Inhomogeneous d-wave superconducting state of a doped Mott insulator

Ziqiang Wang, Jan R. Engelbrecht, Shancai Wang, Hong Ding
Department of Physics, Boston College, Chestnut Hill, MA 02467

Shuheng H. Pan
Department of Physics, Boston University, Boston, MA 02215 (December 30, 2021)

Recent atomic resolution scanning tunneling microscope (STM) measurements discovered remarkable electronic inhomogeneity, i.e. nano-scale spatial variations of the local density of states (LDOS) and the superconducting energy gap, in the high-\(T_c\) superconductor Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+x}\). Based on the experimental findings, we conjectured that the inhomogeneity arises from variations in local oxygen doping level and may be generic of doped Mott insulators. In this paper, we provide theoretical support for this picture. We study a doped Mott insulator within a generalized t-J model, where doping is accompanied by ionic Coulomb potentials centered in the BiO plane located a distance \(d_s\) away from the CuO\(_2\) plane. We solve, at the mean-field level, a set of spatially unrestricted Bogoliubov-de Gennes equations self-consistently to obtain the distributions of the hole concentration, the valence bond and the pairing order parameters for different nominal/average doping concentrations. We calculate the LDOS spectrum, the integrated LDOS, and the local superconducting gap as those measured by STM, make detailed comparisons to experiments, and find remarkable agreement with the experimental data. We emphasize the unconventional screening of the ionic potential in a doped Mott insulator and show that nonlinear screening dominates on nano-meter scales, comparable to the short coherence length of the superconductor, which is the origin of the electronic inhomogeneity. It leads to strong inhomogeneous redistribution of the local hole density and promotes the notion of local doping concentration (LDC). We find that the inhomogeneity structure manifests itself at all energy scales in the STM tunneling differential conductance, and elucidate the similarity and the differences between the data obtained in the constant tunneling current mode and the same data normalized to reflect constant tip-to-sample distance. We also discuss the underdoped case where nonlinear screening of the ionic potential turns the spatial electronic structure into a percolative mixture of patches with smaller pairing gaps embedded in a background with larger gaps to single particle excitations.

PACS numbers: 74.20.Mn, 74.80.-g, 68.37.Ef, 74.25.Jb

I. INTRODUCTION

The parent compounds of the high-\(T_c\) superconductors are stoichiometric Mott insulators \[1\]. In principle, carriers can be introduced into the insulating state either by field effect or by chemical doping, but to date high-\(T_c\) superconductivity in the cuprates has only been found to arise when they are properly doped away from stoichiometry. In the case of YBa\(_2\)Cu\(_3\)O\(_{7-x}\) (YBCO) and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+x}\) (BSCCO), the dopants are the excess oxygen atoms. The latter inject holes into the CuO\(_2\) planes, leaving behind the negatively charged oxygen ions. While for YBCO, the dopant ions go into the copper oxide chains and can be arranged more periodically, \[3\] in the case of BSCCO, the dopants, with a concentration of \(x\), disorder themselves in the semiconducting BiO layer which is about 5\(\AA\) away from the CuO\(_2\) plane where superconductivity is believed to originate.

In addition to doping holes into the CuO\(_2\) planes, the dopant oxygen atoms inevitably introduce long-range random ionic potentials that scatter the carriers in the copper-oxide plane in analogy to the situation encountered in two-dimensional (2D) electron systems in modulation doped semiconductors. This has the potential to cause the electronic structure in the copper-oxide plane to be inhomogeneous. Early neutron scattering \[3\], tunneling \[4\] and STM \[5\] data showed features that could be accounted for by inhomogeneity, but they were usually attributed to sample quality. The common view, which is largely based on the physics of ordinary metals, has been that the ionic potential in a high-quality crystal would be screened by phonons and by the carriers in the plane such that charges distribute uniformly and are accommodated by a homogeneous electronic structure; albeit that the latter has the tendency towards microscopic phase separation \[6\] due to strong electronic correlations. This viewpoint appears to be supported, to a certain extent, by transport \[7\] and photoemission \[8\] measurements on BSCCO which observe quasiparticles with relatively well-defined momentum, a mean-free path of about 100\(\AA\) in the nodal direction, and a transport mean-free path of about 400\(\AA\).

However, this conventional view has been seriously challenged by recent low-temperature STM measurements on BSCCO. \[9-11\] In Ref. \[9\], Pan et al. (here after referred to as we) observed spatially cross-correlated variations in the LDOS and the superconducting energy gap on a remarkably short length scale of about 14\(\AA\). We identified this as the gap amplitude coherence length...
or the pair size. It directly confirms the local pairing nature in the high-$T_c$ superconductor. The magnitude of the superconducting gap has a Gaussian distribution with a mean value of 42 meV, close to the gap value obtained from planar tunneling, and a full-width-half-maximum of about 20 meV. This variance coincides with the intrinsic width ($\sim 20$ meV) of the coherence peak measured by angle resolved photoemission spectroscopic (ARPES) near the antinodes where the d-wave gap is at its maximum. It offers an explanation of the latter as arising, even in the absence of bilayer splitting, from averaging over a distribution of local gap values under the macroscopic ARPES light spot.

Careful analysis of the STM data, combined with those of the ARPES, led us to conjecture in Ref. [9] that the observed inhomogeneous electronic structure arises from the ionic potential associated with the off-stoichiometry oxygen dopants disordered in the BiO layer. We argued that the screening of the ionic potential in the doped Mott insulator is unconventional and incomplete on the nano-meter scale of the pair size, causing the local doping (hole) concentration to exhibit spatial variations. Such a doping profile results in a highly cross-correlated pairing gap profile if the pairing interaction is sufficiently short-ranged.

It should be stressed that the physics involved here is highly unconventional. In an ordinary metal such as copper, the Thomas-Fermi screening length in the linear screening theory is shorter than 1Å, beyond which the ionic potential is perfectly screened and the charge density homogeneous. Such a short screening length is a result of the large thermodynamic density of states or the compressibility ($dn/d\mu$) in ordinary metals. However, adding holes to a doped Mott insulator causes significant shift in the chemical potential due to the strong local Coulomb repulsion. This leads to a small electronic compressibility and thus a larger screening length even within the linear screening theory. We believe that the observed inhomogeneous superconducting state is a result of the strong local correlation in a doped Mott insulator.

It is important to provide theoretical tests for these ideas and to compare theoretical results with experiments. In this paper, we do so by studying the d-wave superconducting state of a doped Mott insulator in a microscopic theory of a generalized t-J model, where doping is accompanied by ionic Coulomb potentials centered at a given strength of the Coulomb interaction, the size of the nonlinear screening is the strong spatially inhomogeneous redistribution of the charge carrier density brought about by the bare ionic potential. The concept of a local doping concentration (LDC) therefore naturally arises. The d-wave pairing amplitude turns out to follow locally the spatially varying hole density, resulting in an inhomogeneous superconducting state. In the resonating valence bond picture, this corresponds to an inhomogeneous state of spinon pairing and local holon condensation. We calculate the local tunneling density of states spectrum, the integrated LDOS, and the local electronic spectrum as measured by the local tunneling density of states. We find that the calculated zero-bias tunneling spectra. We show that the same inhomogeneity structure manifests itself at all energy scales in the calculated tunneling spectra. We find that the calculated zero-bias tunneling
conductance, which is dominated by the nodal quasiparticles, shows spatial variations that are correlated with that of the LDG. We elucidate in detail the mapping, the differences and similarities between the tunneling differential conductance obtained in the constant tunneling current mode, which does not directly represent the electron LDOS, and the same data normalized to reflect a constant tip-to-sample distance that faithfully represent the electronic tunneling density of states. We also provide preliminary evidence that the high superconducting transition temperature $T_c$ can be protected by the short superconducting coherence length and coexist with this type of electronic inhomogeneity.

The rest of the paper is organized as follows. In section II, we describe our generalized t-J model and set up the self-consistent equations for the spatially unrestricted Hartree-Fock-Bogoliubov mean-field solutions. In section III, we study the screening properties of the ionic potential in detail. A single test ion is inserted which imposes a coulombic potential on the otherwise uniform d-wave superconducting state. The charge redistribution and the response of the pairing order parameter to screening of the ionic potential is analyzed. In section IV, we discuss the solution of the inhomogeneous d-wave superconducting state for a finite density of dopant ions and doped holes. We emphasize the concept of LDC and analyze the correlation among these physical observables. In section V, we focus on the inhomogeneity at low energy scales. We study the spatial distribution of the zero-bias tunneling conductance, its correlation with the LDC, and make predictions for experimental tests. In section VI, we discuss the mapping between constant-current differential tunneling conductance and the constant tip-to-sample distance LDOS spectra. The STM topography is calculated for our system together with the constant-current differential tunneling conductance and compared to experiments. A summary of the results and their implications are given in section VII together with discussions of several open issues.

