Screening of long-range Coulomb interactions in the quasi two-dimensional extended Hubbard model: A combined quantum Monte Carlo and Feynman diagram study

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By combining fermion quantum Monte Carlo (QMC) simulations with diagrammatic theory, we have calculated the dielectric screening and the screened electron-electron interaction potential in a quasi two-dimensional extended single-band Hubbard model for cuprate superconductors, with and without a long-range (1/r) extended Coulomb interaction potential, at and near band-filling $\frac{1}{2}$. Our results for the insulating dielectric screening in the $\frac{1}{2}$-filled band case indicate that the Hubbard conduction electron system contributes only a minor fraction, $\Delta \epsilon \cong 0.9$, of the total observed in-plane electronic dielectric constant of the cuprates, $\epsilon_{\infty} \cong 4.7$. With increasing hole doping concentration $x$, the extended (1/r-) part of the Coulomb interaction potential is rapidly suppressed by the metallic screening, due to doping induced charge carriers. Surprisingly, near $x \sim 5\%$, the low-frequency component of the screened potential $V_s$ changes sign and becomes attractive at 1st neighbor and more extended distances in the CuO$_2$-plane. The 1st neighbor screened potential reaches maximum attraction strength at dopings $x \sim 13 - 15\%$ and becomes repulsive again at larger dopings, for $x \sim 23 - 25\%$. Similar results are found for the screened potential of the pure 2D Hubbard model, without extended Coulomb interaction terms, suggesting that the extended Coulomb terms do not qualitatively alter the local screening physics of the doped Hubbard electron system. When included exactly in the screening calculation, the 1st neighbor extended Coulomb term enhances the on-site and 1st neighbor overscreening attraction already present in the pure Hubbard model at finite doping. Our results are potentially relevant for the question of the d-wave pairing mechanism in the cuprates, since they suggest that the screened extended Coulomb interaction potential does not only not suppress a d-wave pairing state but, due to the overscreening, could actually increase the d-wave attraction, in the 5 – 25% doping regime. Our results may also have implications for the explanation of the isotope effect and its doping dependence in the cuprates. At larger dopings, $x > 15\%$, the screened potential becomes attractive even on-site, suggesting the possibility that the screened potential could support or enhance s-wave pairing in the high-doping regime. We also give a rigorous analytical proof that the screened on-site interaction must become attractive near half-filling in the repulsive large-$U$-limit of both the pure Hubbard and the extended Hubbard single-band model. We present a simple physical interpretation of this seemingly paradoxical result in terms of the retardation effects which are inherent in the screening of an instantaneous repulsive interaction potential. We also point out that on-site overscreening implies singularities in the imaginary-frequency dependence of the irreducible polarization insertion and its 3-point vertex function.

I. INTRODUCTION

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 is now supported by experimental evidence, obtained in several cuprate materials, for a non-s-wave pairing state, of $d_{x^2-y^2}$-symmetry. A d-wave pairing state implies a spatially extended Cooper pair wavefunction, involving electrons paired at 1st neighbor or large lattice distances. Such a non-s-wave state is impervious to the on-site $U$-repulsion, but it can still be suppressed by the extended part (1st, 2nd, ... neighbor) of the electron-electron Coulomb repulsion. The bare strength of this extended Coulomb potential may be quite substantial in the cuprates. For any proposed microscopic model of the cuprates, it is therefore crucial to demonstrate that the model can support a d-wave pairing state near $\frac{1}{2}$-bandfilling and that such a pairing state is robust against extended Coulomb repulsions.

In the present paper, we combine diagrammatic and quantum Monte Carlo (QMC) methods to study both the insulating dielectric screening at band-filling $\frac{1}{2}$ and, as a function of doping, the screened electron-electron interaction potential near the $\frac{1}{2}$-filled band limit within the framework of a quasi two-dimensional (2D) Hubbard model with three-dimensional (3D) extended 1/r Coulomb interactions. In the $\frac{1}{2}$-filled band case, our results suggest that the insulating Hubbard electron system
is far less anisotropic, with observed dielectric constants of quite similar magnitude parallel and perpendicular to the CuO$_2$-layer directions. This suggests that the extended $1/r$ part of the electronic Coulomb repulsion is by no means confined to a single CuO$_2$-layer and that the full 3D interaction potential may have to be taken into account. We therefore start from an extended Hubbard Hamiltonian of the form

$$H = \sum_{j,\ell} \left( \frac{1}{2} V(\mathbf{r}_{j\ell}) n_j n_{\ell} - \sum_\sigma t_{j\ell} c^\dagger_{j\sigma} c_{\ell\sigma} \right) \equiv H_V + H_t ,$$

with $c^\dagger_{j\sigma}$ creating an electron of spin $\sigma = \uparrow, \downarrow$ at Cu-site $r_j$ in a three-dimensional (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 $\mu$. Some preliminary results including a 2nd neighbor hybridization $t'$ have also been obtained.

The 3D Coulomb potential

$$V(r) = U \delta_{r,0} + \frac{\epsilon^2_B}{\epsilon_B|r|_{\text{min}}} (1 - \delta_{r,0}) \equiv U \delta_{r,0} + V_e(r)$$

includes the on-site repulsion $U$ and an extended $1/r$-part, $V_e$, 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. On a finite $L(1) \times L(2) \times L(3)$ lattice with periodic boundary conditions and primitive unit vectors $r^{(\alpha)}$, having linear dimension of $L^{(\alpha)}$ unit cells in the $r^{(\alpha)}$ direction for $\alpha = 1, 2, 3$, we define

$$|r|_{\text{min}} = \min_{m_1,m_2,m_3} |r - \sum_{\alpha=1}^3 m_\alpha L^{(\alpha)} r^{(\alpha)}|$$

with the $m_\alpha$ taken over all integers, to ensure proper periodicity of $V(r)$.

The exact screened potential $V_S$, the exact irreducible polarization insertion $P$ and the exact density correlation function $\chi$ of the full Hamiltonian are related by

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

where $V(q)$ denotes the lattice Fourier sum over $V(r)$ and

$$\chi(q,i\omega) = \frac{1}{N} \sum_{j,\ell} \int_0^\beta d\tau e^{i\omega\tau - iq\cdot r_{j\ell}} \langle \Delta n_j(\tau) \Delta n_\ell(0) \rangle$$

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

at wavevectors $q$. Matsubara frequencies $i\omega$ and temperature $T \equiv 1/\beta$ for lattice size $N$ with $\Delta n_j \equiv n_j - \langle n_j \rangle$.  

II. MODEL AND COMBINED DIAGRAMMATIC QUANTUM MONTE CARLO APPROACH

Both theoretical (bandstructure) calculations and experimental observations, specifically the highly anisotropic electronic transport properties of the cuprates, suggest that their electronic structure is close to two-dimensional and it is a reasonable first approximation to neglect interlayer electronic hybridization effects. However, the dielectric screening in the undoped insulating parent compounds contributes only a minor fraction, $\Delta \epsilon \cong 0.9$, to the total observed electronic dielectric constant of the cuprates, $\epsilon_\infty \cong 4.7$, with most of the electronic dielectric screening being provided by non-Hubbard "background" electrons which are not explicitly included in the conventional single-band Hubbard description of the cuprates. In comparing to the observed values for the dielectric constant, we can thus obtain an estimate for the strength of the $1/r$ Coulomb interaction potential of the quasi 2D Hubbard electron system. At finite doping, we find that screening due to the doping induced "metallic" charge fluctuations causes the screened electron-electron interaction potential $V_S$ to become attractive. At low doping concentrations $x$, this "overscreening" effect reverses the sign of the spatially extended part of $V_S$, giving rise to a 1st neighbor attraction in the 5 – 25% doping range, with a attraction strength maximum near $x = 15\%$. At larger $x$, even the on-site part of $V_S$ turns attractive, for $x \gtrsim 15\%$. We give a rigorous analytical proof for the existence of this on-site overscreening effect and show that it is intrinsically a doping induced large-$U$ effect of Hubbard systems near band-filling $\frac{1}{2}$. Possible implications of these overscreening effects for superconducting pairing instabilities in the 2D Hubbard and quasi-2D extended Hubbard model are also discussed.

