Overscreening in Hubbard electron systems

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We show that doping-induced charge fluctuations in strongly correlated Hubbard electron systems near the $\frac{1}{2}$-filled, insulating limit cause overscreening of the electron-electron Coulomb repulsion. The resulting attractive screened interaction potential supports $d_{x^2-y^2}$-pairing with a strongly peaked, doping dependent pairing strength at lower doping, followed by s-wave pairing at larger doping levels.

74.20.-z, 74.20.Mn, 75.25.Dw

In the cuprate high-T_c superconductors, the strong, on-site Hubbard-U Coulomb repulsion is believed to prevent conventional on-site Cooper pair formation. This long-standing theoretical dictum seems to be now supported by experimental evidence, obtained in several cuprate materials, for a non-s-wave pairing state, apparently of $d_{x^2-y^2}$-symmetry [1,2]. Yet, at least one material, the $(Nd,Ce)_2CuO_4$-system, appears to exhibit a fully gapped excitation spectrum, suggesting an s-wave state within the framework of more conventional pairing theories [3,4]. A d-wave pairing state implies a spatially extended Cooper pair wavefunction involving electrons paired at 1st neighbor or larger lattice distances. While impervious to the on-site U repulsion, even non-s-wave extended pairing states *can* be suppressed by the extended (1st, 2nd, ... neighbor) part of the electron-electron Coulomb repulsion. For any proposed microscopic model of the cuprates, it is therefore of crucial importance to demonstrate that, firstly, the model can support at least two qualitatively different pairing states of, possibly, different symmetry [4] and, secondly, that such pairing states are robust against on-site *and* extended Coulomb repulsions.

In the present paper, we use a combination of diagrammatic and quantum Monte Carlo (QMC) techniques to show that the charge fluctuations in a quasi two-dimensional (2D) extended Hubbard model give rise to a screening effect which not only reduces the magnitude, but in fact reverses the sign of the extended part of the three-dimensional (3D) screened Coulomb potential V_S. At larger doping, this overscreening becomes so strong that even the on-site part of V_S changes sign and turns attractive. The overscreening is intrinsically a large-U effect of the Hubbard system at finite doping near band-filling $\frac{1}{2}$. Over a doping range of about $10-20\%$, $|V_S|$ is much weaker than the bare U and thus offers the prospect of developing *controlled* perturbative expansions in terms of V_S, rather than U. Taken as an effective pairing potential, V_S supports $d_{x^2-y^2}$ pairing, with a pairing strength maximum in the $\sim 10-20\%$ doping range, and, in close proximity, s-wave pairing at larger doping.

We start from an extended Hubbard Hamiltonian

$$H = \sum_{j,\ell}\Big(\frac{1}{2}V(r_{j\ell})n_j n_\ell - \sum_\sigma t_{j\ell}c^\dagger_{j\sigma}c_{\ell\sigma}\Big) \equiv H_V + H_t\ , \tag{1}$$

with $c^\dagger_{j,\sigma}$ creating an electron of spin $\sigma=\uparrow,\downarrow$ at Cu-site r_j in a 3D crystal of stacked CuO_2 layers, $n_j=\sum_\sigma c^\dagger_{j\sigma}c_{j\sigma}$ and $r_{j\ell}=r_j-r_\ell$. H_t includes only an in-plane 1st neighbor hybridization t and the chemical potential μ. The 3D Coulomb potential

$$V(r) = U\delta_{r,0} + \frac{e^2}{\epsilon_B|r|}(1-\delta_{r,0}) \equiv U\delta_{r,0} + V_e(r) \tag{2}$$

includes the on-site ($r=0$) repulsion U and an extended $1/|r|$-part, V_e, with a dielectric constant ϵ_B to account for screening by the insulating background not explicitly included in H, that is "non-Hubbard" electrons in lower filled bands and, possibly, phonon degrees of freedom.