II. GENERALIZED t – J MODEL AND THE SELF-CONSISTENCY EQUATIONS

We begin with the generalized t-J model Hamiltonian that includes the long-range Coulomb interaction and the ionic potentials introduced by the process of carrier doping,

$$H = H_{t-J} + H_{\text{Coul}} + H_{\text{ion}}.$$  

Here $H_{t-J}$ is the usual 2D t-J model on a square lattice,

$$H = -t \sum_{\langle i,j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + J \sum_{\langle i,j \rangle} \langle S_i \cdot S_j \rangle - \frac{1}{4} n_i n_j,$$  

where $c_{i\sigma}^\dagger$ is the electron creation operator and $S_i$ is the spin operator $S_i = \frac{1}{2} c_i^\dagger \hat{\sigma}_\alpha c_i \hat{\sigma}_\beta$. The sums over $\langle i,j \rangle$ are among nearest neighbors and sums over repeated spin indices are implied. The most important Mott-Hubbard physics, i.e. the strong on-site Coulomb repulsion, is included in the additional constraint of no double occupancy at each site, $n_i = c_{i\sigma}^\dagger c_{i\sigma} \leq 1$. $H_{\text{Coul}}$ is the long-range Coulomb repulsion,

$$H_{\text{Coul}} = \sum_i V_i n_i, \quad V_i = V_c \sum_{j \neq i} \frac{n_j - \bar{n}}{|r_i - r_j|},$$  

where $\bar{n}$ denotes the average density. The Coulomb interaction strength $V_c$ is given by $V_c = e^2/4\pi \varepsilon a$, with $\varepsilon \approx 8$ the dielectric constant and $a \approx 3.8$ Å the lattice constant corresponding to the Cu-Cu atomic spacing.

The resulting $V_c \sim t$. As emphasized in Ref. [15], the inclusion of the long-range Coulomb interaction is necessary to prevent the mean-field ground state of $H_{t-J}$ from macroscopic phase separation in the interesting parameter regime. The off-plane ionic potential of the dopants is described by $H_{\text{ion}}$,

$$H_{\text{ion}} = \sum_i U_i n_i, \quad U_i = \sum_{\text{ion}=1}^{N_{\text{ion}}} \frac{V_{\text{ion}}}{\sqrt{|r_i - \mathbf{r}_{\text{ion}}|^2 + d_s^2}}.$$  

Here $d_s$ is the distance between the CuO$_2$ plane and the BiO layer where the negatively charged ions reside randomly at $\mathbf{r}_{\text{ion}}$, and $N_{\text{ion}}$ is the number of independent ions in the BiO layer. To model the situation in BSCCO, where each dopant oxygen gives one hole to each of the planes in a bi-layer, we use $N_{\text{ion}} = N_{\text{hole}} = x \times N_s$ where $N_{\text{hole}}$ is the number of doped holes, $x$ is the average doping (hole) concentration on a lattice of $N_s$ sites. We use $J$ as the unit of energy and set $d_s = 1.5a$, $V_{\text{ion}} = V_c = 5J$, and $t = 3J$ in most of our numerical calculations. We verified that varying these parameter in a reasonable range does not qualitatively change our results.

It is convenient to describe the projected Hilbert space in terms of a spin-carrying fermion, the spinon $f_{\alpha\sigma}^\dagger$, creating the singly occupied site with spin-$\sigma$ and a spinless boson, the holon $b_i$, keeping track of the empty site [16]. The electron creation operator becomes $c_{i\sigma}^\dagger = f_{\alpha\sigma}^\dagger b_i$ and the occupancy constraint translates in this slave-boson formulation into $f_{\alpha\sigma}^\dagger f_{\alpha\sigma} + b_i^\dagger b_i = 1$. In the mean-field theory, the antiferromagnetic spin-exchange term is decoupled according to [16]

$$S_i \cdot S_j = -\frac{3}{8} |\chi_{ij}|^2 f_{\alpha\sigma} f_{\alpha\sigma} + \text{h.c.}$$

$$+ \Delta_{ij}^r (f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow}) + \text{h.c.}$$

$$+ \frac{3}{8} (|\chi_{ij}|^2 + |\Delta_{ij}|^2),$$  

Here $H_{t-J}$ is the usual 2D t-J model on a square lattice, $H_{\text{Coul}}$ is the long-range Coulomb repulsion, $H_{\text{ion}}$ is the off-plane ionic potential of the dopants.
where $\Delta_{ij}$ and $\chi_{ij}$ are the spinon pairing and bond order parameters respectively,

$$\Delta_{ij} = \langle f_{i\uparrow} f_{j\downarrow} - f_{i\downarrow} f_{j\uparrow} \rangle, \quad \chi_{ij} = \langle f_{i\sigma} f_{j\sigma} \rangle,$$

defined for each nearest neighbor bond. The inhomogeneous superconducting phase is reached through the local condensation of bosons at low temperatures,

$$\langle b_i^\dagger \rangle = \langle b_i \rangle = \bar{b}_i,$$

(6)

It is important to emphasize that in the presence of the translation symmetry breaking ionic potential in Eq. (4), $(\Delta_{ij}, \chi_{ij}, \bar{b}_i)$ become spatially dependent and must be determined at every site self-consistently. Note that the local doped hole density or the LDC is then directly related to the local boson condensate density,

$$x_i = \bar{b}_i^2,$$

(7)

and the constraint at the mean-field level becomes $n_f = f_{i\sigma} f_{i\sigma} = 1 - x_i$, which is enforced on average at every site by locally shifting the fermion chemical potential $\mu_f$ to $\lambda_i + \mu_f$. Throughout this paper, we use $x$ to denote the average (doped) hole density or the nominal doping concentration,

$$x = \frac{1}{N_s} \sum_{i=1}^{N_s} x_i.$$

(8)

The decoupled Hamiltonian can be written down using the Bogoliubov-Nambu formalism over the Hilbert space of paired spinons,

$$H = \sum_{i,j} (f_{i\uparrow}^\dagger, f_{i\downarrow}) \left( \begin{array}{cc} K_{ij} & F_{ij}^* \\ F_{ji} & -K_{ji}^* \end{array} \right) \left( \begin{array}{c} f_{j\uparrow} \\ f_{j\downarrow}^\dagger \end{array} \right),$$

(9)

where the sums on $i$ and $j$ run over all lattice sites and

$$K_{ij} = \frac{3}{8} \lambda_{ij} \delta_{j,i+\eta},$$

$$F_{ij} = -(\theta_{i}^2 + \frac{3}{8} \lambda_{ij}) \sum_{\eta} \delta_{j,i+\eta} + [V_{sc}(i) - \mu_f] \delta_{ij},$$

with $\eta = \pm \hat{x}, \pm \hat{y}$. In Eq. (9), $V_{sc}(i)$ given by

$$V_{sc}(i) = U_i + \lambda_i + V_i \sum_{j \neq i} \bar{b}_j^2 - x_{ij},$$

(12)

is the nonlinearly screened local potential seen by the spinons implied by the self-consistency conditions. Note that in deriving Eq. (12), only the Hartree potential in the long-range Coulomb interaction is retained, whereas the exchange potential is neglected. The effects of the latter on the superconducting state will be studied elsewhere.

The Hamiltonian in Eq. (9) can be diagonalized in real space by solving the corresponding Bogoliubov-de Gennes equations to obtain the eigenstates $\gamma_n^i$ and $\gamma_n$ with energy $E_n$, $n = 1, \ldots, 2N_s$. The spinon operator can be expanded in this basis according to

$$f_{i\uparrow}(t) = \sum_n u_n(i) \gamma_n^i e^{-iE_n t/h},$$

$$f_{i\downarrow}(t) = \sum_n v_n(i) \gamma_n^i e^{-iE_n t/h},$$

(13)

(14)

where $(u_n(i), v_n(i))$ is the wave-function at site $i$. The order parameters and the local hole density can be expressed in terms of the wave-functions as follows

$$\Delta_{ij} = \sum_n [v_n^*(i) u_n(j) [1 - f(E_n)] - u_n(i) v_n^*(j) f(E_n)],$$

$$\chi_{ij} = \sum_n [v_n^*(i) v_n(j) [1 - f(E_n)] + u_n(i) u_n^*(j) f(E_n)],$$

(15)

(16)

(17)

where $f(E_n)$ is the usual Fermi distribution function.