The remainder of the paper is organized as follows: In Section II, we describe our model and outline the basic approach of combining QMC simulations with diagrammatic theory. In Section III, we present our calculation of the dielectric constant in the $\frac{1}{2}$-filled Hubbard electron system and estimate the "bare" strength of the extended $1/r$ Coulomb interaction, by comparing to experimentally observed values in insulating cuprate parent compounds. In Section IV, we present our results for the on-site and 1st neighbor component of the screened Coulomb potential in the 2D Hubbard and quasi-2D extended Hubbard model. In Section V, we present an exact proof for the existence of on-site overscreening in the asymptotic $U \to \infty$ limit and discuss its implications for the analytical structure of the irreducible polarization insertion and its underlying vertex function. In Section VI, we speculate on possible implications of overscreening for the superconducting pairing instabilities of the 2D Hubbard and quasi-2D extended Hubbard model. Section VII contains a brief summary.
Here, \(\langle \ldots \rangle\) and \(\ldots (\tau)\) denote, respectively, thermal averaging and imaginary-time evolution with respect to \(H\). Note that \(V_s\) and \(P\) depend on the choice of representation for \(H_V\). Eqs. (2) are based on the diagrammatic expansion in the charge representation where the \(U\)-term is written as \(U \sum n_j^2\), rather than the more familiar spin representation \(U \sum n_j^o n_j^\ell\). While both are equivalent when all diagrams are summed exactly to all orders, the former, as we will discuss, may offer some advantages for approximate diagram resumations.

The basic idea of our QMC approach is to calculate \(V_s\), via Eq. (4), from the polarization insertion \(P\) which, in turn, is extracted, via Eq. (5), from QMC results for the density correlation function \(\chi\). In order to include the full 3D extended Coulomb repulsion into this approach, we treat only a certain 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 \(V_i(r) \equiv V(r) - V_o(r)\), is then handled perturbatively.

By retaining only in-plane terms in \(V_o\), the QMC simulation can be restricted to a single 2D layer. We thus calculate, by QMC, the density correlation function

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

\[
\equiv -P_o(q, i\omega)[1 - V_o(q)P_o(q, i\omega)]^{-1}
\]

for the QMC Hamiltonian

\[
H_o \equiv H_{V_o} + H_t
\]

on a single 2D \(CuO_2\)-plane, with the interaction potential \(V\) in Eq. (2) replaced by \(V_o\). Here, \(\langle \ldots \rangle_o\) and \(\ldots (\tau)_o\) denote, respectively, thermal averaging and imaginary-time evolution with respect to \(H_o\) and \(P_o\) is the exact irreducible polarization insertion of \(H_o\), which can be extracted from the QMC results for \(\chi_o\) via Eq. (5).

Our essential approximation is to replace the exact \(P\) of the full Hamiltonian \(H\) in Eqs. (2) by \(P_o\), i.e., we set

\[
P(q, i\omega) \approx P_o(q, i\omega) = [V_o(q) - 1/\chi_o(q, i\omega)]^{-1}
\]

in Eqs. (2) and (5). All renormalizations of \(P\) due to the short-range part of the interaction potential, \(V_o\), are thus included exactly, to all orders of \(V_o\). Renormalizations due to the weaker long-range part \(V_i\) are neglected in \(P\), but approximately included in \(V_s\), via Eq. (3), and in \(\chi\) via Eq. (6), i.e., by setting \(V_s(q, i\omega) \equiv [1 - V(q)P_o(q, i\omega)]^{-1}V(q)\) and \(\chi(q, i\omega) \equiv -P_o(q, i\omega)[1 - V(q)P_o(q, i\omega)]^{-1}\). Note that this approximation for \(P\) becomes exact if we replace \(H\) by \(H_o\), as, e.g., in our calculations of \(P\) and \(V_s\) for the pure 2D Hubbard model discussed below.

As a simple cuprate system, we consider \(La_{2-x}Sr_xCuO_4\), with a body-centered tetragonal \((bct)\) 3D model crystal structure, in-plane lattice constant \(a = 3.80\text{\,Å}\), inter-layer spacing \(d = 6.62\text{\,Å}\), \(t = 0.35\text{\,eV}\) and \(U = 8t\). (Small orthorhombic or larger-unit-cell tetragonal distortions from this idealized structure are neglected.) Note that the foregoing values for \(U\) and \(t\) are consistent with the values derived by the systematic mapping of the low-energy Hilbertspace of the three-band onto the single-band Hubbard model. The values of \(U\) and \(t\) are also consistent with (and, essentially, determined by) the observed values of the antiferromagnetic exchange constant \(J \approx 0.13eV\) and of the Mott-Hubbard charge excitation gap \(\Delta_{MH} \approx 1.8-2.6eV\) in the undoped \(La_2CuO_4\) parent compound.

Using standard finite-temperature fermion determinant QMC methods, \(\chi_o\) 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 square lattices with periodic boundary conditions at \(\beta \equiv 1/T\) up to \(\beta t \approx 10\), with imaginary-time step \(\Delta\tau \equiv \beta/L_t \lesssim 0.0625t^{-1}\) where \(L_t\) is the Trotter number. In most simulations, we use for \(H_o\) the pure Hubbard model with

\[
V_o(r) = U \delta_{r,0}
\]

In order to explore the effects arising from inclusion of extended \(V\)-terms in the polarization insertion \(P_o\), we have also performed a few simulations for the 1st neighbor extended Hubbard model, with

\[
V_o(r) = U \delta_{r,0} + V_1 \sum_{s \in N_1} \delta_{r,s}
\]

where

\[
V_1 \equiv \frac{e^2}{\epsilon_B a}
\]

is the strength of the bare in-plane 1st neighbor Coulomb repulsion and \(N_1\) denotes the set of in-plane 1st neighbor lattice vectors, \(s = (\pm a, 0, 0)\) and \((0, \pm a, 0)\).

### III. DIELECTRIC SCREENING IN THE \(\frac{1}{2}\)-FILLED MOTT-HUBBARD INSULATOR

Our first objective is to calculate the dielectric constant of the insulator from our model and thereby obtain an estimate for the background screening \(\epsilon_B\) [in Eq. (4)] from the measured long-wavelength external field dielectric tensor \(\epsilon_{ex}(\omega)|_{q \to 0}\) in the undoped, insulating \(La_2CuO_4\) material. Note here that the observed \(\epsilon_{ex}(\omega)|_{q \to 0}\) contains contributions from both the conduction electron system, explicitly included in our Hubbard model description, and from the “background” electron and phonon degrees of freedom which are not explicitly included in our single-band Hubbard description. Note also that in our simplified model, \(\epsilon_B\) is represented as a momentum- and frequency-independent constant, i.e., in effect the background is treated as a structureless homogeneous dielectric medium, down to atomic length scales. We should caution from the outset that such an
approach can provide only reasonable order of magnitude estimates.

In a more quantitative modeling approach, based e.g., on a shell model representation of the insulating non-Hubbard electron and phonon background, one may include more realistically the momentum and frequency structure of $\epsilon_B$. However, as discussed briefly below, the “local field” effects in such a model, arising from the momentum dependence of $\epsilon_B$, will not qualitatively alter our main conclusions. Also, the frequency dependence of the electronic contribution to $\epsilon_B$ is likely of lesser importance, due to the high charge excitation energy scale of the background electrons which is expected to be in the several eV range, exceeding the Hubbard electron bandwidth $8t$. Via the phonon contribution to $\epsilon_B$, on the other hand, the low phonon frequency scale $\Omega_{ph} \lesssim 0.1eV \ll 8t$, enters into the screening of the Coulomb interaction, and, along with it, isotopic mass dependence. This may have implications for the explanation of the isotopic effect observed in the superconducting properties of the cuprates, especially in the underdoped regime, as discussed further in Section IV. However, as we will also explain in Section IV, neither the presence of the phonon contribution nor its low frequency scale, will substantially alter the Hubbard electrons’ “metallic” screening at finite doping which is the central focus of the present paper.

Within the framework of our simplified background dielectric model, we obtain the longitudinal (scalar) dielectric function $\epsilon_{ex}$ from

$$\frac{1}{\epsilon_{ex}(q, i\omega)} = \frac{1}{\epsilon_B} \left[ 1 - \frac{4\pi e^2}{\epsilon_B V_c |q|^2} \chi(q, i\omega) \right]$$  \hspace{1cm} (12)

at $i\omega = 0$. Here, $V_c$ denotes the 3D unit cell volume and as discussed above, $\chi = -P[1-V(q)P]^{-1}$ from [1] with $P \equiv P_o$. The components of the static dielectric tensor $\epsilon_{ex}$ in the long-wavelength limit can then be extracted from

$$\hat{e} \cdot \epsilon_{ex} \cdot \hat{e} = \lim_{|q| \to 0} \lim_{L \to \infty} \epsilon_{ex}(|q|\hat{e}, i\omega = 0)$$ \hspace{1cm} (13)

for arbitrary unit vectors $\hat{e}$ with $L$ denoting the linear lattice size. Note here that it is crucial to take the thermodynamic limit $L \to \infty$ at finite $|q| > 0$ before taking the long-wavelength limit $|q| \to 0$.