The basic idea of our approach is to treat some short-range portion of $V(r)$, denoted by $V_o(r)$, exactly by QMC methods. The remaining weaker, but long-range part of V, denoted by $V_\ell(r)$, is then handled perturbatively. By including only short-range in-plane terms in V_o, the QMC simulation can be restricted to a single 2D layer for which we obtain, by QMC, the density correlation function

$$\chi_o(q,i\omega) = \frac{1}{N}\sum_{j,\ell}\int_0^\beta d\tau e^{i\omega\tau - iq\cdot r_{j\ell}}\langle \Delta n_j(\tau)_o \Delta n_\ell(0)_o\rangle_o \equiv -P_o(q,i\omega)[1-V_o(q)P_o(q,i\omega)]^{-1} \tag{3}$$

at wavevectors q, Matsubara frequencies $i\omega$ and temperature $T\equiv 1/\beta$ for lattice size N with $\Delta n_j \equiv n_j - \langle n_j\rangle_o$. Here, $\langle ...\rangle_o$ and $...(\tau)_o$ denote, respectively, thermal averaging and imaginary-time evolution with respect to the QMC Hamiltonian $H_o \equiv H_{V_o}+H_t$. P_o is the corresponding irreducible polarization insertion [5].

The exact screened potential V_S, irreducible polarization insertion P and density correlation function χ of the full Hamiltonian (1) are related by [5]

$$V_S(q,i\omega) = [1 - V(q)P(q,i\omega)]^{-1}V(q) \\ = V(q) - V(q)\chi(q,i\omega)V(q)\ , \qquad (4)$$

where $V(q)$ denotes the lattice Fourier sum over $V(r)$. Our essential approximation is to replace the exact P of the full Hamiltonian H by P_o, extracted from the QMC results for χ_o via Eq.3. All renormalizations of P due to V_o are thus included exactly, to all orders in V_o. Renormalizations due to the weaker long-range part V_ℓ are neglected in P, but approximately included in V_S via Eq. 4. Note here that Eqs. 3, 4 for V_S, P and P_o are based on the diagrammatic expansion in the *charge* representation where the U-term is written as $\frac{U}{2}\sum_j n_j^2$, rather than the more familiar *spin* representation $U\sum_j n_{j\uparrow}n_{j\downarrow}$. While both are equivalent when summed exactly to all orders, the former, as we will show, has some crucial advantages for approximate diagram resummations.

As a simple cuprate, we consider $La_{2-x}Sr_xCuO_4$, with a body-centered tetragonal (*bct*) model crystal structure, in-plane lattice constant $a = 3.80\mathring{A}$, inter-layer spacing $d = 6.62\mathring{A}$ [6], $t = 0.35eV$ and $U = 8t$ [7]. Using standard determinant QMC methods, χ_o is simulated with up to 2×10^7 MC sweeps and typically $\lesssim 0.5\%$ statistical error on 6×6, 8×8 and 10×10 2D lattices with periodic boundary conditions, taking $V_o(r) = U\delta_{r,0}$, at $\beta \equiv 1/T$ up to $\beta t = 10$, with imaginary-time step $\Delta\tau \equiv \beta/L \leq 0.0625t^{-1}$ where L is the Trotter number.

To estimate ϵ_B from the measured long-wavelength external field dielectric function $\epsilon_{ex}(\omega)|_{q\to0}$ in the undoped, insulating La_2CuO_4 [8,9] we calculate [10]

$$\frac{1}{\epsilon_{ex}(q,i\omega)} = \frac{1}{\epsilon_B}\Big[1 - \frac{4\pi e^2}{\epsilon_B \mathcal{V}_c|q|^2}\chi(q,i\omega)\Big]\ , \qquad (5)$$

at the smallest q-vectors with non-zero in-plane component available on our finite model lattices and $i\omega = 0$, with $\mathcal{V}_c$ denoting the 3D unit cell volume, $\chi = -P[1 - V(q)P]^{-1}$ from (4) and $P \cong P_o$. In the undoped Hubbard system at temperatures $T \geq 0.1t$, we find that ϵ_{ex} from (5) varies roughly linearly with ϵ_B. The excess $\Delta\epsilon \equiv \epsilon_{ex} - \epsilon_B \cong 0.75 - 0.85$, that is, the Hubbard electrons' contribution to the dielectric screening, is approximately independent of ϵ_B for $\epsilon_B \geq 3$. From the measured dielectric function ϵ_{ex} of undoped La_2CuO_4 in the static limit $\omega \to 0$, $\epsilon_0 \equiv \epsilon_{ex}(0) \cong 30$ [8], we thus estimate $\epsilon_B = \epsilon_{ex} - \Delta\epsilon \cong 29$. However, this includes a large, in fact, dominant phonon contribution [11]. The purely electronic dielectric screening is observed at frequencies $\omega_\infty \sim 0.5 - 1$eV, well above the phonon spectrum $\Omega_{ph} \lesssim$ 0.1eV, but still well below the electronic Mott-Hubbard charge gap $\Delta_{MH} \sim 1.5 - 2$eV, where $\epsilon_\infty \equiv \epsilon_{ex}(\omega_\infty) \cong 5$ [9]. Hence we get $\epsilon_B \cong 4.2$ for the purely electronic background screening. ¿From the estimated values $\epsilon_B \cong 4.2$ (without phonons) or even $\epsilon_B \cong 29$ (including phonons), one obtains a quite substantial 1st neighbor repulsion strength $V_1 = e^2/(\epsilon_B a) \cong 0.90$eV $\cong 2.6t$ in the former and $V_1 \cong 0.13$eV $\cong 0.37t$ in the latter case. Thus, $V_e(r)$ could severely suppress spatially extended pairing potentials [12].