We solve the self-consistency Eqs. (15,17) through numerical iterations. Typically, we start with a random set of $(\Delta_{ij}, \chi_{ij}, \lambda_i, x_i, \mu_f)$, insert them into Eq. (9) and diagonalize the resulting matrix to obtain the wave-functions $(u_n(i), v_n(i))$ and the eigenvalues $E_n$. Then we update the set of $(\Delta_{ij}, \chi_{ij}, \lambda_i, x_i, \mu_f)$ according to Eqs. (15,16,17) and insert them back into the Hamiltonian (9). The procedure is iterated until convergence is reached. In general we allow $\chi_{ij}$ and $\Delta_{ij}$ to be complex at the beginning of the iteration, but both of these order parameters converge to real values at the end of the iteration in the average doping range $(0.06 < x < 0.32)$ studied.

In order to compare to STM data, we calculate the local tunneling density of states,

$$N_i(\omega) = \text{Im} \int dt e^{i\omega t} G_i^{\text{ret}}(t),$$

(18)

where $G_i^{\text{ret}}(t)$ is the retarded local Green’s function of the electrons,

$$G_i^{\text{ret}}(t) = -\theta(t) \langle \{ c_{i\sigma}^\dagger(0), c_{i\sigma}(t) \} \rangle.$$

(19)

In the mean-field theory, since the bosons locally condense, we have

$$G_i^{\text{ret}}(t) = -\bar{b}_i^2 \theta(t) \langle \{ f_{i\sigma}^\dagger(0), f_{i\sigma}(t) \} \rangle.$$

(20)

Notice that the local electron Green’s function and therefore the local tunneling density of states is equal to the
local holon condensate density times the local spinon Green’s function. From Eq. (7), it is clear then that the LDOS is overall proportional to the LDC $x_i$. Using Eqs. (13,14), we obtain,

$$N_i(\omega) = x_i \sum_n (|u_n(i)|^2 \delta(\omega - E_n) + |v_n(i)|^2 \delta(\omega + E_n)).$$

(21)

The role played by the LDC is two-fold: it enters as an overall prefactor through essentially the wave-function renormalization of the electrons as well as through the LDOS of spinons from the response of $\Delta_{ij}$ and $\chi_{ij}$ to a spatially varying $x_i$. This is a property of the tunneling density of states which is different from the thermodynamic density of states.

Our choice of the t-J model for quantitative calculations is a natural one, because it is the simplest model that captures the physics of a doped (antiferromagnetic) Mott-insulator. In this strong coupling approach, the carrier concentration is proportional to the doping concentration (rather than the electron density), which is the most fundamental property of a doped Mott-insulator. More specifically, as can be clearly seen from Eq. (20), the coherent weight of the quasiparticle is small at small doping and scales with the LDC. This is in excellent agreement with the recent ARPES measurements [13,22] on BSCCO, where the weight of the emergent quasiparticle peak below $T_c$ near the anti-node was found to be proportional to the doping concentration at low temperatures.

III. A SINGLE OFF-PLANE ION AND NONLINEAR SCREENING

To understand the screening properties of the ionic potential better, we start with the case where a single off-plane ion (i.e. $N_{\text{ion}} = 1$) is placed above the center of a $25 \times 25$ lattice with a setback distance $d_s = 1.5a$. The ion imposes a Coulomb potential on the otherwise uniform superconducting state at a doping level $x$. This situation is similar to that of a single nonmagnetic impurity (say Zn) extensively studied using the t-J model recently, [23–25] except that the impurity is located out of the plane and the impurity potential is long-ranged. The scattering is presumably not in the unitary limit. In addition, fully self-consistent solution in $(\bar{b}_i, \Delta_{ij}, \chi_{ij})$ has not been studied before.

Fig. 1 shows the bare ionic potential $U_i$ from Eq. (4) and the screened potential $V_{sc}(i)$ from Eq. (12) coming out of the self-consistent solution. The average doping concentration in the plane is $x = 0.12$. It is clear that the long-range impurity potential in Fig. 1a is perfectly screened at distances much larger than $d_s$ but poorly screened at short distances resulting in a short-range impurity potential in Fig. 1b.

FIG. 1. The Coulomb potential from a single negatively charged ion located at a distance $d_s = 1.5a$ above the center of an otherwise uniform 2D d-wave superconductor. The lattice size is $25 \times 25$ and the average doping $x = 0.12$. (a) The long-range bare ionic potential from Eq. (4). (b) The screened potential from Eq. (12).
concentration of screening. The self-consistently determined local hole at the redistribution of the carrier density as a result of changes in the hole concentration

ion, the hole density is strongly inhomogeneous, namely Fig. 2a, which shows that in the vicinity of the dopant, the hole density is defined in Eq. (22). The solid line is a Gaussian fit to the data, which gives a decay length \( \xi \times 1.86a \).

The nature of the screening is revealed when we look at the redistribution of the carrier density as a result of screening. The self-consistently determined local hole concentration \( x_i \) is plotted in a 2D hole density map in Fig. 2a, which shows that in the vicinity of the dopant ion, the hole density is strongly inhomogeneous, namely the changes in the hole concentration \( \delta x_i \), brought about by the dopant ionic potential, are comparable to the averaged concentration \( x \) itself. Fig. 2b shows the hole density distribution along a horizontal line-cut passing through the center of the lattice. This clearly demonstrates that the screening of the ionic impurity potential in the doped Mott insulator is highly unconventional and is entirely dominated by nonlinear screening on the scale of the ionic setback distance \( d_s \). The nonlinearity in screening is further verified by its nonlinear response to changes in the strength of the Coulomb potential \( V_{\text{ion}} \).

It is instructive to compare to conventional screening in the linear response theory described by the Thomas-Fermi screening length, which is applicable to ordinary metals and superconductors. For an electron gas in 2D, the Thomas-Fermi screening length is \textit{independent} of electron density and is given by \( q_{\text{TF}}^{-1} = a_B^2/2 \), where \( a_B^2 = \hbar^2/\epsilon m^* e^2 \) is the effective Bohr radius. Taking \( \epsilon \approx 8 \) and a thermodynamic effective mass \( m^* / m \approx 3 \), which is appropriate for the cuprates, gives \( a_B^2 \approx 1.4\AA \). The resulting Thomas-Fermi screening length \( \sim 0.7\AA \) which is much less than a lattice spacing \( a \approx 3.8\AA \). Thus linear screening theory would have predicted that the ionic Coulomb potential is screened on the length scale of a lattice spacing and the charge redistribution induced by the bare potential is small. In our case, Figs. 2a and 2b clearly show that linear screening is only valid when the distance to the center of the ionic potential is much greater than the distance \( d_s \), where the hole density is essentially uniform and its value close to the average concentration \( x = 0.12 \).

Thus, the profile of the screened impurity potential and that of the hole density distribution and, as we shall see later, that of the d-wave pairing OP (see Fig. 2b), are controlled by the crossover from nonlinear to linear screening as one moves away from the center of the ionic potential. To better quantify this crossover behavior, we study the auto-correlation function of the local hole density variations \( \delta x_i = x_i - x \),

\[
C_x(r_j) = \frac{1}{N_x} \sum_i \langle \delta x_i \delta x_{i+j} \rangle.
\] (22)

In Fig. 2c, we show the azimuthally averaged \( C_x \), which decays very fast with the distance, indicative of strong short-range correlation in the LDC. The short-distance behavior can be fitted very well by a Gaussian with a decay length \( \xi = 1.86a \). For convenience, let us define the correlation length by the decay length of the Gaussian function. We arrive at a hole-density correlation length \( \xi_x = 1.86a \), which is quite close to the setback distance \( d_s = 1.5a \), suggesting the latter as the length scale over which the crossover between linear and nonlinear screening takes place.
local hole density from its average value. We plot, in Fig. 3a, the variation of the doped Mott insulator in the presence of a periodic lattice.

To study this question in the d-wave superconducting state of a 2D electron gas in the continuum. We next study the average doping dependence of the decay lengths extracted from the Gaussian fits to the correlation functions at the corresponding doping levels, shown in Fig. 3c. Thus, for a given strength of the ionic Coulomb potential, the size of the nonlinear screening cloud around the center of the potential is controlled entirely by the setback distance $d_s$.

In Fig. 3c, we show the spatial variation of the LDC $\delta x_i$ along the center horizontal cut for the case of a larger setback distance $d_s = 5a$ at $x = 0.06$ and 0.12. It is clear that as the screened potential becomes smoother, the size of the screening cloud becomes larger, characterized by a decay length on the order of $d_s$.

We next study the average doping dependence of the screening in the nonlinear regime. In the linear screening theory, the fact that the 2D Thomas-Fermi screening length is independent of carrier density is a consequence of the properties of the density of states and the polarizability of the 2D electron system. This suggests that the insensitivity of screening to average doping is true even for nonlinear screening. Analytical solutions of the 2D nonlinear screening problem only exists for the special case of an antidot in a semiconductor 2D electron gas in the continuum. To study this question in the d-wave superconducting state of a doped Mott insulator in the presence of a periodic lattice potential, we plot, in Fig. 3a, the variation of the local hole density from its average value $\langle \delta x_i \rangle$ as a function of distance along the center horizontal cut for several different average hole concentrations. The fact that the data points almost completely collapse onto a single curve shows that the screening is indeed insensitive to the carrier density in both the linear and the nonlinear screening regime.