Since the finite-system QMC simulations provide us with density correlation data $\chi_o(q, i\omega)$ only on a finite, discrete $q$-grid, some special care must be taken to extract the foregoing limits from the QMC data. To do so, we have developed a simple, physically motivated $r$-space embedding procedure which provides us with a continuous $q$-space interpolation and gives a reasonable approximation of $\chi_o(q, i\omega)$ in the thermodynamic limit. Our embedding procedure is based on the observation that, in the $\frac{1}{2}$-filled limit at large $U$, $U \sim 8t$, and low temperature $T$, the single-layer density correlation function $\chi_o(r, i\omega)$ in $r$-space is actually of quite short range and, already on rather small lattices, exhibits very little finite-size dependence. Physically, this is simply a manifestation of the fact that the charge excitation spectrum exhibits a large Mott-Hubbard gap, $\Delta_{\text{MH}} \sim U \gg t, T$. The Mott-Hubbard gap not only suppresses all charge correlations; it also endows them with a very short charge correlation length, $\xi$. In fact, from our QMC data taken on $8 \times 8$ lattices at $T = 0.1t$ we estimate $\xi$ to be substantially less than the in-plane lattice constant $a$.

Based on this observation, we approximate $\chi_o^{(L)}(r, i\omega)$ for a large $L \times L$ square lattice by the QMC result $\chi_o^{(QMC)}(r, i\omega)$, obtained on a smaller lattice of size $L_o \times L_o$, for those $r$-vectors which fall within the (properly symmetrized) boundaries of the smaller lattice; for $r$-vectors outside of those small-lattice boundaries, we simply set $\chi_o^{(L)}(r, i\omega)$ to zero. Specifically, for 2D lattice vectors $r \equiv (m_1a, m_2a)$ on the $L \times L$ “host” lattice, with integer $m_1$, $m_2$ and $|m_1|, |m_2| \leq L/2$, we set

$$\chi_o^{(L)}(r, i\omega) = w(r, L_o)\chi_o^{(QMC)}(r, i\omega)$$ \hspace{1cm} (14)

where, for even $L_o$,

$$w(r, L_o) = \begin{cases} 1 & \text{if } |m_1| < L_o/2 \text{ and } |m_2| < L_o/2 \\ \frac{1}{2} & \text{if } |m_1| = L_o/2 \text{ and } |m_2| < L_o/2 \\ \frac{1}{2} & \text{if } |m_1| < L_o/2 \text{ and } |m_2| = L_o/2 \\ 0 & \text{otherwise} \end{cases}$$ \hspace{1cm} (15)

In principle, we could also set the embedding weight factors $w(r, L_o)$ to zero for those lattice vectors which fall “on the boundary” (i.e., for $|m_1| = L_o/2$ or $|m_2| = L_o/2$), without noticeably changing our final results, since even for our small QMC lattices, our $\chi_o^{(QMC)}(r, i\omega)$ are already negligibly small on the boundary. With the above choice of $w$, Eq. (14), we are ensuring that the large-lattice $\chi_o^{(L)}$ provides a “natural” interpolation of the small-lattice $\chi_o^{(QMC)}$ in $q$-space, in the sense that, after Fourier transform, identically

$$\chi_o^{(L)}(q, i\omega) = \chi_o^{(QMC)}(q, i\omega)$$ \hspace{1cm} (16)

for those discrete 2D $q$-points $q \equiv (2\pi/a)(p_1/L_o, p_2/L_o)$, with integer $p_1, p_2$, which lie on the discrete $q$-grid of the smaller $L_o \times L_o$ lattice.

An additional complication in extracting $\epsilon_{ex}$ from the QMC data arises from the fact that the QMC simulations are performed at finite temperature where the system exhibits a small, but non-zero, concentration of electron and hole charge carriers due to thermal excitation across the Mott-Hubbard gap. In our QMC simulations in the grand-canonical ensemble, these thermally excited carriers manifest themselves by the fact that

$$\chi_o^{(T)}(q, i\omega = 0) > 0$$ \hspace{1cm} (17)

i.e., at finite $T$ there is a finite thermal fluctuation in the system’s total particle number. From QMC simulations at different temperatures, we have verified that this thermal carrier contribution to $\chi_o$ does indeed exhibit
the expected activated behavior, i.e., roughly $\chi_o^{(T)} \sim \exp(-\Delta_{MH}/T)$. If included in the calculation of $\chi(q, i\omega)$ this finite $q = 0$ charge fluctuation would give rise to a "quasi metallic" singularity contribution to the scalar dielectric function which would completely dominate the $q \to 0$ limit, with

$$\epsilon_{ex}(q, i\omega = 0) \sim \frac{4\pi e^2}{V_c q^2} \chi_o^{(T)}.$$  

(18)

Physically this reflects the fact that the thermally excited charge carriers are screening out any macroscopic Coulomb field with a finite screening length, which is simply a manifestation of the general principle that no physical system can be a true insulator at finite temperature.

To estimate the $(T = 0)$ insulator contribution to $\chi_o$, we thus subtract out the thermally activated carrier contribution and use as our $\chi_o$-input into Eq. (8)

$$\chi_{o,ins}^{(L)}(q, i\omega) = \chi_o^{(L)}(q, i\omega) - \chi_o^{(T)} \delta_{i\omega,0}$$

(19)

to calculate $P_o(q, i\omega)$. With this subtraction, the resulting $\chi$ from Eq. (8) indeed, by construction, acquires the correct "insulating" long-wavelength behavior to give a finite $\epsilon_{ex}$ for $|q| \to 0$.

Taking the limit $L \to \infty$ on $\chi_{o,ins}^{(L)}$ and then expanding the resulting $\chi_{ins}^{(\infty)}$ around $q = 0$, we can write

$$\chi_{o,ins}^{(\infty)}(q, i\omega) = \hat{e} \cdot \hat{B} \cdot \hat{e} |q|^2 + O(|q|^4)$$

(20)

for $q \equiv |q|\hat{e}$ with unit vector $\hat{e}$ and with the cartesian components of the $\hat{B}$-tensor given by

$$B_{\alpha\beta} = \frac{1}{2} \lim_{|q|\to 0} \frac{\partial^2 \chi_{o,ins}^{(\infty)}(q, i\omega = 0)}{\partial q_\alpha \partial q_\beta}$$

(21)

for $\alpha, \beta = 1, 2, 3$.

Inserting $\chi_{o,ins}^{(\infty)}(q, i\omega = 0)$ from Eq. (20) into Eq. (8), combining with Eqs. (11) and (12), and comparing to Eq. (13), we get

$$\overline{\epsilon}_{ex} = \epsilon_B \overline{1} + \frac{4\pi e^2}{V_c} \hat{B} .$$

(22)

With the cartesian coordinate axes chosen along the conventional tetragonal symmetry directions, only the diagonal components of $\hat{B}$ and $\overline{\epsilon}_{ex}$ are non-zero with the in-plane component given by

$$\epsilon_\| \equiv \epsilon_{ex,11} = \epsilon_{ex,22} = \epsilon_B + \frac{4\pi e^2}{V_c} B_\| .$$

(23)

Since, in our approximation, we do not include any interlayer charge correlations in $\chi_o$, the out-of-plane ("c-axis") component of $\hat{B}$ vanishes and we get

$$\epsilon_\perp \equiv \epsilon_{ex,33} = \epsilon_B ,$$

(24)

i.e. the Hubbard electron system does not contribute to the c-axis dielectric screening.

From our QMC results for $\chi^{(QMC)}(q, T)$ on a $L_o \times L_o = 8 \times 8$ lattice, embedded in large $L \times L$ lattices with $L$ up to 512, we estimate $B_\|$, using Eq. (22), and from it the Hubbard electron system’s contribution to the in-plane dielectric constant

$$\Delta \epsilon \equiv \epsilon_\| - \epsilon_\perp = \frac{4\pi e^2}{V_c} B_\| .$$

(25)

Using the pure on-site Hubbard potential, Eq. (1), as our interaction potential $V_o$ in the QMC Hamiltonian, with the standard Hubbard model parameters stated in the previous section, we find $\Delta \epsilon \equiv 0.70$ from QMC data obtained $T = 0.333t$ and $\Delta \epsilon \equiv 0.93$ from QMC data obtained $T = 0.11t$. Note that this value of $\Delta \epsilon$ is independent of $\epsilon_B$, since $\chi_o$ and $B_\|$ depend only on the QMC Hamiltonian $H_o$ which is independent of $\epsilon_B$ for the pure Hubbard case.

The slight ($\sim 25\%$) $T$-dependence of the foregoing $\Delta \epsilon$ result suggests that the thermal fluctuations, due to thermally excited carriers, are still noticeably (but not substantially) affecting the "insulating" charge correlations in the Mott-Hubbard insulator itself, at $T = 0.333t$. This is not entirely surprising since, e.g., the thermal carrier subtraction $\chi_o^{(T)}$ at that $T$ is about $10 - 20\%$ of typical $\chi_o$-values at typical non-zero $|q| \sim \pi/a$, e.g. $\chi_o^{(T)}/\chi_o(q, i\omega = 0)|_{BZ} \approx 0.15$ where $\langle \ldots \rangle_{BZ}$ denotes the Brillouin zone average over $q$. However, it is reasonable to assume that the $T = 0.1t$ result approximates the $T = 0$ limit to within a percent or better, since the thermal carrier subtraction $\chi_o^{(T)}$ at $T = 0.1t$ is already 5 orders of magnitude smaller than, say, typical $\chi_o$, e.g., $\chi_o^{(T)}/\chi_o(q, i\omega = 0)|_{BZ} \approx 2 \times 10^{-5}$.