In Fig.1(a) and (b), we explore how screening affects the 3D Coulomb potential V_S, calculated from (4) at $i\omega = 0$, Fourier transformed back to r-space and plotted *vs.* doping concentration $x \equiv 1 - \langle n_j\rangle$ for the on-site ($r = 0$) and in-plane 1st neighbor r-vector. The surprising result in Fig. 1(b) is that a small amount of doping, of order 5%, will not only suppress the extended $1/|r|$-repulsion for $r \neq 0$, but will in fact cause a sign change in the 1st neighbor and similarly (not shown) in the 2nd and 3rd neighbor screened potential. Thus $V_S(r)$ becomes attractive at short-range distances. The attraction strength at $r \neq 0$ shows a pronounced doping dependence, reaches a maximum at $x \sim 10 - 14\%$ and becomes repulsive again at $x \sim 23 - 28\%$. Even more surprising, as shown in Fig. 1(a), is the doping dependence of the on-site ($r = 0$) potential which is also rapidly suppressed with increasing x and becomes strongly attractive at larger doping, near $x \cong 15\%$. Minus sign problems at finite doping unfortunately limit our simulations to $T \geq 0.33t$. However, at least in that temperature regime, we find $|V_S|$ to be increasing with decreasing T. This suggests that the overscreening becomes stronger than shown in Fig. 1 at lower T.

The presence of a strong Hubbard-U *and* finite doping density $x > 0$ are crucial for the overscreening. If one replaces the V_o-renormalized P_o in (4) by, say, the non-interacting ("RPA") polarization bubble P_{RPA}, one also obtains a suppression of $V_S(r)$. However, both the on-site ($r = 0$) and the short-range extended part ($r \neq 0$) of V_S remain repulsive in RPA [13]. Likewise, in the undoped large-U system, $V_S(r)$ is only reduced relative to $V(r)$, by a roughly r-independent factor, comparable to the ratio ϵ_{ex}/ϵ_B, for $r \neq 0$. Thus, V_S retains a $1/|r|$-dependence and remains repulsive. This is expected for the screening of a Coulomb potential in an insulator and confirms the insulating character of the $\frac{1}{2}$-filled Hubbard system.

To understand the central role of U and finite doping x in the overscreening effect, consider the pure 2D Hubbard model where $V(r) = V_o(r) = U\delta_{r,0}$, our approximation $P \cong P_o$ becomes exact and, from Eq. 4,

$$V_S(r,i\omega) = U\delta_{r,0} - U^2\chi_o(r,i\omega) \qquad (6)$$

with $\chi_o(r,i\omega)$ denoting the Fourier transform of $\chi_o(q,i\omega)$. Clearly, the on-site potential $V_S(r = 0, i\omega)$ at finite doping *must* become attractive for $U \to \infty$, since $\chi_o(r = 0, i\omega)$ is always positive and approaches a non-zero U-independent limit [of, at least, $\mathcal{O}(x/t)$, by a simple $U = \infty$ scaling argument] for $U \gg t$. By contrast, at $\frac{1}{2}$-filling, all charge fluctuations are suppressed, with $\chi_o(r, i\omega = 0) \sim \mathcal{O}(t^2/U^3)$, and $V_S(r = 0, i\omega = 0) \cong U$ is repulsive for $U \gg t$. For near (1st, 2nd, ...) neighbor r's, $\chi_o(r, i\omega = 0)$ is negative at small U and becomes positive only at finite doping and only when U exceeds some