This situation is quite reminiscent of a single in-plane nonmagnetic impurity, e.g. an intentionally doped Zn atom, that replaces a copper atom causing strong scatter-

FIG. 3. The average doping and setback distance dependence of screening. (a) The spatial variations in hole concentration $\langle \delta x_i \rangle$ along the central line-cut at four different average doping concentrations, showing screening is insensitive to average doping $x$. (b) The decay lengths of the hole-density (diamonds) and the d-wave pairing OP (triangle) auto-correlations, and that of the cross-correlation (circle) between the two as a function of average doping $x$. (c) Same as in (a), but for a larger setback distance $d_s = 5a$.

FIG. 4. The 2D maps showing the spatial variations in the dominant d-wave (a), and the accompanying extended s-wave (b) pairing OPs in the vicinity of the ionic potential.

In Fig. 4, we show the spatial variation of the self-consistently determined superconducting order parameter near the center of the ionic potential for $d_s = 1.5a$. We find that the nonlinear screening region where the hole concentration exhibits strong inhomogeneity is accompanied by spatial variation of the order parameter $\Delta_{ij}$. Moreover, when $\Delta_{ij}$, defined in Eq. (24), is decomposed into a $d_{x^2-y^2}$ and an extended s-wave component at a site $i$ according to,

$$\Delta_d(i) = \frac{1}{4}(\Delta_{i,i+\hat{x}} + \Delta_{i,i-\hat{x}} - \Delta_{i,i+\hat{y}} - \Delta_{i,i-\hat{y}}), \quad (23)$$

$$\Delta_s(i) = \frac{1}{4}(\Delta_{i,i+\hat{x}} + \Delta_{i,i-\hat{x}} + \Delta_{i,i+\hat{y}} + \Delta_{i,i-\hat{y}}), \quad (24)$$

we find that the spatially varying d-wave order parameter $\Delta_d(i)$ shown in Fig. 4a is complimented by a much smaller nonuniform $\Delta_s(i)$ shown in Fig. 4b. The magnitude of $\Delta_d$ along the center line cut in Fig. 4a has been shown in Fig. 2b.
ing in the unitary limit. The inhomogeneity induced $\Delta_s$ shows an interesting four-fold (d-wave) symmetry, i.e. it is vanishingly small along the nodal direction of $\Delta_d(i)$ and changes sign upon a 90° rotation. These properties can be qualitatively understood from the Ginzburg-Landau theory that permits by symmetry a mixed gradient term proportional to $\partial \Delta_d \partial \Delta_s$. Note that the order parameters in this $d + s$ state are both real and that spontaneous time-reversal symmetry breaking, such as in a $d + i s$ state, does not occur. It is interesting to point out that the reduction is greater in the anti-nodal direction where the d-wave gap is at its maximum.

The auto-correlation function of the spatial variation of the d-wave OP $\delta \Delta_d(i) = \Delta_d(i) - \bar{\Delta}_d$ and the cross-correlation function between $\delta \Delta_d(i)$ and the local doping variation $\delta x_i$ are defined by

$$C_{\Delta_d}(r_j) = \frac{1}{N_s} \sum_i (\delta \Delta_d(i) \delta \Delta_d(i + j)), \quad (25)$$

$$C_{\delta x - \Delta_d}(r_j) = \frac{1}{N_s} \sum_i (\delta x_i \delta \Delta_d(i + j)). \quad (26)$$

We plot the azimuthally averaged correlation functions in Fig. 5a and 5b. The $\Delta_d$-correlation length $\xi_{\Delta_d} \simeq 2.53a$, which is close to the hole density correlation length. The fact that the cross-correlation length, $\xi_{\delta x - \Delta_d} \simeq 2.26a$, is close to $\xi_d$ and $\xi_{\Delta_d}$ shows that the spatial variations in $\Delta_d$ and the LDC are strongly (anti-)correlated. This is an important character of the d-wave superconducting state emerged from the short-range resonating valence bond state, where the local spinon pairing produced by the nearest-neighbor antiferromagnetic exchange interaction is directly affected by the local holon condensate density.

To summarize this section, an out-of-plane negatively charged ion induces a nonlinear screening cloud in its vicinity, wherein the doping concentration is significantly higher and the d-wave pairing parameter significantly smaller than their averaged values in the bulk of the 2D superconductor. The size of the nonlinear screening cloud is essentially independent of the averaged doping concentration. It is controlled by the setback distance $d_s$ of the dopant ions to the 2D plane. This local picture for the response of the d-wave superconducting state to a single ionic test charge will be important for understanding the real situations of many ions, particularly in the case of dilute dopants in the underdoped regime. In the rest of the paper, we use $d_s = 1.5a$. This comes out naturally from the lattice constants of BSCCO which is about 3.8Å in the plane and 5Å in the c-direction. We will come back to this issue in the last section and discuss other physical processes, such as dielectric screening from interband transitions and electron-phonon coupling, that could complicate the choice of $d_s$, but would not change the essential physics described in this paper.

FIG. 5. The azimuthally averaged auto-correlation function for the d-wave OP variation (a) and the absolute value of the cross-correlation function between the hole density variation and the d-wave OP variation (b). The solid lines are Gaussian fits to the data.

FIG. 6. 2D density plot of the bare (a) and the screened (b) ionic potential on a 32 × 32 lattice at average doping $x = 0.12$. The data has been smoothed to reduce the effects of the lattice discreteness.

8
IV. FINITE DENSITY OF IONS — INHOMOGENEOUS SUPERCONDUCTING STATE OF A DOPED MOTT INSULATOR

Having studied how an external out-of-plane charge is screened by the d-wave superconductor, we now turn to the situation in BSCCO where \( N_{\text{ion}} \) number of negatively charged ions resides in the BiO layer donating \( N_{\text{hole}} = N_{\text{ion}} \) number of doped holes to each of the CuO bilayers. Without the knowledge of the detailed chemical frustration encountered by the dopant ions, we assume that they distribute randomly in the BiO layer. This can lead to accidental clustering of the dopant oxygen atoms which may or may not happen in real materials depending on the details of the chemistry. Since very strong clustering happens rarely and locally, it does not affect the essential physics we describe.

A. Inhomogeneous electronic structures

The bare ionic potential calculated from Eq. (4) is shown in Fig. 6a for a \( 32 \times 32 \) lattice at \( x = 0.12 \). The self-consistently determined screened potential of Eq. (12) is plotted in Fig. 6b. The large fluctuations in the bare ionic potential are dramatically screened as can be seen by comparing Fig. 6a and Fig. 6b. The spatial variations of the self-consistently determined LDC in Eq. (7) and \( \Delta_d \) in Eq. (23) are shown as 2D maps in Figs. 7a and 7b. It is clearly seen from Fig. 7a that the variations in the hole density closely track the screened potential in Fig. 6b. The local ionic dopant configurations are shown as black dots. The reverse color-coding for the \( \Delta_d \)-map makes it easy to observe the (anti-)correlation between \( x_i \) and \( \Delta_d(i) \). The average inter-hole distance at this doping is \( d_x \simeq 2.86a \), which is smaller than the size of the screening cloud \( 2\xi_x \simeq 3.72a \) of a single isolated ion discussed in the previous section. The fact that the number of dopant ions is the same as the number of doped holes then implies that the screening clouds associated with individual ions overlap and interfere such that nonlinear screening dominates and leads to significant inhomogeneity in the electronic structure throughout the entire system. This confirms the conjecture we made in Ref. [9] that the inhomogeneity results from the lack of conventional metallic screening of the dopant ionic potential in doped Mott insulators.

![FIG. 7. The spatial variations of the local hole concentration \( x_i \) (a) and the d-wave order parameter \( \Delta_d(i) \) (b) shown as 2D maps for \( x = 0.12 \) on a \( 32 \times 32 \) lattice. The location of the negatively charged ions projected on the 2D plane is shown as black dots in (a), together with the contours of the doped hole density. Reversed color-coding is used in (b) for easy visualization of the anti-correlation between \( x_i \) and \( \Delta_d(i) \).](image-url)
from their averaged values.

The azimuthally averaged auto-correlation for the d-wave order parameter variations is plotted in Fig. 8c which shows the same structure with a decay length $\xi_{d} \simeq 2.2a$. We remark that at this average hole concentration, which is slightly below optimal doping, the oscillatory structures are rather weak and are just beginning to emerge. Interestingly, the azimuthally averaged correlation functions obtained from the experimental STM data on optimally doped BSCCO, shown in Fig. 2 (e-f) of Ref. 9, have the same structure, including the weak oscillations in the tails. We expect the secondary peak to develop more prominently in more underdoped systems where percolative-like patches are likely to become more pronounced with increasing average inter-hole distance.

