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-\( T \) 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. Yet, at least one material, the (\( Nd, Ce \))\(_2\)CuO\(_4\)-system, appears to exhibit a fully gapped excitation spectrum, suggesting an \( s \)-wave state within the framework of more conventional pairing theories. 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 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 \( V_3 \). At larger doping, this overscreening becomes so strong that even the on-site part of \( V_3 \) 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 \( 10 - 20\% \), \(|V_3|\) is much weaker than the bare \( U \) and thus offers the prospect of developing controlled perturbative expansions in terms of \( V_3 \), rather than \( U \). Taken as an effective pairing potential, \( V_3 \) supports \( d_{x^2-y^2} \) pairing, with a pairing strength maximum in the \( 10 - 20\% \) doping range, and, in close proximity, \( s \)-wave pairing at larger doping.

We start from an extended Hubbard Hamiltonian

\[
H = \sum_{j,\ell} \left( \frac{1}{2} V(r_j) n_j n_{\ell} - \sum_{\sigma} t_{j\ell} c_{j\sigma}^\dagger c_{\ell\sigma} \right) \\
\equiv H_V + H_t ,
\]

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

\[
V(r) = U\delta_{r,0} + \frac{e^2}{\epsilon_B |r|} (1 - \delta_{r,0}) \equiv U\delta_{r,0} + V_c(r)
\]

includes the on-site \((r=0)\) repulsion \( U \) and an extended \( 1/|r| \)-part, \( V_c \), with a dielectric constant \( \epsilon_B \) 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 \( V_t(r) \), 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

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

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 \( \langle ... \rangle \) denote, respectively, thermal averaging and imaginary-time evolution with respect to the QMC Hamiltonian \( \hat{H}_o \equiv \hat{H}_V + \hat{H}_t \). \( P_o \) is the corresponding irreducible polarization insertion.

The exact screened potential \( V_3 \), irreducible polarization insertion \( P \) and density correlation function \( \chi \) of the full Hamiltonian \((\mathbf{3})\) are related by \((\mathbf{3})\).
\[ V_S(q, \omega) = [1 - V(q)P(q, \omega)]^{-1}V(q) = V(q) - V(q)\chi(q, \omega)V(q), \]  

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 \( \chi_0 \) 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 \( i\omega \) representation where the \( U \)-term is written as \( U \sum q n_q^2 \), rather than the more familiar \( \text{spin} \) representation \( U \sum j n_j^+ n_j^- \). While both are equivalent when summed exactly to all orders, the former, as we will show, has some crucial advantages for approximate diagram resumations.

As a simple cuprate, we consider \( La_{2-x}Sr_xCuO_4 \), with a body-centered tetragonal (\( \text{bct} \)) model crystal structure, in-plane lattice constant \( a = 3.80 \AA \), inter-layer spacing \( d = 0.62 \AA \), \( t = 0.35eV \) and \( U = 8t \). Using standard determinant QMC methods, \( \chi_0 \) is simulated with up to \( 2 \times 10^7 \) MC sweeps and typically \( \lesssim 0.5% \) statistical error on \( 6 \times 6, 8 \times 8 \) and \( 10 \times 10 \) 2D lattices with periodic boundary conditions, taking \( V_o(r) = U\delta_{r,0} \), at \( \beta = 1/T \) up to \( \beta t = 10 \), with imaginary-time step \( \Delta t \equiv \beta/L \leq 0.0625t^{-1} \) where \( L \) is the Trotter number.

To estimate \( \epsilon_B \) from the measured long-wavelength external field dielectric function \( \epsilon_{ex}(\omega)|_{q \to 0} \) in the undoped, insulating \( La_{2-x}Sr_xCuO_4 \) we calculate

\[ \frac{1}{\epsilon_{ex}(q, \omega)} = \frac{1}{\epsilon_B} \left[ 1 - \frac{4\pi e^2}{\epsilon_B V_c|q|} \chi(q, \omega) \right], \]  

(5)

at the smallest \( q \) vectors with non-zero in-plane component available on our finite model lattices and \( \omega = 0 \), with \( V_c \) denoting the 3D unit cell volume, \( \chi = -P[1 - V(q)P]^{-1} \) from (4) and \( P \equiv P_o \). In the undoped Hubbard system at temperatures \( T \geq 0.1t \) we find that \( \epsilon_{ex} \) varies roughly linearly with \( \epsilon_B \). The excess \( \Delta \epsilon \equiv \epsilon_{ex} - \epsilon_B \approx 0.75 - 0.85, \) that is, the Hubbard electrons' contribution to the dielectric screening, is approximately independent of \( \epsilon_B \) for \( \epsilon_B \geq 3 \). From the measured dielectric function \( \epsilon_{ex} \) of undoped \( La_{2-x}Sr_xCuO_4 \) in the static limit \( \omega \to 0 \), \( \epsilon_0 \equiv \epsilon_{ex}(0) \approx 30 \), we thus estimate \( \epsilon_B = \epsilon_{ex} - \Delta \epsilon \approx 29 \). However, this includes a large, in fact, dominant phonon contribution [11]. The purely electronic dielectric screening is observed at frequencies \( \omega_{\gamma} \approx 0.5 - 1eV \), well above the phonon spectrum \( \Omega_{ph} \approx 0.1eV \), but still well below the electronic Mott-Hubbard charge gap \( \Delta_{MH} \approx 1.5 - 2eV \), where \( \epsilon_{ex}(\omega) \approx 5 \). Hence we get \( \epsilon_B \approx 4.2 \) for the purely electronic background screening. From the estimated values \( \epsilon_B \approx 4.2 \) (without phonons) or even \( \epsilon_B \approx 29 \) (including phonons), one obtains a quite substantial 1st neighbor repulsion binding strength \( V_1 \approx 0.13eV \approx 0.37t \) in the former and \( V_1 \approx 0.13eV \approx 0.37t \) in the latter case. Thus, \( V_o(r) \) 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 \( \omega = 0 \), Fourier transformed back to \( r \)-space and plotted vs. doping concentration \( x \approx 1 - \langle n_j \rangle \) for the on-site \( (r = 0) \) and in-plane 1st neighbor \( r \)-vector. The surprising result in Fig. 1(b) 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 \( V_S \) 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 \( x \approx 15\% \). 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, \( V_S \) is only reduced relative to \( V(r) \), by a roughly \( r \)-independent factor, comparable to the ratio \( \epsilon_{ex}/\epsilon_B \), 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 \( 1/2 \)-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 \( P \equiv P_o \) becomes exact and, from Eq. 4,