To explore the effects of including renormalizations due to extended Coulomb interactions in the polarization insertion $P_o$, we have also performed simulations for a $\frac{1}{2}$-filled 1st neighbor extended Hubbard model, Eq. (10), with $V_1 = t = 0.35eV$ at $T = 0.333t$. The resulting change in $\Delta \epsilon$, $\delta \Delta \epsilon \equiv \Delta \epsilon|_{V_1=\frac{1}{2}} - \Delta \epsilon|_{V_1=0} \approx -0.014$, is only about $2\%$ of $\Delta \epsilon$. Unfortunately, minus problems in the QMC simulations prevent us from extending these $V_1$-dependent studies to lower $T$ and/or more realistic larger $V_1$-values, with, say, $V_1 = 2 - 3 \times t$. However, the foregoing result clearly suggests that the extended Coulomb effects on the polarization insertion are entirely negligible, at least as far as the long-wavelength limit at $\frac{1}{2}$-filling is concerned.

The measured values for the dielectric tensor $\epsilon_{ex}(\omega)$ of undoped La$_2$CuO$_4$ in the static limit $\omega \to 0$ are $\epsilon_{0,||} \equiv \epsilon_{11}(\omega = 0) \approx 30 \pm 3$ for the in-plane component, and $\epsilon_{0,\perp} \equiv \epsilon_{33}(\omega = 0) \approx 25 \pm 3$ for the c-axis component. However, these values include a large, in fact, dominant phonon contribution. 

[^1]: The measured values for the dielectric tensor $\epsilon_{ex}(\omega)$ of undoped La$_2$CuO$_4$ in the static limit $\omega \to 0$ are $\epsilon_{0,||} \equiv \epsilon_{11}(\omega = 0) \approx 30 \pm 3$ for the in-plane component, and $\epsilon_{0,\perp} \equiv \epsilon_{33}(\omega = 0) \approx 25 \pm 3$ for the c-axis component. However, these values include a large, in fact, dominant phonon contribution.
The purely electronic contribution to the dielectric screening is observed at frequencies \( \omega_\infty \sim 0.5 - 1 \text{eV} \), which are well above the phonon spectrum \( \Omega_{\text{ph}} \lesssim 0.1 \text{eV} \), but at the same time still well below the electronic Mott-Hubbard charge gap \( \Delta_{BH} \sim 1.5 - 2 \text{eV} \). In this frequency regime, one finds approximately frequency independent values of \( \varepsilon_{\infty,||} \equiv \varepsilon_{\|}(\omega_\infty) \approx 4.73 \) for the in-plane component and \( \varepsilon_{\infty,\perp} \equiv \varepsilon_{\perp}(\omega_\infty) \approx 4.56 \) for the c-axis component. The corresponding anisotropy \( \Delta \varepsilon_\infty = \varepsilon_{\infty,||} - \varepsilon_{\infty,\perp} \approx 0.2 \) is substantially smaller than our estimated value \( \Delta \varepsilon = 0.9 \). However, in our model estimate, we are assuming an isotropic background \( \varepsilon_B \), whereas, in the real material, the background itself could also be anisotropic. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term. If we generalize our model to allow for such a background anisotropy, we can estimate the background anisotropic term.

One of the main conclusions from the foregoing analysis is that the background degrees of freedom dominate the dielectric constant at \( \frac{1}{2} \) filling, with the Hubbard “conduction band” electrons contributing only about 25% to the total electronic dielectric constant, as observed in the \( \omega_\infty \) frequency range. The other main conclusion is that both in the background dielectric screening and in the full dielectric screening (including Hubbard electrons), the anisotropy is insignificant, compared to the actual values of the dielectric tensor components. This conclusion holds equally well for the purely electronic contribution to the dielectric screening and for the phonon contribution, as evidenced by the nearly identical values of \( \varepsilon_0 \sim 30 \) and \( \varepsilon_{0,\perp} \sim 25 \) in the static limit. We will therefore in the following continue to work with an isotropic background model, with the electronic \( (\omega_\infty) \) value \( \varepsilon_B = \sqrt{\varepsilon_B^c \varepsilon_B^T} \approx 4 \) and the analogously obtained static \( (\omega \to 0) \) value \( \varepsilon_B \approx 27 \), providing, respectively, reasonable lower and upper limits for \( \varepsilon_B \).

From the estimated \( \varepsilon_B \approx 4 \) (without phonons) or even \( \varepsilon_B \approx 27 \) (including phonons), one obtains substantial 1st neighbor repulsion strengths of \( V_1 \equiv e^2 / (\varepsilon_B a) \approx 0.95 \text{eV} \approx 2.7 t \) in the former and \( V_1 \approx 0.14 \text{eV} \approx 0.4 t \) in the latter case. Thus, the extended part of the Coulomb potential, \( V_S(r) \), appears to be indeed strong enough, that it could severely suppress extended (1st neighbor) pairing potentials which are commonly invoked in both phenomenological models and microscopic scenarios of d-wave pairing. It is therefore of considerable interest to find out how this bare Coulomb interaction potential between the Hubbard electrons is modified due to the metallic screening generated by the doped Hubbard electron system itself. In the next section, we will turn to this question.
IV. QMC RESULTS FOR $V_S$

In Fig. 3(a) and (b), we show results for $V_S(r, i\omega)$ at $i\omega = 0$, plotted vs. doping $x \equiv 1 - (n_j)$ for the on-site ($r = 0$) and in-plane 1st neighbor $r$-vector in the quasi-2D extended Hubbard model on the $La_2CuO_4$ bet crystal structure with $\epsilon_B = 4$ and $\epsilon_B = \infty$. Note that the latter $\epsilon_B$ represents just the pure 2D Hubbard model, with the extended part of the Coulomb potential, $V_o$, set to zero. The results for $V_S$ were extracted from QMC data for the single-plane density correlation function $\chi_o$ of the pure 2D Hubbard model, i.e., with $V_o$ given by Eq. (3), as explained in Section I, and with $V_S(r, i\omega)$ obtained from $V_S(q, i\omega)$ by Fourier transform over the finite-lattice 1st Brillouin zone. Since we are only interested in the short-distance behavior of $V_S$, here, we have not attempted to embed our 2D $\chi_o$-data in larger 2D lattices, as was done in the previous Section for the insulating dielectric function calculations. Rather, all results shown are for $L_o \times L_o \times L_o$ 3D lattices, using QMC data for $\chi_o$ obtained on corresponding $L_o \times L_o$ 2D lattices, with $L_o = 6, 8, \text{and } 10$.

As shown in Fig. 3(b) a small amount of doping suppresses the extended $1/|r|$-repulsion for $r \neq 0$ and causes a sign change in the 1st neighbor and (not shown) in the 2nd and 3rd neighbor screened potential. Thus, $V_S(r)$ at short-range in-plane distances $r \neq 0$ becomes attractive, for $x$ of order 5%, the attraction strength reaches a maximum at $x \sim 10 - 14\%$, and $V_S(r)$ turns repulsive again at $x \sim 23 - 28\%$.

As shown in Fig. 3(a), the on-site ($r = 0$) potential, while largely unaffected by screening at $x = 0$, is also rapidly suppressed with increasing $x$ and it also becomes attractive at larger doping, near $x \geq 15\%$. Over the doping range studied, the screened on-site potential varies monotonically with $x$, in contrast to the extended $(r \neq 0)$ part of $V_S$.

As a function of $\epsilon_B$, $V_S$ varies generally monotonically, in the directions indicated in Figs. 3(a) and (b). If we increase $\epsilon_B$ from 4 to the upper estimated value of $\epsilon_B = 27$, we find that the resulting $V_S$ will be within $1 - 2\%$ of the $\epsilon_B = \infty$ (pure 2D Hubbard) results shown in Figs. 3(a) and (b). Overall, in comparing the quasi-2D extended Hubbard model with $\epsilon_B = 4$ to the pure 2D Hubbard model ($\epsilon_B = \infty$), we note that all the foregoing results are qualitatively unaffected by the extended Coulomb repulsion. The primary effect of the extended Coulomb terms is to move the 1st neighbor $V_S$ slightly in the repulsive direction, thereby suppressing the maximal 1st neighbor attraction strength in Fig. 3(b) by less than 10%. In addition, the extended Coulomb interaction shifts the “optimal” doping, where the 1st neighbor attraction maximum occurs, from $x \approx 10\%$ in the pure 2D Hubbard model to $x \approx 13\%$ in the quasi-2D extended Hubbard model with $\epsilon_B = 4$. The screened on-site potential is shifted slightly in the attractive direction, but, again, for doping concentrations up to 20%, the effect is typically smaller than 10%.