![Graphs showing auto- and cross-correlation analyses.](image)

**FIG. 8.** The auto- and cross-correlation analysis of the spatial variations in the doping concentration $\delta x_i$ and the d-wave order parameter $\delta \Delta_d(i)$. (a) 2D auto-correlation of $\delta x_i$. (b) Azimuthally averaged auto-correlation function of $\delta x_i$. (c) Azimuthally averaged auto-correlation function of $\delta \Delta_d(i)$. (d) The absolute value of the azimuthally averaged cross-correlation function of $\delta x_i$ and $\delta \Delta_d(i)$. The solid lines in (b), (c) and (d) are Gaussian fits to the correlation functions with the corresponding decay lengths $\xi_{d}$ shown in legends.

Comparison of the $x_i$-map in Fig. 7a and the $\Delta_d$-map in Fig. 7b shows that the order parameter gap is bigger where the doping rate is lower and vice versa, in agreement with the general trend of the doping dependence of $\Delta_d$ in a clean system. This (anti-)correlated behavior is confirmed by the cross-correlation analysis of $\delta x_i$ and $\delta \Delta_d$ in Fig. 8d, where the absolute value of the azimuthally averaged correlation function is plotted versus separation. The fact that the cross-correlation length, $\xi_{x-\Delta_d} \simeq 2.1a$, is very close to that of the auto-correlations indicates that the correlation between the spatial variations in $\Delta_d$ and $x_i$ is very strong.

![Graphs showing correlations and order parameter distributions.](image)

**FIG. 9.** (a) A scatter-plot of the d-wave order parameter $\Delta_d(i)$ and the extended s-wave order parameter $\Delta_s(i)$ versus local doping concentration $x_i$. The solid line corresponds to $\Delta_d$ as a function of $x$ obtained in the absence of the ionic dopant potential. (b) A histogram showing the statistical distribution of $\Delta_d(i)$ in this single $32 \times 32$ system. The solid line is a Gaussian fit.

We proposed, in Ref. 9, the concept of local doping concentration to emphasize the local nature of the physics associated with screening and pairing in a doped Mott insulator. To further substantiate this idea, we produce a scatter-plot of the local d-wave order parameter $\Delta_d(i)$ versus the local doping $x_i$ in Fig. 9a. For a range of doping near the average doping value of $x = 0.12$, the data points scatter around the $\Delta_d$ v.s. $x$ curve (solid line) obtained in the homogeneous case without the ionic dopant potential. In the regions where the local doping is low, the scatter in $\Delta_d$ is small and the correlation between $\Delta_d(i)$ and $x_i$ is extremely strong. On the other hand, the $\Delta_d(i)$ values show significant scatter in the locally overdoped regimes and deviate appreciably from the values in a clean system at the corresponding doping level. Also shown in Fig. 9a is the scatter plot of the much...
smaller, extended s-wave order parameter $\Delta_s(i)$ versus $x_i$. It scatters around a zero mean and shows a slightly larger variance with decreasing LDC. The statistical distribution of $\Delta_d$ in this single 32 × 32 system is plotted as histograms in Figs. 9b. It can be fitted reasonably well by a Gaussian distribution.

B. Local tunneling density of states as measured by STM spectroscopy

To enable further comparisons with the STM experiments, we next calculate the local tunneling density of states $N_i(\omega)$ according to Eq. (21). The $\delta$ functions in Eq. (21) are replaced by the derivatives of the corresponding Fermi distribution function [32] at an inverse temperature of $\beta J = 30$. Parallel to our presentation of the experimental data [9], we extract the local pairing energy gap (full gap), denoted by $\Delta_T(i)$ to differentiate from the $d$-wave OP $\Delta_d(i)$ discussed above, from the peak-to-peak distance in the electron LDOS spectrum $N_i(\omega)$ at every site $i$. Simultaneously, we obtain the integrated LDOS (ILDOS) at every site $i$ from

$$I_i = \int_{-\omega_0}^{0} d\omega N_i(\omega),$$

where the integration limit is typically taken to be $-\omega_0 = -J$. Note that $N_i(\omega)$ at $\omega < 0$ corresponds to the LDOS of the occupied states below the chemical potential. It should be compared to the STM tunneling spectrum at negative sample bias where electrons tunnel out of the occupied states in the sample. The energy $\omega$ is related to the bias $V$ according to $\omega = eV$.

The spatial variations of $\Delta_T(i)$ and $I_i$ are shown as the gap and the ILDOS maps in Figs. 10a and 10b respectively. As used in Ref. [9], the reverse color coding in the gap map (brighter color for a smaller tunneling gap) makes it easy to observe its (anti-)correlation with the ILDOS map, namely, bigger gap regions correspond to smaller ILDOS and vice versa, in agreement with the STM data. In Fig. 11a, we construct a scatter plot of the superconducting gap versus the ILDOS consisting of a total of $32 \times 32 = 1024$ data points, which suggests an approximate linear relationship between the two quantities, in remarkable agreement with the STM data we presented in Fig. 4 of Ref. [9].

It is easy to notice the great similarity between the ILDOS map in Fig. 10b and the 2D hole density map shown in Fig. 7a. This supports within our model the conjecture made in Ref. [8] that the ILDOS as measured by STM should be approximately proportional to the LDC.

To examine this relationship in more detail, we show a scatter-plot of the ILDOS $I_i$, obtained from Eq. (27), versus the local doping level $x_i$ in Fig. 11b. Remarkably, the ILDOS is indeed linearly proportional to the LDC when $x_i$ is small, i.e. when the local region is underdoped. This is consistent with the Mott-Hubbard picture in which doping a Mott insulator introduces spectral weight near the Fermi energy necessary to transform the insulator into a superconductor. As observed in recent ARPES experiments, the integrated quasiparticle weight scales with the average doping concentration in the underdoped regime. The idea of LDC that we advocate extends this Mott-Hubbard picture, commonly used to interpret macroscopic spectroscopy properties, to microscopic scales. It remains valid in describing the local spectroscopies of the short-coherence length superconducting state of the doped Mott-insulator. However, for larger hole concentration, i.e. further away from the
Mott insulator, the ILDOS in Fig. 11b tends to taper off and saturate. It shows that the two quantities are more intricately connected than the overall proportionality stemming from the quasiparticle wave-function renormalization which is apparent in Eq. (21). This result turns out to be important for the analysis of the low energy inhomogeneity structures in the following section.

![Graph](image)

**FIG. 11.** (a) A scatter-plot of the superconducting gap \( \Delta_T(i) \) in the tunneling spectrum versus the ILDOS. (b) A scatter-plot of the ILDOS versus the LDC \( x_i \).

The statistical properties of the tunneling gap \( \Delta_T \) and the ILDOS \( I_i \) are in general quite similar to those of the d-wave pairing order parameter \( \Delta_d \) and the local hole concentration \( x_i \). The histogram of \( \Delta_T \) in the 32 \( \times \) 32 system is plotted in Fig. 12a, which shows an approximate Gaussian distribution. The azimuthally averaged auto-correlation of the spatial gap variation \( \delta\Delta_T(i) \) is shown in Fig. 12b, and that of the cross-correlation of the gap variation and the ILDOS variation,

\[
C_{T-\Delta_T}(r_j) = \frac{1}{N_x} \sum_i \langle \delta\Delta_T(i) \delta I_{i+r_j} \rangle,
\]

(28)

is shown in Fig. 12c in the absolute value. The extracted gap correlation length \( \xi_{\Delta_T} \approx 2.9a \) is somewhat larger than that of d-wave order parameter \( \xi_{\Delta_d} \). Although the values of the decay lengths depend on the value of the setback distance \( d_s \) of the dopant oxygen ions, we find for \( d_s = 1.5a \), and \( a = 3.8 \text{Å} \), \( \xi_{\Delta_T} \approx 11 \text{Å} \) which is close to the corresponding value of 14Å obtained by analyzing the experimental data. The similar cross-correlation length is consistent with the observation that these two quantities are strongly (anti-)correlated.

![Graph](image)

**FIG. 12.** Statistical properties of the tunneling gap \( \Delta_T \). (a) A histogram of \( \Delta_T \) in the 32 \( \times \) 32 system at \( x = 0.12 \), showing approximate Gaussian distribution (solid line). (b) The azimuthally averaged auto-correlation function of the tunneling gap variations. (c) The absolute value of the azimuthally averaged cross-correlation function between the variations in \( \Delta_T \) and the ILDOS. The solid lines are Gaussian fits.