\[ V_S(r, \omega) = U\delta_{r,0} - U^2\chi_0(r, \omega) \]  

(6)

with \( \chi_0(r, \omega) \) denoting the Fourier transform of \( \chi_0(q, \omega) \). Clearly, the on-site potential \( V_S(r = 0, \omega) \) at finite doping must become attractive for \( U \to \infty \), since \( \chi_0(r = 0, \omega) \) is always positive and approaches a non-zero \( U \)-independent limit [of, at least, \( O(x/t) \)], by a simple \( U = \infty \) scaling argument for \( U \gg t \). By contrast, at \( 1/4 \)-filling, all charge fluctuations are suppressed, with \( \chi_0(r, \omega = 0) \sim O(t^2/U^3) \), and \( V_S(r = 0, \omega = 0) \approx U \) is repulsive for \( U \gg t \). For near (1st, 2nd, ...) neighbor \( r \)'s, \( \chi_0(r, \omega = 0) \) is negative at small \( U \) and becomes positive only at finite doping and only when \( U \) exceeds some
based on 8 at (a) on site (\(r\) and (b), results are for 6 \(\times\) 1st neighbor all plotted vs. hole doping concentration \(x\).

FIG. 1. Screened Coulomb potential \(V_S(r)\equiv V_S(r, \nu \omega = 0)\) at (a) on site \((r = 0)\) and (b) at in-plane 1st neighbor lattice vectors \(r\) and (c) Eliashberg \(\lambda\) 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 \(x = 1 − \langle n_i \rangle\) at \(\beta t \equiv t/T = 3.0\) and \(\Delta rt = 0.0375\) 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 \(V_S\). \(\lambda_d\) is scaled \(\times 4\) 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. [4] are almost independent of \(V_e\) for \(\epsilon_B \geq 4\). (The \(\epsilon_B = 30\) data are within 1 – 2\% of the pure Hubbard \((\epsilon_B \rightarrow \infty)\) 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, \(P \approx P_o\), we have also carried out QMC simulations with both \(U-\) and 1st neighbor \(V_e\)-term included in \(V_e\). Preliminary results suggest that setting \(P \approx P_o\) in (3) reproduces the main \(V_e\)-effect on \(\chi\), 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 \(U^2\chi_{\sigma^\alpha}\)-term in (3) by a factor of order \(V_1\chi_o\) for \(U \gg t\) and finite \(x \gg t/U\). By simple \(U \rightarrow \infty\) scaling arguments this is of order \(V_1x/t\), i.e. small if \(V_1 \ll t/x\). At sufficiently large \(V_1\); i.e. low \(\epsilon_B\), our basic approach does break down due to charge density wave instabilities, signaled by \(1/\chi(q, \nu \omega = 0\) → 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 \(\lambda\)-parameters, defined in terms of the Fermi surface (FS) “expectation values” of \(V_S(k−k', \nu \omega = 0\) 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 \(\lambda_s\) for on-site s-wave (and, identically, for in-plane 1st neighbor s-wave), and \(\lambda_d\), for in-plane 1st neighbor \(d_{x^2−y^2}\) pairing, with respective pair wavefunctions \(\eta(k)\) \(\equiv 1\) and \(\eta_d(k) = \cos(ak_x) − \cos(ak_y)\). For the required FS integrals, we have interpolated our 3D \(V_S(q, \nu \omega)\) 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 \(\lambda_d\) reaching a maximum of \(\sim 0.15 – 0.17\) near \(x \sim 10 – 14\%\). \(\lambda_s\) is repulsive at low doping, but becomes strongly attractive at larger doping \(x \gtrsim 15\%. Thus, as expected on symmetry grounds, \(\lambda_s\) and \(\lambda_d\) reflect the doping dependence of the on-site and 1st neighbor attraction \(V_S\) shown in Fig. 1(a) and (b), respectively. The
$\lambda$-values for near-neighbor pair wavefunctions of other symmetries $(p, d_{xy}, q)$ are small compared to $\lambda_s$ and $\lambda_d$.

The spectral weight of $\chi(q, i\omega)$ extends up to values $\Omega_\chi \sim 8 - 10t [1]$. In the EM analysis [4], this "boson" energy scale, together with $\lambda$, determines the superconducting $T_c$, roughly as $T_c \sim 1/\Omega_\chi$ (Ref. [1]). Because of the large $\Omega_\chi$-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 [3]. 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 $\frac{1}{2}$ 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 transition 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. [3], can unambiguously rule out non-s-wave states in (Nd,Ce)$_2$CuO$_4$.
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. Wisser, 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 $\epsilon_B$, 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).