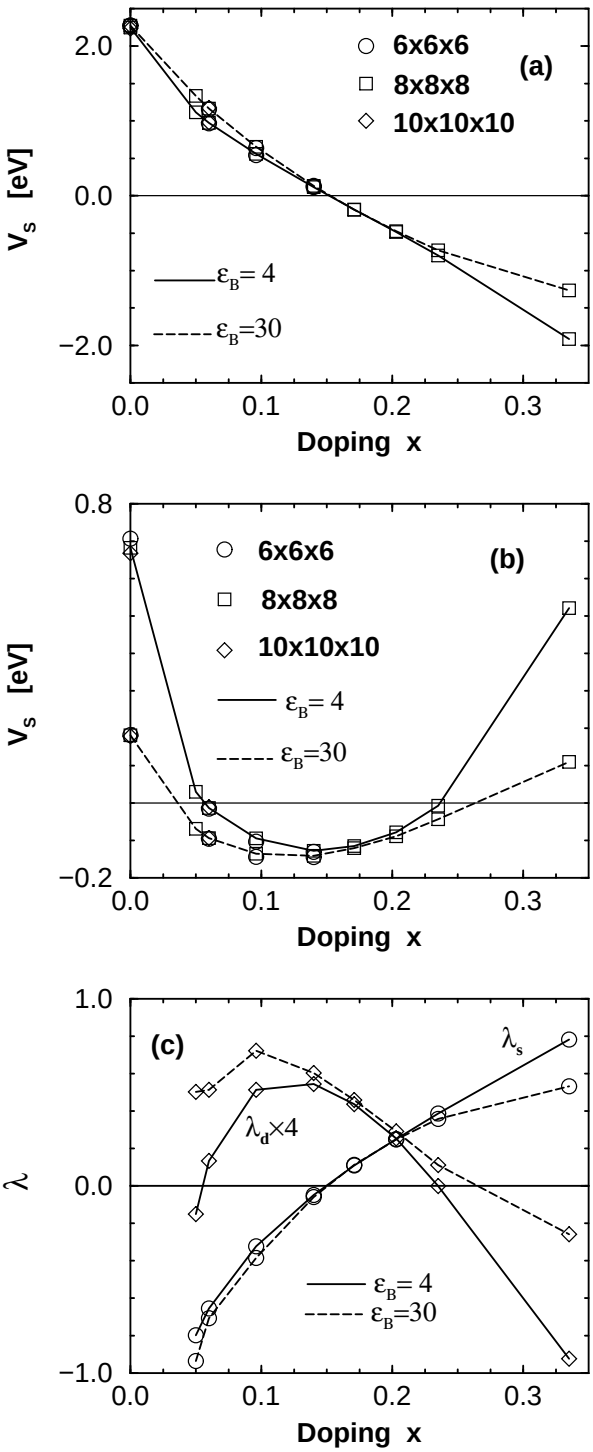

FIG. 1. Screened Coulomb potential $V_S(r) \equiv V_S(r, i\omega = 0)$ at (a) on site ($r = 0$) and (b) at in-plane 1st neighbor lattice vectors r and (c) Eliashberg λ-parameters for in-plane 1st neighbor $d_{x^2-y^2}$ and on-site/1st neighbor s-wave pairing, all plotted vs. hole doping concentration $x = 1 - \langle n_j \rangle$ at $\beta t \equiv t/T = 3.0$ and $\Delta\tau t = 0.0375$ for $\epsilon_B = 4$ and 30. In (a) and (b), results are for La_2CuO_4 with *bct* lattice sizes $6 \times 6 \times 6$, $8 \times 8 \times 8$ and $10 \times 10 \times 10$, with estimated statistical uncertainties in V_s of less than 0.01eV. In (c), results are based on $8 \times 8 \times 8$ data for V_S. λ_d is scaled ×4 for display.

doping dependent threshold of order several t. The near neighbor attraction in V_S therefore also requires large U and finite doping.