Next we turn to the details of the spatial variations of the local tunneling spectrum and make comparisons to experiments. Fig. 13a shows a three-dimensional rendering of the tunneling spectra along a horizontal line-cut marked in Fig. 10(a), exemplifying the detailed variations of the LDOS, the pairing energy gap, and the correlation between them.
The projection of Fig. 13a onto the 2D plane is shown in Fig. 13b. It is clear that regions with higher ILDOS also exhibit smaller pairing gaps and higher coherence peaks. The black dotted lines trace the positions of the coherence peaks. Combined with the gap-map in Fig. 10a, one can see that the gap varies somewhat less rapidly near the center of a “patch” than at its “edges”. We expect this feature to become more prevalent for smaller average doping concentrations, i.e. more underdoped samples. In Fig. 13c, we show five characteristic tunneling spectra calculated at the five positions marked in Fig. 10a. The LDC at these points are given in the captions. Notice that the spectral lines plotted versus the bias voltage show remarkable resemblance to the experimental data shown in Fig. 3 of Ref. [9]. The most striking feature is that the spatial inhomogeneity exists all the way down to low energies as can be clearly seen from the the systematic scatter in the zero-bias tunneling conductance. [4] The broad range of agreements between the results presented in Figs. 11, 12 and 13, and the experimental findings including such details add to our confidence that the present theory of the inhomogeneous d-wave superconducting state with spinon pairing and local holon condensation captures the essential physics of the superconducting state in BSCCO.

V. ZERO-BIAS TUNNELING DENSITY OF STATES

One of the most striking results of both the STM measurements (see Fig. 3 of Ref. [8]) and the present theory (see Fig. 13) is that the spatially inhomogeneous electronic structure not only appears at the energy scale of the superconducting gap, but persists all the way down to low energies, including the zero-bias tunneling conductance. On the experimental side, the low energy inhomogeneity can only be observed clearly when the tunneling matrix element effect along the \( c \)-axis is removed by a normalization procedure introduced in Ref. [8]. Let’s take a brief detour and study this matrix element effect. The tunneling current at site \( \mathbf{r}_i \) is given by

\[
I_E(\mathbf{r}_i, V) = \int d\omega f(\omega)[1 - f(\omega + eV)] \times N_i(\omega)\rho(\omega + eV)|M(\mathbf{r}_i, z)|^2,
\]

where \( \rho(\omega) \) is the density of states of the STM tip which is usually taken to be a constant, and \( M(\mathbf{r}_i, z) \) is the tunneling matrix element. Our knowledge of \( M \) is scarce in complicated materials, but in general one should be able to factor out its dependence on \( z \) which corresponds to the tip distance to the tunneling surface,

\[
M(\mathbf{r}_i, z) = \text{const.} \times m(\mathbf{r}_i)e^{-\alpha \delta z(\mathbf{r}_i)}.
\]

Here \( \delta z(\mathbf{r}_i) \) is the spatial variation of the tip-to-surface distance in the constant-current scanning mode, and \( \alpha \)
is a constant determined by the work-function. The detailed behavior of $m(r_i)$ is presently unknown and can at best be assumed to have no or very weak spatial dependence. However, the spatial variation in the tip distance $\delta z(r_i)$ is known in the form of the surface topography from experiments. The normalization procedure we used in Ref. 3 is precisely to remove this part of the matrix element effect such that the resulting data represent tunneling measurements carried out with the tip-to-surface distance effectively held constant. While it has been common practice to present STM data without such a normalization, in which case the low energy inhomogeneity of the tunneling conductance is not clearly revealed, we believe that the constant tip distance normalization is physical and should be carried out in order to obtain the true electronic contribution to the tunneling spectra. Our theoretical calculations in the inhomogeneous d-wave superconducting state based on local spinon pairing and local holon condensation indeed support the experimental observation 3 that the low energy STM tunneling spectra is spatially inhomogeneous. We next provide a careful analysis of the theoretical data at zero-bias and make a few predictions that can be tested and used to guide further experiments.

Fig. 14a shows a 2D map of the zero-bias LDOS at every point on our $32 \times 32$ lattice. The spatial variations are obvious, but what is striking is that this is the same pattern of inhomogeneity that we saw at the energy scale of the superconducting gap as shown in the gap map in Fig. 10a, in complete agreement with experiments. 30 Moreover, comparing Fig. 14a to the local hole density map in Fig. 7a shows that they are directly correlated. This strongly suggests that the same kind of inhomogeneity pattern should be observable at all energy scales in the STM tunneling spectroscopy. To further illustrate the correlation between them, we construct a scatter-plot of the zero-bias LDOS $N_i(0)$ versus the LDC $x_i$ in Fig. 14b. It suggests a strong correlation via a linear relationship between the two quantities in the regions of low doping. The scatter increases gradually with increasing LDC and the linear relationship tappers off and saturates. This is quite similar to the behavior of the ILDOS and points to the more intricate $x_i$-dependence of the LDOS in Eq. (21) beyond the overall linear proportionality.

Since the local doping concentration is not directly accessible experimentally, in Fig. 14c we present the scatter plot of the zero-bias LDOS versus the ILDOS. Interestingly, due to the weaker variation of the ILDOS in regions of higher hole concentration (see Fig. 14b), the scatter of the zero-bias LDOS exhibits a slight upward curvature with increasing ILDOS. Such a scatter plot can be directly constructed from the STM experimental data for comparison, 30 which serves as another test for the present theory. Two remarks are in order.

(i) It is important to emphasize the difference between the electron tunneling DOS that spectroscopy measurements probe and the thermodynamic DOS or the compressibility that shows up in thermodynamic measurements such as the specific heat. While the former depends on both the quasiparticle wave-function renormalization $Z$ and the self-energy corrections, the latter is insensitive to $Z$. 21 Although the inhomogeneity in the tunneling spectra at low energies emerges from the spatial variations in the LDC $x_i$ through both the wave-function renormalization and the spinon tunneling spectra as described by Eq. (21), its implications on the thermodynamic DOS and the transport properties require a different analysis. We stress that the difference between these two density of states even at our unrestricted mean-field level is more than the local doping concentration $x_i$, the prefactor in the electron tunneling LDOS, due to the presence of the spinon wave-functions in Eq. (21).

![FIG. 14. Spatial inhomogeneity at zero bias. (a) A 2D map of the zero bias LDOS, $N_i(0)$, showing the same pattern of inhomogeneity as the tunneling gap map and the ILDOS map in Fig. 10. (b) A scatter-plot of $N_i(0)$ versus the LDC $x_i$. (c) A scatter-plot of $N_i(0)$ versus the ILDOS.](image-url)
(ii) Although the spinon tunneling DOS is not directly accessible by STM measurements, since only the physical electrons can tunnel in and out of the sample, it can be, nevertheless, readily extracted from Eq. (21). Dividing out the prefactor $x_i$, we show in Fig. 15a the spinon tunneling spectra, $N_i^f(\omega) = N_i(\omega)/x_i$, at the five locations marked in Fig. 10a. Comparing to the corresponding spectral lines for electron LDOS at the same locations shown in Fig. 13c, it is clear that the degree of inhomogeneity remains large at the energy scale of the superconducting gap. This is not surprising because the gap inhomogeneity results from local spinon pairing in our picture. However, the degree of inhomogeneity appears to have been somewhat reduced at low energies near zero-bias, suggesting that the spinons near the gap nodes, unlike the (electron) nodal quasiparticles, experience less inhomogeneity. The scatter plot of the spinon zero-bias LDOS versus local hole concentration is shown Fig. 15b. Although the relative magnitude of the variations is reduced by about 30% from the electron case in Fig. 14a, the spatial variation of the zero-bias conductance for spinons is not only clearly visible, but shows a very well defined correlation with the local hole concentration at the zero-bias, suggesting that the spinons near the gap nodes will experience the same type of inhomogeneity as the spinons at the gap edge.

![Graph](image)

Fig. 15. The tunneling LDOS for spinons. (a) The spinon tunneling spectra at the five positions marked in Fig. 10a, in comparison to those of the electron tunneling spectra shown in Fig. 13c where the LDC $x_i$, $i = 1, \ldots, 5$ were given. (b) A scatter-plot of the spinon zero-bias LDOS versus the LDC $x_i$, showing remarkable similarity to that of $\Delta_d(t)$ versus $x_i$ presented in Fig. 9a.

VI. STM TOPOGRAPHY AND THE TUNNELING SPECTRA AT CONSTANT CURRENT

We next derive from our numerical data, a theoretical STM topographic image at constant tunneling current for the $32 \times 32$ system we study. We then use the result to reconstruct the local tunneling spectra at constant current, which corresponds to the original STM data before normalization. In doing so, we will further illustrate the physics behind the normalization procedure used in Ref. 13, which is essentially a mapping from a constant current topography to the electron LDOS measured at constant tunneling barrier width.