These results suggest that, despite the substantial strength of the bare extended Coulomb potential $V_e$ at near-neighbor distances, the local screened potential in the Hubbard electron system at finite doping is largely unaffected by extended Coulomb interactions. Recall from the previous section that the Hubbard electrons are largely ineffective in providing dielectric screening in the $\frac{1}{2}$-filled insulator. By contrast, the results in Fig. 3 suggest that the Hubbard electrons’ metallic screening is very strong, in fact, strong enough to completely overwhelm the extended Coulomb repulsion, once a sufficient amount of doping and sufficient electronic background screening, with $x > 5\%$ and $\epsilon_B \geq 4$, say, is present. Additional background screening due to phonons will not have any significant effect on $V_S$ under these conditions.

From the foregoing discussion, it also becomes clear that the presence and frequency dependence of the phonon contribution to $\epsilon_B$ will not substantially affect the Hubbard electrons’ metallic screening at finite doping. If one were to include a phononic frequency dependence in $\epsilon_B$, with a typical phonon frequency scale $\Omega_{ph} \ll \delta t$, then as a function of $i\omega$, one would find that $V_S(r, i\omega)$ is given roughly by the pure Hubbard result (i.e. the dashed lines in Fig. 3) at frequencies $|i\omega| \ll \Omega_{ph}$ where the phonons contribute to the background screening; and $V_S(r, i\omega)$ is given roughly by the extended Hubbard result with $\epsilon_B \equiv 4$ (i.e. the full lines in Fig. 3) at frequencies $|i\omega| \gtrsim \Omega_{ph}$ where the phonons do not contribute to the background screening. Over most of the doping range of interest, e.g., between $x \sim 10\%$ and $x \sim 20\%$, this additional “phononic” frequency dependence of $V_S$, for $|i\omega|$ on the scale of $\Omega_{ph}$, is thus quite small, since the $\epsilon_B = 4.0$ extended Hubbard results are not very different the $\epsilon_B = \infty$ pure Hubbard results for $V_S$. More importantly, the qualitative features of $V_S$, such as its doping dependence and the overscreening effects at finite doping will not be changed by the phononic effects. The foregoing argument implicitly assumes that the characteristic frequency scale of the electronic density correlations, i.e., of $\chi_o(q, i\omega)$, is much higher than $\Omega_{ph}$. From earlier QMC studies, it appears that this condition is indeed satisfied, since the spectral weight for density fluctuations in the Hubbard model extends over a frequency range comparable to the electronic bandwidth.

By the same arguments, the phononic frequency dependence of $V_S$ will become increasingly important at low doping concentrations where the metallic screening of the Hubbard electrons is too weak to suppress the extended Coulomb effects. This observation may offer a possible explanation for the doping dependence of the isotope effect in the superconducting transition temperature of the cuprates. The observed isotope exponent $\alpha$ is generally a decreasing function of doping, in the underdoped regime, and becomes negligibly small (compared to the classical BCS value of $\alpha = \frac{1}{2}$) in the “optimal” doping range near $x \sim 15\%$. This behavior is qualitatively consistent with the notion that, with increasing
doping, the phonon effect becomes less and less important in the screened potential. Along with its doping dependence, also the overall magnitude of the isotope exponent in underdoped cuprates (which can exceed the classical BCS value) has been a long-standing theoretical puzzle given the assumption of an electronic pairing mechanism. It remains to be explored within specific pairing models whether the phononic frequency dependence of the screened Coulomb potential is large enough to also explain the observed magnitudes of $\alpha$ in the underdoped regime.

Minus sign problems at finite doping unfortunately limit our simulations to $T \geq \Delta T$. However, at least in that temperature regime, we find $V_S$ to be increasing with decreasing $T$. This suggests that the over-screening effects ($i.e.$ the attraction in $V_S < 0$) becomes stronger than shown in Fig. 1 at lower $T$.

The presence of both a strong Hubbard-$U$ and finite doping density $x > 0$ are crucial for these over-screening effects to arise. If we replace the fully $V_o$-renormalized $P_o$ in $V(r)$ by, say, the non-interacting ("RPA") polarization bubble $P_{RPA}$, we also obtain 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 over the whole doping range studied here.

In the undoped large-$U$ system, $V_S(r)$ is reduced relative to $V(r)$, by a roughly $r$-independent factor comparable to the ratio $\epsilon_{\omega}/\epsilon_B$, for $r \neq 0$, i.e. $V_S$ is reduced relative to $V$ but retains a repulsive $1/|r|$-dependence. This is expected for the screening of a $1/|r|$ potential in an insulator and confirms the insulating character of the $1/2$-filled Hubbard system. The $1/r$ long-distance behavior of $V_S(r)$ can of course again be traced back to the fact that long-wavelength charge fluctuations are suppressed in the $1/2$-filled insulating state. For $x = 0$, $\chi(q, i\omega) \sim |q|^2 \to 0$, and hence also $P(q, i\omega) \sim |q|^2 \to 0$ for $|q| \to 0$. As a consequence, the screening denominator $1 - V(q)P(q, i\omega)$ in Eq. (3) remains finite for $q \to 0$ and $V_S(q, i\omega)$ inherits the $1/|q|^2$ singularity of $V(q)$, thus its $1/|r|$-dependence upon Fourier transforming back to $r$-space.

By contrast, in the doped system, the screening takes on a noticeably metallic character and the $r$-dependence of $V_S$ changes dramatically, even on the finite lattice sizes and high temperatures accessible with our QMC approach. Already at small doping concentrations, $x \gtrsim 5\%$, $V_S(r, i\omega)$ dies out much faster with $|r|$ than in the undoped case. For example, at "optimal doping" where the 1st neighbor $V_S$ is maximally attractive, the in-plane 2nd neighbor $V_S$ [at $r = (a, a, 0)$] is about 4 times smaller in magnitude than the in-plane 1st neighbor $V_S$ [at $r = (a, a, 0)$]. The metallic screening also strongly suppresses the inter-layer Coulomb repulsion, with $V_S$ at the nearest inter-layer distance $r = (a/2, a/2, d)$ being reduced by a factor of probably more than 500 relative to the bare $V$ at that distance and by a factor of more than 100 relative to the in-plane 1st neighbor $V_S$. Notice here that the quasi-2D Hubbard electron system can produce inter-layer screening even though our model does not include any matrix elements for inter-layer electron transfer. Unlike the in-plane components of $V_S$, its inter-layer components remain repulsive at finite dopings, over the doping range explored in Fig. 1, i.e., we do not find any evidence for inter-layer overscreening.

The essential features of $V_S$ are robust against substantial modifications of the extended Coulomb terms. Note here that, in real materials, the simple $1/|r|$-dependence of $V_{1}(r)$ can be modified locally by local field effects. However, our results do not change by more than $20 - 30\%$ if we in- or decrease $V_{1}(r)$ locally, at 1st, 2nd, and/or 3rd neighbor distances, by up to $30\%$, relative to Eq. (4). The latter is a conservative upper limit for such local field effects, based on the cuprates’ Wannier orbital and crystal structure. Using different layered 3D geometries, such as a $YBa_2Cu_3O_7$ bi-layer structure, also does not change the results in Fig. 1 by more than a few percent.

We have also carried out QMC simulations with the 1st neighbor extended Hubbard model, Eq. (11), at finite doping, thereby including extended Coulomb effects in our in our polarization insertion $P$. Surprisingly, we find that this actually increases the 1st neighbor attraction of $V_S$ and, to a lesser extent, also the on-site attraction. For example, if we simulate and analyze according to Eqs. (15) in an in-plane 1st neighbor Hubbard model, with $V(r) = V_o(r)$ given by Eq. (10), and a 1st neighbor repulsion strength $V_1 = 0.5t = 0.175$eV, then the magnitude of the 1st neighbor attraction in $V_S(r, i\omega = 0)$ at a near-optimal doping of $x = 14\%$ increases by about 16% relative to the pure on-site Hubbard model results shown in Fig. 1(c). Notice that this is a comparison of two exact results, since we have used the same potential $V(r)$ in Eq. (4), as was used as our QMC potential $V_o(r)$, both in the pure Hubbard and in the 1st neighbor extended Hubbard calculation, i.e. $\chi_o = \chi$ and $P_o = P$ exactly. The foregoing result implies that the 1st neighbor overscreening (in the 5 – 25% doping range) is not only robust against extended Coulomb interactions, but, in fact, could be enhanced if extended Coulomb interactions are included exactly in the polarization insertion. This result also suggests the interesting possibility that extended Coulomb interactions may actually contribute constructively to the pairing attraction for extended superconducting pair wavefunctions and specifically to $d_{x^2-y^2}$-pairing, as discussed in Section V. The effects of including extended Coulomb interactions in the polarization insertion need to be investigated further. Specifically, the effects of longer-range Coulomb terms (2nd, 3rd, ...) neighbor need to be explored.