The results in Fig. 1 are almost independent of V_e for $\epsilon_B \geq 4$. (The $\epsilon_B = 30$ data are within $1-2\%$ of the pure Hubbard ($\epsilon_B \to \infty$) results.) By using spatially truncated versions of V_e, different layered geometries, and more realistic dielectric background models [10], we have also verified that neither 3D Coulomb interlayer terms, nor the long-range $1/|r|$-tail in V_e, nor our particular choice of crystal structure, nor local field effects will substantially affect the overscreening. To test our approximation, $P \cong P_o$, we have also carried out QMC simulations with both U- *and* a 1st neighbor V_e-term included in V_o. Preliminary results suggest that setting $P \cong P_o$ in (4) reproduces the main V_e-effect on χ, but tends to underestimate the attraction in V_S. Thus, the essential features of V_S are very robust against extended Coulomb terms. This result can be rationalized by expanding (4) to leading order in V_e. The corrections are smaller than the $U^2\chi_o$-term in (6) by a factor of order $V_1\chi_o$ for $U \gg t$ and finite $x \gtrsim t/U$. By simple $U \to \infty$ scaling arguments this is of order $V_1 x/t$, *i.e.* small if $V_1 \ll t/x$. At sufficiently large V_1, i.e. low ϵ_B, our basic approach *does* break down due to charge density wave instabilities, signaled by $1/\chi(q, i\omega = 0) \to 0$. For the present parameter set and doping range, this happens only for $\epsilon_B \lesssim 1.8$.

A crucial advantage of our diagrammatic expansion in the charge representation is the large reduction of the overall strength of V_S in the $10-20\%$ doping range. This suggests the possibility of carrying out *controlled*, self-consistent weak-coupling expansions in which the fully screened V_S, rather than the bare V or U, serves as the small parameter. As a first step in that direction, we have explored possible V_S-induced or -enhanced superconducting pairing instabilities, using the standard Eliashberg-McMillan (EM) approach [14]. A convenient measure of the pairing strength of V_S are the dimensionless EM λ-parameters, defined in terms of the Fermi surface (FS) "expectation values" of $V_S(k - k', i\omega = 0)$ for relevant Cooper pair trial wavefunctions $\eta(k)$ in electron momentum (k-) space, as described in detail in Refs. [14].

In Fig. 1(c), we show the EM parameters λ_s for on-site s-wave (and, identically, for in-plane 1st neighbor s-wave), and λ_d, for in-plane 1st neighbor $d_{x^2-y^2}$ pairing, with respective pair wavefunctions $\eta_s(k) \equiv 1$ and $\eta_d(k) = \cos(ak_x) - \cos(ak_y)$. For the required FS integrals, we have interpolated our 3D $V_S(q, i\omega)$ from the finite-lattice $8 \times 8 \times 8$ onto a $200 \times 200 \times 200$ q-mesh. At low doping, the dominant attractive ($\lambda > 0$) channel is $d_{x^2-y^2}$ with λ_d reaching a maximum of $\sim 0.15 - 0.17$ near $x \sim 10 - 14\%$. λ_s is repulsive at low doping, but becomes strongly attractive at larger doping $x \gtrsim 15\%$. Thus, as expected on symmetry grounds, λ_s and λ_d reflect the doping dependence of the on-site and 1st neighbor attraction V_S shown in Fig. 1(a) and (b), respectively. The

λ-values for near-neighbor pair wavefunctions of other symmetries (p, d_{xy}, g) are small compared to λ_s and λ_d.

The spectral weight of $\chi(q, i\omega)$ extends up to values $\Omega_\chi \sim 8 - 10t$ [15]. In the EM analysis [14], this "boson" energy scale, together with λ, determines the superconducting T_c, roughly as $T_c \sim \Omega_\chi \exp(-1/\lambda)$. Because of the large Ω_χ-scale, it may be possible to achieve high T_c's even at moderate coupling values $\lambda < 1$.

It is quite possible that near-neighbor, d-wave-attractive charge correlations $\chi(r \neq 0, i\omega) > 0$ are very closely related to short-range antiferromagnetic spin correlations in Hubbard systems near $\frac{1}{2}$-filling. The charge fluctuation picture developed here may thus provide a description of the physics in near-$\frac{1}{2}$-filled Hubbard systems which is complementary to that of a spin fluctuation based approach [2]. The overscreening of the on-site potential, and hence the possibility of s-wave pairing in the Hubbard model, is one aspect of this problem which is obvious in the former, but difficult to capture in the latter approach.