The STM measurements are usually carried out at a constant tunneling current $I_0$ which is equivalent to the integrated LDOS from the sample bias voltage $-V_0$ to the Fermi level. Thus we can write,

$$I_0 = \int_{-V_0}^{0} dV \frac{dI}{dV}(r, V, z(r)),$$

(31)

where $\frac{dI}{dV}(r, V, z(r))$ is the LDOS or the tunneling differential conductance. It is a function of the 2D coordinates $r$ on the tunneling surface, the sample bias $V$, and the tip to surface distance $z(r)$ (topography) that must vary at every $r$ in order to keep the current $I_0$ a constant. Note that $\frac{dI}{dV}$ in Eq. (31) corresponds precisely to the original STM data before normalization. From our discussion following Eq. (24), it is clear that $\frac{dI}{dV}$ is related to the physical electronic tunneling spectra $N(r, eV)$ obtained at constant $z(r)$ according to,

$$N(r, eV) = \frac{dI}{dV}(r, V, z(r))e^{\alpha z(r)}.$$

(32)

Integrating Eq. (32) over $V$ from $-V_0$ to 0 gives, after using Eq. (31),

$$I(r) = I_0 e^{\alpha z(r)},$$

(33)

where $I(r)$ is the electronic ILDOS given by Eq. (27) in terms of the normalized or the calculated tunneling spectra. Eq. (34), together with Eq. (32), completely describes the mapping between the constant current topography and the local electron tunneling spectra at constant tunneling barrier width.

From our calculated LDOS map and using Eq. (33), we obtain the constant current STM topographic image $z(r)$ on our $32 \times 32$ lattice using $\alpha = 2.3 \AA^{-1}$ which corresponds to a work-function of about 4eV. The topography is presented in Fig. 16a, which exhibits identical structures as the electron LDOS map shown in Fig. 10b. We next covert the entire local tunneling spectra $N(r, V)$ at constant tip-sample distance to the tunneling differential conductance at constant current using Eq. (32) and the topography map. The procedure turns out to be equivalent to normalizing the LDOS spectra by the corresponding ILDOS.
FIG. 16. Calculated STM spectroscopy of the $32 \times 32$ lattice in the constant current mode. (a) The topographic image of our system, showing the same inhomogeneity structures as the electron ILDOS map plotted in Fig. 10b. (b) The characteristic tunneling differential conductance spectra at the same five positions marked in Fig. 10a. The integrated area under the spectral lines on the negative bias side is the same, i.e. the constant tunneling current. Note that the inhomogeneous distribution of tunneling differential conductance near zero bias is hardly visible. (c) A scatter-plot of the zero-bias conductance versus the LDC.

In Fig. 16b, we show five differential conductance curves at the same five positions marked in Fig. 10a. Notice that, typical of the raw STM data, the spectral lines on the negative bias side cross approximately at one value of the voltage as a result of the constraint that the integrated area under each curve, i.e. the tunneling current, must be the same. The spatial inhomogeneity on the energy scale of the superconducting gap remains, albeit that the peak height does not show the same systematics — smaller gap with higher coherence peak — as in the experimental data with or without normalization. This discrepancy may be due to the simplification of the mean-field theory which ignores the effects of fluctuations, and perhaps also, to a certain extent, due to the complication of the matrix element effects in the STM tunneling data. The spatial variations of the tunneling differential conductance spectra at low energies are, however, much less visible. The scatter-plot of the zero-bias conductance versus local doping concentration is shown in Fig. 16c. Comparing to the same plot for the electron zero-bias LDOS shown in Fig. 14b, we find that the relative magnitude of the variations in the zero-bias conductance is suppressed by about 65% and it shows almost no systematic dependence on the LDC. These findings are in good qualitative agreement with the experimental observation that the original STM data before normalization show much less spatial inhomogeneity at low energies.

VII. SUMMARY AND DISCUSSIONS

We have investigated in this paper, through microscopic calculations based on a generalized $t$-$J$ model, the effects of the off-plane ionic potential associated with off-stoichiometry doping in the $d$-wave superconducting state of a doped Mott insulator. We find that nonlinear screening dominates the response of the doped Mott insulator to the ionic potential. One of the main characteristics of nonlinear screening is the emergence of a percolative-type of inhomogeneity in the electronic structure. In 2D electron systems formed in modulation doped semiconductors, nonlinear screening of the ionic dopant potential at low electron densities can tear the 2D electrons into an inhomogeneous mixture of metallic and dielectric regions. What we have shown here is a striking analogy of the physics in a doped Mott insulator: nonlinear screening of the dopant ionic potential leads to an inhomogeneous $d$-wave superconducting state wherein the LDC and the $d$-wave superconducting gap exhibit significant spatially correlated variations on the scale of a nanometer comparable to the short coherence length. In this context, the concept of a local doping concentration augmented by the generalization of the Mott-Hubbard picture to local spectroscopies that we advocate is very useful. We have shown that, within our self-consistent, spatially unrestricted mean-field approach, local spinon pairing and local holon condensation capture the essential physics of the inhomogeneous superconducting state and provide remarkably consistent descriptions of the experimental data.

We have shown that there is one length scale controlled by the ionic setback distance $d_s$ that characterizes the inhomogeneity. The decay lengths of the auto-correlations of the spatial variations in the LDC and the $d$-wave pair-
ing order parameter are found to be close to \( d_s \), suggesting that the superconducting pair-size is determined by \( d_s \). In this paper, we have chosen \( d_s = 1.5a \) based on the physical distance of \( \sim 5 \text{Å} \) between the CuO\(_2\) plane and the BiO layer where the dopant oxygen ions reside and \( a \simeq 3.8 \text{Å} \) for the Cu-Cu atomic spacing. However, it is important to emphasize the effects of anisotropy in the background dielectric screening constant which enters the ionic potential. It was pointed out to us by Kivelson that, for the high-\( T_c \) cuprates, the background dielectric constant, determined by the electronic interband polarization and phonon contributions, is highly anisotropic, i.e., it has a different value along the \( c \)-direction, \( \epsilon_{\perp} \), than in the \( ab \)-plane \( \epsilon_{\parallel} \). If this anisotropy is taken into account, the ionic potential given in Eq. (3) must be modified by replacing \( V_d \rightarrow V_{d_s} \) and \( d \rightarrow d_s^* \) with \( d_s^* = \sqrt{\epsilon_{\parallel}/\epsilon_{\perp}} d_s \). Thus the effective distance between the BiO layer and the CuO\(_2\) plane can be significantly larger than 5Å. Taking \( \epsilon_{\perp} \simeq 8.0 \) and \( \epsilon_{\parallel} \simeq 1.5 \), it follows that the effective setback distance \( d_s^* \simeq 3.5a \simeq 13 \text{Å} \). Our results then imply that the pair-size, determined by the decay length in the spatial variation of the d-wave order parameter, would be on the order of one to two nanometers, in good agreement with our experimental findings.

The physics discussed here can be continued to more underdoped cases where the percolative structures resulting from nonlinear screening are expected to be more pronounced. Already in the case of 12\% average doping studied here, the tunneling spectra along particular line-cuts in Fig. 10a show patches over which the superconducting gap is nearly flat in the center and changes quickly near the edges, indicative of a percolative electronic structure which is often referred to as microscopic phase separation. As we have shown that the size of the screening cloud around an isolated ion is determined by its effective setback distance \( d_s^* \), it is likely that, with increasing doping, a percolation transition/crossover takes place near optimal doping where the average inter-hole distance becomes comparable to an effective setback distance \( d_s^* \).

We have not discussed the very underdoped physics in detail because in that case it will become important to include the effects associated with magnetism that is not important and has thus been left out in the average doping range considered in this paper. We have tested that if magnetism is included, locally antiferromagnetic ordered insulating regions emerge and percolate at sufficiently low averaged doping. This is left for further studies. Nevertheless, the present theory implies that in underdoped BSCCO, the local tunneling spectra should reveal a percolative structure of superconducting patches embedded in a background where larger tunneling gaps to single-particle excitations arise.

A frequently asked question is how does the high transition temperature coexist with the inhomogeneity. While we do not have a complete answer, we would like to discuss a few relevant issues related to this question.

One of the most obvious reasons for high-\( T_c \) superconductivity to survive the inhomogeneity is its short coherence length. In our theory, the latter, determined by the effective setback distance \( d_s^* \), is also the scale of the inhomogeneity and will therefore remain shorter than the mean-free path which is usually much larger than the correlation length of the screening centers for a reasonable scattering strength. Moreover, as we have pointed out in Ref. [8], the scattering by the out-of-plane ionic potential involves predominantly small momentum transfers limited by the small scattering angle on the order of \( 1/d_s^* k_F \), where \( k_F \) is the Fermi momentum. This type of scattering is much less effective at reducing \( T_c \) than at increasing the single-particle scattering rate.