Only at unphysically large $V_1$, i.e. unphysically small $\epsilon_B$, does our approach break down, due to charge density wave instabilities. These instabilities are signaled by $1/\chi(q, i\omega = 0) \to 0$ at some point in $q$-space. For the parameter range explored in the present paper, this occurs only for $\epsilon_B \lesssim 2.0$. 

8
V. EXACT PROOF OF ON-SITE OVERSCREENING AND ITS IMPLICATIONS FOR THE POLARIZATION INSERTION

In order to see why a sufficiently large \( U \) at finite doping \( x \equiv 1 - \langle n_j \rangle \) must cause an on-site overscreening effect, we consider first the pure Hubbard model, \( V(r) \equiv U\delta_{r,0} \), where, from the exact Eq. (4),

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

with \( V_S(r, i\omega) \) and \( \chi(r, i\omega) \) denoting the respective Fourier transforms of \( V_S(q, i\omega) \) and \( \chi(q, i\omega) \) back into \( r \)-space. Clearly, the on-site \(-U^2\chi\)-term in Eq. (26) is attractive for all \( i\omega \), since \( \chi(r=0, i\omega) \), the autocorrelation function of \( \Delta n_j \), is always positive.

At \( x = 0 \), i.e. in the \( \tfrac{1}{2} \)-filled insulator, charge fluctuations are suppressed by the Mott-Hubbard gap. For \( U \rightarrow \infty \), one finds from a large-\( U \) expansion that \( \chi(r, i\omega = 0) \sim O(t^2/U^2) \), and, in Eq. (26), \( V_S(r=0, i\omega = 0) \equiv U - O(t^2/U) > 0 \) which remains repulsive for large \( U \gg t \). The crucial point here is that, at finite \( |x| > 0 \), even an infinitely large \( U \) cannot completely suppress the charge fluctuations, since \( n_j \) is not conserved at finite \( |x| \), regardless of \( U \). Specifically, the on-site component \( \chi(r=0, i\omega) \) approaches a positive, non-zero limit \( \sim O(x/t) \), by a simple \( U = \infty \) scaling argument for \( U \rightarrow \infty \). Hence, the \(-U^2\chi\)-term will overcome the bare \( U \)-term in Eq. (26) and \( V_S(r=0, i\omega) \) must become attractive, i.e. on-site overscreening must occur, for sufficiently large \( U \). Also, as a consequence, for sufficiently large \( U \), \( V_S(r=0, i\omega=0) \) must change sign as a function of \( x \).

Formally, the suppression of \( \chi \) at the \( \tfrac{1}{2} \)-filling arises in the strong-coupling expansion because the large repulsive \( U \) effectively projects out the low-energy Hilberspace sector containing only states without doubly occupied sites. Upon projection onto the low-energy sector, the on-site charge operators \( n_j \) become exactly conserved with \( n_j = 1 \) and \( \Delta n_j = 0 \) at all sites for \( U \rightarrow \infty \), giving \( \chi \equiv 0 \) from Eq. (3). At large, but finite \( U \), inter-site charge transfer processes via the hybridization term \( H_t \), must necessarily go through “virtual” intermediate states containing at least one doubly occupied site. To 2nd order in the hybridization \( H_t \), each of the two matrix elements exciting from the low-energy sector into this high-energy sector and back is of order \( t/U \) while the inverse energy denominator associated with the virtual excitation is of order \( 1/U \), resulting in \( \chi \sim t^2/U^3 \). At finite doping, on the other hand, the projected \( n_j \) are not conserved. Even for \( U = \infty \), the doping induced holes can still move through the lattice, via the \( H_t \)-term, since the inter-site charge transfer can proceed without having to go through high-energy intermediate states involving double occupancy. Hence, \( \chi \) approaches a non-zero limit, \( \chi_\infty \neq 0 \), at finite doping concentration for \( U \rightarrow \infty \).

Note that the foregoing large-\( U \) argument constitutes an exact analytical proof of on-site overscreening in the asymptotic limit \( U \rightarrow \infty \). The proof holds both on finite and infinite lattices in any spatial dimension and it immediately generalizes to the full extended Hubbard model, Eqs. (4) since the \(-U^2\chi\)-term remains the dominant screening contribution for \( U/t \rightarrow \infty \) at finite \( x > 0 \), even in the presence of a finite extended interaction term \( V_c \neq 0 \). Our QMC results in Fig. [a] not only confirm these exact large-\( U \) results; they also show that the large-\( U \) scenario is realized in the physically relevant parameter regime \( U \sim 8 - 12t \).

The occurrence of on-site overscreening, or close proximity to it, is accompanied by profound effects in the polarization insertion \( P(q, i\omega) \), namely, by \( q \)-dependent singularities of \( P \) on the (analytically continued) \( i\omega \)-axis. To see this, recall that \( V_S(r=0, i\omega) \) is just the Brillouin zone average of \( V_S(q, i\omega) \). Hence, in order to get \( V_S(r=0, i\omega) < 0 \), there must be some region in \( q \)-space, for which \( V_S(q, i\omega) < 0 \). On the other hand, since \( \chi(q, i\omega) \sim O(1/\omega^2) \) for \( |\omega| \rightarrow \infty \), it follows from Eq. (4) that \( V_S(q, i\omega) \rightarrow V(q) > 0 \) for \( |\omega| \rightarrow \infty \), i.e., in the high frequency limit the screened potential approaches the repulsive bare potential. Hence, for those \( q \) for which \( V_S(q, i\omega) < 0 \) at some (low) frequency \( \omega \), there must exist at least one \( i\omega(\omega(q)) \), on the imaginary frequency axis, such that \( V_S(q, i\omega) \), analytically continued onto the continuous \( i\omega \)-axis, goes through zero,

\[
\lim_{\omega \rightarrow i\omega(\omega(q))} V_S(q, i\omega) = 0.
\]

By Eq. (6), this implies

\[
\lim_{\omega \rightarrow i\omega(\omega(q))} 1/\chi(q, i\omega) = V(q)
\]

and, by Eq. (6), which is equivalent to \( 1/P(q, i\omega) = V(q) - 1/\chi(q, i\omega) \), this implies

\[
\lim_{\omega \rightarrow i\omega(\omega(q))} 1/P(q, i\omega) = 0.
\]

In other words, \( 1/P(q, i\omega) \) changes sign and \( P(q, i\omega) \) must be singular at \( i\omega(\omega(q)) \).

Note that this clearly is a strong correlation effect. Weak coupling approximations to \( P(q, i\omega) \), notably RPA, do not give such a singularity in \( P(q, i\omega) \). In RPA, \( 1/P(q, i\omega) < 0 \) at all \( q \) and \( \omega \). It is therefore not surprising that RPA cannot reproduce the on-site overscreening effect. Note also that this singularity in \( P \) does not imply any singularities \( i.e. \) instabilities) in physically observable quantities, such as \( \chi(q, i\omega) \). In fact, \( \chi(q, i\omega) \) is perfectly regular at \( i\omega(\omega(q)) \), as implied by Eq. (25) and \( V(q) > 0 \).

However, the singularity of \( P(q, i\omega) \) does imply singularities of certain vertex functions to which both \( P \) and the single-particle self-energy \( \Sigma \) are diagrammatically related. For example, both \( P \) and \( \Sigma \) can be expressed in terms of an appropriately defined 3-point vertex function \( \Lambda(k, iv; q, i\omega) \), entering boson momentum-energy \( (q, i\omega) \), entering fermion momentum-energy \( (k, iv) \) (where \( iv \) is an odd Matsubara frequency)
and exiting fermion momentum-energy \((k + q, iv + i\omega)\), such that

\[
P(q, i\omega) = \left(\frac{T}{N}\right) \sum_{k, iv} G(k, iv) G((k + q, iv + i\omega) \Lambda(k, iv; q, i\omega)) \tag{30}
\]

and

\[
\Sigma(k, iv) = \Sigma_{H}(k) - \left(\frac{T}{N}\right) \sum_{q, i\omega} V_{S}(q, i\omega) G(k + q, iv + i\omega) \Lambda(k, iv; q, i\omega) \tag{31}
\]

where \(G(k, iv)\) is the single-particle Green’s function and \(\Sigma_{H}\) denotes the self-energy contribution from the Hartree diagram. Note that the singularity of \(P\) implies an analogous singularity in the \(i\omega\)-dependence of \(\Lambda\) for \(i\omega \rightarrow i\omega^{(s)}(q)\). However, in the foregoing expression for \(\Sigma\), which is, in principle, a physically observable quantity, the singularity of \(\Lambda\) is cancelled by the vanishing of the other factor in the summand, \(V_{S}(q, i\omega) \rightarrow 0\) for \(i\omega \rightarrow i\omega^{(s)}(q)\). The formal implications of this singularity in \(P\) and \(\Lambda\) need to be further investigated.