In summary, we have studied the effect of screening on the electron-electron interaction potential in a quasi-2D Hubbard model for CuO_2-layers, coupled by an extended $1/|r|$ 3D Coulomb repulsion. While contributing only a minor portion of the total insulating dielectric constant at $\frac{1}{2}$-filling, the Hubbard electron system, when doped away from $\frac{1}{2}$-filling, exhibits a strong overscreening effect which causes the extended part of the screened potential to change sign and become attractive, at 1st and further neighbor distances. This screened potential gives rise to a pairing attraction in the $d_{x^2-y^2}$ channel which, as a function of doping, exhibits a maximum near $\sim 10 - 15\%$, reminiscent of the doping dependence of the superconducting T_c in the cuprates. At larger doping, even the on-site part of the screened potential becomes attractive and gives rise to an s-wave pairing attraction which increases strongly with doping, suggesting the possibility of a doping-induced transisition or cross-over from d- to s-wave pairing. The overscreening effect is robust against 3D extended Coulomb repulsions, independent of the 3D crystal structure, and represents intrinsically a *charge* fluctuation aspect of the Hubbard electron system at large U and finite doping density near $\frac{1}{2}$-filling.

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[1] For a review of the experiments see D. J. van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).

[2] For a review of the theoretical aspects see D. J. Scalapino, Phys. Rep. **250**, 329 (1995).

[3] Q. Huang *et al.*, Nature **347**, 369 (1990); D.H. Wu *et al.*, Phys. Rev. Lett. **70**, 85 (1993); A. Andreone *et al., ibid.* **49**, 6392 (1994); S.M. Anlage *et al.,ibid.* **50**, 523 (1994); J.W. Ekin *et al., ibid.* **56**, 13746 (1997); S. Kashiwaya *et al., ibid.* 57, 8680 (1998).

[4] Non-s-wave pairing states with a fully gapped quasiparticle spectrum are not fundamentally prohibited by any symmetry principles; c.f. H.-B. Schüttler *et al.*, J. Supercond. **8**, 555 (1995), and references therein. Only phase sensitive Josephson experiments, c.f. Ref. [1], can unambiguously rule out non-s-wave states in $(Nd, Ce)_2CuO_4$.

[5] G. D. Mahan, *Many-Particle Physics*, 1st ed. (Plenum Press, New York, 1981).

[6] J. D. Jorgensen *et al.*, Phys. Rev. Lett. **58**, 1024 (1987).

[7] H.-B. Schüttler and A.J. Fedro, Phys. Rev. B **45**, 7588 (1992); and references therein.

[8] C. Y. Chen *et al.*, Phys. Rev. B **43**, 392 (1991);

[9] J. P. Falck *et al.*, Phys. Rev. B **48**, 4043 (1993).

[10] S. L. Adler, Phys. Rev. **126**, 413 (1962); N. Wiser, *ibid.* **129**, 62 (1963); S. K. Sinha, *ibid.* **177**, 1256 (1969); L. J. Sham Phys. Rev. B **6**, 3584 (1972); W. Hanke, *ibid.* **8**, 4585 (1973); W. Hanke and L. J. Sham, Phys. Rev. Lett. **33**, 582 (1974); S. K. Sinha, *CRC Critical Reviews in Solid State Sciences* **3**, 273 (1973).

[11] D. Emin, Phys. Rev. Lett. **62**, 1544 (1989).

[12] Pairing mechanisms based on the t-J model will certainly not survive without, and just barely with, the phonon part of ϵ_B, a point overlooked in recent work proposing a "purely electronic mechanism" in the t-J context; see *e.g.* C. Gazza *et al.*, xxx.lanl.gov/cond-mat/9803314.

[13] D. Z. Liu and K. Levin [Physica C **275**, 81 (1997)], have reported a weak attraction in the $d_{x^2-y^2}$ pairing channel for RPA-screened Coulomb matrix elements, due to local field effects.

[14] P. B. Allen and B. Mitrovic, in *Solid State Physics*, eds. H. Ehrenreich *et al.*, Vol 37, pp. 1-91, Academic Press (New York, 1982); H.-B. Schüttler and M. N. Norman, Phys. Rev. B **54**, 13295 (1996).

[15] R. Preuss *et al.*, Phys. Rev. Lett. **79**, 1122 (1997).