![FIG. 17. The temperature dependence of the averaged d-wave order parameter (open squares) on a 16 × 16 lattice at an average doping \( x = 0.15 \). Also shown in open circles is the temperature dependence of the d-wave order parameter in the uniform d-wave state without the ionic potential.](image_url)
tain degree of dopant ordering. To this end, we studied a case where the dopant ions are periodically ordered and the average doping \( x = 0.14 \). We found that the LDC and the \( d \)-wave order parameter show spatial variations that are periodic with the same periodicity as that of the dopant ions. The widths of the distribution functions are significantly reduced when compared to the disordered case. We therefore expect that, although the spatial inhomogeneity would remain after thermal annealing, the spatial variations would be more periodic in structure with a noticeably smaller magnitude.

Based on these results, we expect that the microscopic variations in the electronic properties of YBCO, particularly in its ortho-phase, \([3]\) should be more periodic in space because the oxygen dopants can be ordered in the copper-oxygen chains. However, there exists an important difference in the role of the dopant ions. In BSCCO, the BiO plane is essentially insulating which allows us to treat the dopants as solely providing the dielectrically screened ionic potential. The situation can be very different in YBCO because the chains themselves are conducting and have low energy dynamics of their own. The electrons in the chains will scatter off the dopant ions giving rise to charge density oscillations along the chains that may complicate the way by which carriers are doped into the \( \text{Cu}O_2 \) plane. The present theory would predict the appearance of inhomogeneous electronic structures in the \( \text{Cu}O_2 \) planes of YBCO that are most pronounced directly under/above the doped chains. This type of spatial inhomogeneity on YBCO may have been recently observed. \([3]\)

We have investigated here one of the most direct consequences of off-stoichiometry doping of a Mott insulator, namely the ionic potential. There are potentially others. For example, the presence of dopants can affect the transverse inhomogeneity on YBCO may have been recently observed. \([3]\)

VIII. ACKNOWLEDGMENTS

The authors thank Sasha Balatsky, Seamus Davis, Misha Fogler, Jung-Hoon Han, Hae-Young Kee, Steve Kivelson, Dung-Hai Lee, Patrick Lee, Alex de Lozanne, and Allan MacDonald for useful discussions and comments. They are especially grateful to Steve Kivelson, Dung-Hai Lee, and Patrick Lee for sharing their insights and to Jung-Hoon Han for his involvement and contributions during the early stage of this work. They thank Jared O’Neal and Robert Badzey for their help with data analysis. Z.W. would like to thank Patrick Lee for hosting his sabbatical leave at MIT where a part of this work was completed. This work is supported in part by DOE Grant No. DE-FG02-99ER45747, NSF Grant No. DMR-0072205, and by the Sloan Foundation and Research Corporation. The authors also thank the Institute for Theoretical Physics at UCSB where this work was begun during the workshop on High Temperature Superconductivity and acknowledge the generous support of NSF Grant No. PHY94-07194.

[1] P. W. Anderson, Science, 235, 1196 (1987).
[2] R. X. Lian, D. A. Bonn, and W. H. Hardy, Physica C336, 56 (2000).
[3] H. F. Fong, et al. Nature 398, 588 (1999).
[4] H. Hasegawa, et al. in Physical Properties of High Temperature Superconductors III, edited by D. M. Ginsberg, (world Scientific, 1992).
[5] E. L. Wolf, et al. Journal of Superconductivity, 70, 355 (1994).
[6] V. J. Emery and S. A. Kivelson, Physica C209, 597 (1993); S. A. Kivelson and V. J. Emery, in Strongly Correlated Electronic Materials, edited by K. S. Bedell, et al. (Addison-Wesley, 1994).
[7] Y. Zhang, et. al. Phys. Rev. Lett. 86, 890 (2001). Recent measurements on BSCCO by the same group show a 400Å mean-free-path.
[8] T. Valla, et al. Science 285, 2110 (1999); A. Kaminski, et al. Phys. Rev. Lett. 84, 1788 (2000); P. V. Bogdanov, et al. Phys. Rev. Lett. 85, 2581 (2000).
[9] S. H. Pan, et al. Nature, 413, 282 (2001).
[10] C. Howald, P. Fournier, and A. Kapitulnik, Phys. Rev. B64, 100504, (2001).
[11] K. Lang, et al. Bull. Amer. Phys. Soc. 46, 804 (2001).
[12] Ch. Renner, et al. Phys. Rev. Lett. 80, 149 (1998); N. Miyakawa, et al. Phys. Rev. Lett.83, 1018 (1999).
[13] H. Ding, et al. Phys. Rev. Lett. 87, 227001 (2001).
[14] A. L. Efros, Solid State Commun. 65, 1281 (1988); A. L. Efros, F. G. Pikus, and V. G. Burnett, Phys. Rev. B47, 2233 (1993); B. I. Shklovskii and A. L. Efros, Electronic Properties of Doped Semiconductors, (Springer-Verlag, 1984).
[15] M. S. Hybertsen, et al. Phys. Rev. B45, 10032 (1992).
[16] J. H. Han, Q.-H. Wang, and D.-H. Lee, cond-mat/0006046, (2000).
[17] We find that in the presence of the dopant ionic potential, the tendency towards phase separation is suppressed even without the long-range Coulomb interaction in the doping range of interest here.
[18] G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. 63, 973 (1987); G. Kotliar and J. Liu, Phys. Rev. B38, 5142 (1988).
[19] M. U. Ubbens and P. A. Lee, Phys. Rev. B46, 8434 (1992).
[20] Z. Wang, Y. Bang, and G. Kotliar, Phys. Rev. Lett. 67, 2733 (1991); Z. Wang, Int. J. Mod. Phys. B 36, 603 (1992).
[21] E. Abrahams, P. W. Anderson, P. A. Lee, and T. V. Ramakrishnan, Phys. Rev. B 24, 6783 (1981).
[22] D. L. Feng, et al. Science 289, 277 (2000).
[23] H. Tanaka, K. Kuboki, and M. Sigrist, Int. J. Mod. Phys. B 12, 2447 (1998).
[24] H. Tsuchiura, Y. Tanaka, M. Ogata, and S. Kashiwaya, J. Phys. Soc. Jpn. 68, 2510 (1999); H. Tsuchiura, Y. Tanaka, M. Ogata, and S. Kashiwaya, Phys. Rev. Lett. 84, 3165 (2000).
[25] J.-X. Zhu, T. K. Lee, C. S. Ting, and C.-R. Hu, Phys. Rev. B 61, 8667 (2000).
[26] T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. 54, 437 (1982).
[27] T. Deruelle, et al. Phys. Rev. B 45, 9082 (1992).
[28] A. V. Balatsky and M. I. Salkola, Phys. Rev. Lett. 76, 2386 (1996); A. V. Balatsky, M. I. Salkola, and A. Rosen- gren, Phys. Rev. B 51, 15547 (1995).
[29] M. Franz, C. Kallin, and A. J. Berlinski, Phys. Rev. B 54, R68907 (1996).
[30] A. J. Berlinski, et al. Phys. Rev. Lett. 75, 2200 (1995).
[31] D. Rokshar and S. Kivelson, Phys. Rev. Lett. 61, 2376 (1988).
[32] Y. Wang and A. H. MacDonald, Phys. Rev. B 52, R3876 (1995).
[33] A. Ino, et al. Phys. Rev. Lett. 81, 2124 (1998).
[34] We note that in Fig. 3 of Ref. [9], the two tunneling spectra taken at locations where the ILDOS is very small do not show the coherence peaks and the superconducting gaps are absent indicative of insulating behavior. The tunneling spectra in these rare insulating regimes cannot be described by our present mean-field theory which does not include the incoherent contributions that dominates the insulating behavior.
[35] Q.-H. Wang, J. H. Han, and D.-H. Lee, cond-mat/0106038 (2001).
[36] S. H. Pan, et al. to be published.
[37] S. A. Kivelson, private communications.
[38] Hae-Young Kee, Phys. Rev. B 64, 012506 (2001).
[39] A. de Lozanne, et al. to be published (2001); private communications.
[40] A. I. Larkin and Yu. N. Ovchinnikov, Sov. Phys. JETP 34, 1144 (1972); L. B. Ioffe and A. I. Larkin, Sov. Phys. JETP 54, 378 (1981).
[41] J. S. Meyer and B. D. Simons, Phys. Rev. B 64, 134516 (2001).
[42] W. A. Atkinson, P. J. Hirschfeld, and A. H. MacDonald, Phys. Rev. Lett. 85, 3922 (2000).
[43] A. Ghosal, M. Randeria, and N. Trivedi, Phys. Rev. B 65, 014501 (2002).