As discussed in Section IV, RPA results show that, for near \(1\text{st}, 2\text{nd}, \ldots\) neighbor \(r\)’s, \(\chi(r, i\omega = 0)\) is negative at small \(U\), whereas QMC results suggest that the near-neighbor \(\chi(r, i\omega = 0)\) becomes positive at finite doping when \(U\) exceeds a doping dependent threshold of order several \(t\). From Eq. (26) one sees that this positive near neighbor \(\chi(r, i\omega = 0)\) gives rise to the near neighbor attraction in \(V_{S}\) at large \(U\) and finite \(x\), as displayed in Fig. 1b. Hence, the QMC and RPA results taken together suggest that near-neighbor overscreening is fundamentally also a large-\(U\) effect, just like on-site overscreening. However, note here that \(\chi(r, i\omega)\) for \(r \neq 0\) is not an autocorrelation function and its sign is allowed to be either positive or negative, depending on the model parameters. Because of this, it does not seem to be possible to generalize the above large-\(U\) overscreening proof to show the existence of near- \(1\text{st}, 2\text{nd}, \ldots\) neighbor overscreening in \(V_{S}(r, i\omega)\) by analytical means. Also, unlike the on-site overscreening case, the existence of near-neighbor overscreening does not necessarily imply the existence of singularities in \(P(q, i\omega)\).

V. D- AND S-WAVE PAIRING STRENGTHS

Given the attractive nature of the screened potential at finite doping, it is tempting to ask whether this attraction could give rise to superconductivity and, if so, of what pairing symmetry. A potential 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, compared to the bare Hubbard-\(U\). 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. Such an expansion can be formulated diagrammatically by retaining only skeleton diagrams in which none of the interaction lines contain any polarization insertions and each interaction line represents a \(V_{S}(q, i\omega)\). Superconducting instabilities can then be studied in terms of such a perturbative approximation to the irreducible particle-particle vertex, expanded to 1st order in \(V_{S}\).

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. A convenient measure of the pairing strength of \(V_{S}\) are the dimensionless EM \(\lambda\)-parameters, defined in terms of the Fermi surface “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, e.g., in Refs. 13 and 25.

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 \(\eta_{s}(k) \equiv 1\) and \(\eta_{d}(k) = \cos(ak_{x}) – \cos(ak_{y})\). To carry out the required Fermi surface integrals, our 3D \(V_{S}(q, i\omega)\) was interpolated from the finite \(8\times8\times8\) lattice \(q\)-grid onto a \(200\times200\times200\) \(q\)-grid, using the 3D version of the \(q\)-interpolation scheme described in Section I for the 2D \(q\)-interpolation of \(\chi_{\lambda}\).

Applying this interpolation scheme to \(V_{S}(q, i\omega)\) is justified here, analogous to the above \(\chi_{\lambda}\)-interpolation, by the fact that, at finite doping, \(V_{S}(r, i\omega)\) is of very short-range in \(r\)-space, due to the “metallic” character of the screening.

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. We note in passing that the doping dependence of \(\lambda_{d}\) is reminiscent of the observed doping dependence of the superconducting \(T_{c}\) in the cuprates. The \(\lambda\)-values for near-neighbor pair wavefunctions of other symmetries \((p, d_{xy}, q)\) are small compared to \(\lambda_{s}\) and \(\lambda_{d}\) and for that reason not further discussed here.

The spectral weight of \(\chi(q, i\omega)\) extends up to values \(\Omega_{\chi} \sim 8 – 10\). In the EM analysis, this ”boson” energy scale, together with \(\lambda\), determines the superconducting \(T_{c}\), roughly as \(T_{c} \sim \Omega_{\chi} \exp(-1/\lambda)\). Because of the large \(\Omega_{\chi}\)-scale, it may be possible, at least within the EM approximation, to achieve high \(T_{c}\)’s even for moderate coupling values \(\lambda < 1\).

We should caution here that the foregoing QMC results can of course only suggest the general, qualitative trends in \(V_{S}\) and \(\lambda\) parameters, due to the high temperatures and small lattice size limitations inherent in the QMC
approach. Also, our EM approach is based formally on a perturbative expansion of the exact irreducible particle-particle vertex to 1st order in $V_S$. This approximation should be relied upon, if at all, only close to the "cross-over" $x_C \approx 15\%$ when $V_S(r=0, i\omega) = 0$, so that $|V_S(q, i\omega)| \ll 8t$, at least for low frequencies $|i\omega| \ll 8t$. i.e. roughly in the 10 $\sim$ 20% doping range. At large over- or underdoping ($x \gtrsim 20\%$ or $x \lesssim 10\%$), where $|\lambda_\sigma| \sim O(1)$, corrections of higher order in $V_S$ are likely to contribute strongly to the self-energy and to the irreducible particle-particle vertex, thereby causing the EM approximation, with $V_S$ as the effective pairing potential, to break down. The increasingly attractive $\lambda_\sigma$-values at $x \gtrsim 25\%$ doping, in Fig. 1c, do therefore not necessarily imply increasingly strong s-wave pairing tendencies. The effects of vertex corrections, of higher order in $V_S$, need to be further explored, both in the over- and underdoped regimes.

It is also important to realize that the strong reduction in overall screened potential strength $|V_S|$ is only a necessary, not a sufficient condition for the applicability of the EM approach. Note in particular, that $V_S$ is "weak" (and, where applicable, attractive) only at low frequencies. At large frequencies, with $|i\omega|$ of the order of the bandwidth $8t$, the charge correlation function begins to die out, with $\chi(q, i\omega) \sim 1/|i\omega|^2$, and, by Eq. (3), $V_S(q, i\omega) \rightarrow V(q)$ for $|i\omega| \rightarrow \infty$. In other words, at high frequencies, the screened potential recovers the full strength of the bare potential. Physically, this simply reflects the fact that at high frequencies, $|i\omega| \gg 8t$, the conduction electron system is "too slow" to provide a screening response to very rapidly varying fields. Since the characteristic frequency scale of these charge fluctuations is quite high, of the order of the bandwidth, the conventional underpinnings of the EM approximation, such as the Migdal theorem, are not necessarily satisfied. Thus, even in the "near-optimal" doping regime where the low-frequency $V_S$ is weak, it needs to be re-examined whether corrections to the irreducible particle-particle vertex of higher order in $V_S$ are indeed small.

With these caveats in mind, we should compare our results for the pairing strengths in the Hubbard model to earlier studies of the superconducting pairing correlations and of the effective pairing potential $\Delta_{\sigma}$ in the Hubbard model. Early studies of pair correlation functions indicated a tendency towards $d_{x^2-y^2}$-pairing. In finite-T simulations this was suggested by an increase in $d_{x^2-y^2}$ pairing correlations with decreasing temperature. However, due to the QMC minussign problem, these exact QMC studies were limited to small lattice sizes and rather high temperatures (in physical units about an order of magnitude higher than the observed $T_c$ scale in the cuprates). It may therefore be difficult to draw meaningful conclusions about the low-temperature long-range pairing correlations of the model from the finite-system and/or finite-T exact QMC data for pair correlation functions.

Also, by contrast, more recent studies of pairing correlations in the groundstate of the Hubbard model, based on the "constrained path Monte Carlo" (CPMC) approach, did not provide any evidence for long-range pairing correlations of either $d_{x^2-y^2}$- or s-wave symmetry. However, the CPMC approach is based on a (in principle uncontrolled) variational approximation which, albeit remarkably successful in reproducing exactly known groundstate energies, may not necessarily reproduce the exact pairing correlations. Thus, existing QMC studies of pair correlation functions in the Hubbard model are, at best, inconclusive as far as $d_{x^2-y^2}$-pairing is concerned and, with all the above-cited limitations, they do not provide evidence for s-wave pairing in the near-$\frac{1}{2}$-filled Hubbard model.

In addition to the above-cited "technical" limitations, there is a further, physical reason why especially long-range s-wave pairing correlations, if existent in the Hubbard model, may escape detection in QMC simulations of pair correlation functions. To understand this, note that retardation plays a central role in the physical origin of the screening attraction in our $V_S$. For example, for the pure Hubbard model, Eq. (26) Fourier transformed to the (imaginary) time ($\tau$) domain, becomes

$$V_S(r=0, \tau) = U\delta(\tau) - U^2\chi(r=0, \tau). \quad (32)$$

A pair of electrons, $e$ and $\bar{e}$, say, is subject to the instantaneous, bare repulsive $U$ interaction term only if they both occupy the same site $j$ at the same time. By contrast, the attractive screening term, $-U^2\chi$, is retarded, i.e., physically speaking, the charge polarization caused by $e$ at site $j$ can still be felt by $\bar{e}$ after a time lag $\theta > 0$, when $\bar{e}$ has already left $j$. Thus, the on-site screening arises from processes wherein the two electrons interact on the same site, but at different times, via their local charge polarizations, thereby evading their bare, instantaneous repulsion. The time scale for this retarded interaction is governed by the frequency spectrum of the dynamical density correlation $\chi$, i.e., for the relevant parameter range it is of order of the inverse bandwidth $(8t)^{-1}$. Pair correlations induced by such a potential, with retarded attractive and instantaneous repulsive contributions, should be most easily detected via time-delayed pair creation order parameters of the general form

$$\Delta_\theta = c_j^\dag(\theta)c_{\bar{j}}^\dag \quad (33)$$

where $c_j^\dag(\theta) = e^{i\theta H}c_j^\dag e^{-i\theta H}$. In other words, $\Delta_\theta$ creates the second electron $\bar{e}$ with time lag $\theta$ relative to the first electron $e$. For the on-site s-wave ($j = \bar{j}$) case, one should thus consider time-delayed pair correlation functions of the general form

$$C(r_j - r_{\bar{j}}, \tau, \theta, \theta') = \langle T \{ c_j(\tau + \theta)c_{\bar{j}}(\tau) c_{\bar{j}}^\dag(\theta')c_j^\dag(0) \} \rangle \quad (34)$$
where $T[...]$ implies fermion time ordering. The strongest signal for pairing correlations should then be detected for typical values of $\theta$ and $\theta'$ which are comparable to the retardation time scale of the attractive part of the potential, i.e., in the case of our $V_S(r, \tau)$, for $\theta, \theta' \sim \langle 8t \rangle^{-1}$. By contrast, the existing QMC studies of pairing correlation functions in the Hubbard model have so far considered only simultaneous pair correlations $C(r_j - r_\tau, \tau, \theta, \theta')$ with $\theta = \theta' = 0$. In such a simultaneous pair correlation function, the detectable signal for $s$-wave pairing is expected to be very weak (and, in the case of pairing with odd frequency parity, identically zero) if the underlying pairing potential happens to have a time-dependent structure of the sort described above for $V_S(r, \tau)$, i.e., a strong instantaneous repulsion superimposed on a retarded attraction. We note that for such a temporal structure of the pairing potential the possibility of a triplet $s$-wave pairing state with odd frequency parity can not be ruled out.

In using QMC simulations to find superconducting instabilities via the pair correlation function approach one thus faces at least three major difficulties: (i) long-range pair correlations develop only at low temperatures, of order $T_c$; (ii) it requires large lattice sizes to detect such long-range correlations in finite systems (a problem compounded at finite $T$ in two dimensions by the expected algebraic decay of the correlations); and, (iii) depending on the structure of the superconducting order parameter, the simulated pair correlation function may provide only an undetectably weak signal if one chooses the “wrong” pair creation operators (and one doesn’t know a priori which operators are the “right” ones). A potentially promising route to circumvent some of these difficulties is to focus instead on the underlying exact effective pairing potential, i.e., in precise diagrammatic terms, on the irreducible particle-particle vertex function $\chi^{\lambda}_{x \tau}(8t)^{-1}$. The basic idea here is that, in contrast to long-range pair correlations, the effective pairing potential may be (i) of short range and may (ii) develop strong signatures of the pairing attraction already at high temperatures. Also, (iii) by solving for the dominant pairing eigenvalues and eigenfunctions of the the corresponding particle-particle ladder equation, the particle-particle vertex approach automatically reveals the symmetry and space-time structure of the dominant superconducting order parameter.

The existing QMC results for the exact irreducible particle-particle vertex of the 2D Hubbard model near $\frac{1}{2}$-filling suggest that there is indeed a noticeable 1st neighbor pairing attraction and that a pairing eigenfunction of spin-singlet $d_{x^2-y^2}$ symmetry becomes dominant (i.e., develops the largest pairing eigenvalue) as the temperature is lowered. In addition, sub-dominant pairing eigenvalues of comparable magnitude with eigenfunctions of odd-frequency triplet $s$- and odd-frequency singlet $p$-wave symmetry are found. The effective “on-site” interaction extracted from the irreducible particle-particle vertex is found to be repulsive.

We should emphasize here that, aside from some preliminary studies at $\frac{1}{2}$-filling all of the foregoing exact irreducible particle-particle vertex results were obtained at a doping concentration of $x \cong 13\%$ and, at that concentration, they are not inconsistent with our results for the pairing $\lambda$-parameters shown in Fig. 2(c). At $x = 13\%$, our $d_{x^2-y^2}-\lambda$ is indeed the dominantly attractive one; the $s$-wave-$\lambda$ is repulsive at $x = 13\%$ and becomes attractive only for $x > 15\%$.

Also, unfortunately, the reported results for the real-space interaction strengths extracted from the irreducible particle-particle vertex were for smaller Hubbard $U$, $U = 4t$, whereas a physically more realistic larger value of $U = 8t$ was used in our calculations of $V_S(r, \omega)$. Recall here that, as discussed above, the on-site overscreening is a large-$U$ effect and $U = 4t$ may simply be too small to produce on-site overscreening. Interestingly, from a comparison of the pairing eigenvalues extracted from the irreducible particle-particle vertex at $U = 4t$ and at $U = 8t$, it appears that the (odd frequency triplet) $s$-wave eigenvalues are increasing with $U$. This observation is not inconsistent with the notion that one moves towards on-site overscreening with increasing $U$.

It would therefore be of considerable interest to check whether the irreducible particle-particle vertex develops an on-site attraction and stronger $s$-wave pairing tendencies at larger doping, $x > 15\%$, and larger Hubbard repulsion $U$, e.g., for $U = 8t$. This would provide a very stringent test as to whether our screened potential $V_S$ in the charge representation indeed provides a reasonable approximation to the exact irreducible particle-particle vertex or whether particle-particle vertex corrections of higher order in $V_S$ are important.

In analyzing the irreducible particle-particle vertex, it was also found that its momentum and real-space structure, and the $T$-dependence of that momentum and real-space structure, closely resembles that of an appropriately defined spin fluctuation mediated pairing potential of the Hubbard model, suggesting that spin fluctuations are indeed responsible for the $d$-wave pairing attraction. It is possible that the positive near-neighbor charge correlations [i.e. $\chi(r, \omega = 0) > 0$ at near-neighbor $r$-vectors], responsible for the $d$-wave pairing attraction in our approach, are closely (and perhaps causally) related to short-range antiferromagnetic spin correlations in Hubbard systems near $\frac{1}{2}$-filling. The charge representation approach 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. 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 may be (with all the above-stated caveats !) “obvious” in the former, but difficult to reproduce in the latter approach. The relationship between our charge representation formulation and the spin fluctuation picture of the Hubbard model needs to be further investigated.
VII. SUMMARY

In summary, by a combination of diagrammatic and quantum Monte Carlo techniques and by exact analytical approaches, we have studied the dielectric screening and the screening of electron-electron Coulomb repulsions in the charge representation of the 2D Hubbard model. We find that finite doping gives rise to a 1st neighbor overscreening effect which causes the exact screened on-site Coulomb potential $V_S$ in the charge representation to become attractive. We have shown that this is indeed an intrinsic local property of both large-$U$ Hubbard and extended Hubbard models at finite doping which exists independent of dimensionality, 3D crystal structure or system size. Our QMC results thus show that this asymptotic large-$U$ scenario is indeed realized in the finite-$U$ parameter range relevant to the cuprates. We have also shown that on-site overscreening implies singularities in the imaginary-frequency dependence of the irreducible polarization insertion and of its underlying 3-point vertex function.

When analyzed as an effective pairing potential $i.e.$, formally, as a 1st order approximation to the irreducible particle-particle vertex, the screened potential $V_S$ gives rise to a 1st neighbor $d_{x^2-y^2}$ pairing attraction in the doping range between $x \gtrsim 5\%$ and $x \lesssim 20 - 25\%$ and to an on-site $s$-wave pairing attraction for $x > 15\%$. The doping dependence of the $d_{x^2-y^2}$ Eliashberg $\lambda$-parameter closely tracks that of the extended (1st neighbor) attraction of $V_S$, with a maximum of pairing strength near $x = 10 - 15\%$, reminiscent of the observed doping dependence of the superconducting $T_c$ in the cuprates. The doping dependence of the on-site $s$-wave $\lambda$-parameter closely tracks that of the on-site $V_S$, increasing monotonically with $x$ and becoming strongly attractive for $x \sim 15\%$. This suggests the possibility of a doping induced transition or cross-over from $d$- to $s$-wave pairing.

We have argued that retardation plays an essential role in the on-site overscreening of the interaction potential and that this should be reflected in the temporal / frequency structure of the corresponding $s$-wave superconducting order parameter.

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