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High-temperature superconductivity and charge segregation in a model with strong long-range electron–phonon and Coulomb interactions

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Abstract

An analytical method of studying strong long-range electron–phonon and Coulomb interactions in complex lattices is presented. The method is applied to a perovskite layer with anisotropic coupling of holes to the vibrations of apical atoms. Depending on the relative strength of the polaronic shift E_p and the inter-site Coulomb repulsion V_c, the system is either a polaronic Fermi liquid, $V_c > 1.23E_p$, a bipolaronic superconductor, $1.16E_p < V_c < 1.23E_p$, or a charge segregated insulator, $V_c < 1.16E_p$. In the superconducting window, the carriers are mobile bipolarons with a remarkably low effective mass. The model describes the key features of the underdoped superconducting cuprates.

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There is clear experimental [1–5] and theoretical [6–15] evidence for strong electron–phonon (el–ph) interaction in high-T_c superconducting cuprates (HTSC). Electron correlations are also important in shaping the Mott–Hubbard insulating state of parent undoped compounds [16]. The theory of high-T_c cuprates must treat both interactions on equal footing as was suggested some time ago [6]. In recent years many publications addressed the fundamental problem of competing el–ph and Coulomb interactions in the framework of the Holstein–Hubbard model [11–15] where both interactions are short-range (on-site). The mass of bipolaronic carriers in this model is very large and the critical temperature is suppressed down to a Kelvin scale. However, in the cuprates the screening is poor so that the el–ph interaction necessarily has to be long-range. Motivated by this fact, we have proposed that a long-range Fröhlich, rather than short-range Holstein, interaction should be the adequate model for the cuprates [17,18]. Differently from the usual continuum Fröhlich model (for review see [6,7]), we introduced a multipolaron Fröhlich-like lattice model with electrostatic forces fully taking into account the discreteness of the lattice, finite electron bandwidth, and the quantum nature of phonons. A single small polaron with the Fröhlich interaction was discussed long time ago [19]. Analytical [17] and ex-

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act Monte-Carlo [18] studies of the simple chain and plane lattices with a long-range el–ph coupling revealed a several-order lower effective mass of this polaron than that of the small Holstein polaron. Later, the polaron and bipolaron cases of the chain model were analyzed in more detail in Refs. [20] and [21], confirming low masses of both types of carriers. Qualitatively, a long-range el–ph interaction results in a lighter mass because the extended lattice deformation changes gradually as the carrier moves through the lattice.

In this Letter, we study a realistic *multi*-polaron model of the copper–oxygen perovskite layer which is the major structural unit of the HTSC compounds. The model includes the infinite on-site repulsion (Hubbard U term), long-range inter-hole Coulomb repulsion V_c, and long-range Fröhlich interaction between in-plane holes and apical oxygens. We find that, within a certain window of V_c, the holes form inter-site bipolarons with a remarkably low mass. The bipolarons repel and the whole system is a superconductor with a high critical temperature. At large V_c, the system is a polaronic Fermi liquid and at small V_c it is a charge segregated insulator.

To deal with the model's considerable complexity we first describe a theoretical approach that makes the analysis of complex lattices simple in the strong coupling limit. The model Hamiltonian explicitly includes long-range electron–phonon and Coulomb interactions as well as kinetic and deformation energies. An implicitly present infinite Hubbard term prohibits double occupancy and removes the need to distinguish fermionic spins. Introducing fermion operators $c_{\mathbf{n}}$ and phonon operators $d_{\mathbf{m}\alpha}$, the Hamiltonian is written as

$$\begin{aligned} H = &- \sum_{\mathbf{n}\neq\mathbf{n}'} \left[T(\mathbf{n}-\mathbf{n}')c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}'} - V_c(\mathbf{n}-\mathbf{n}')c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}}c^{\dagger}_{\mathbf{n}'}c_{\mathbf{n}'} \right] \\ &- \omega \sum_{\mathbf{nm}} g_{\alpha}(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}}) \\ &\qquad \times c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}}\left(d^{\dagger}_{\mathbf{m}\alpha}+d_{\mathbf{m}\alpha}\right) \\ &+ \omega \sum_{\mathbf{m}\alpha}\left(d^{\dagger}_{\mathbf{m}\alpha}d_{\mathbf{m}\alpha}+\frac{1}{2}\right). \end{aligned} \tag{1}$$

Here $\mathbf{e}_{\mathbf{m}\alpha}$ is the polarization vector of αth vibration coordinate at site $\mathbf{m}$, $\mathbf{u}_{\mathbf{m}-\mathbf{n}} \equiv (\mathbf{m}-\mathbf{n})/|\mathbf{m}-\mathbf{n}|$ is the unit vector in the direction from electron $\mathbf{n}$ to ion $\mathbf{m}$, and $g_{\alpha}(\mathbf{m}-\mathbf{n})$ is a dimensionless el–ph coupling function. ($g_{\alpha}(\mathbf{m}-\mathbf{n})$ is proportional to a *force* acting between $\mathbf{m}$ and $\mathbf{n}$.) We assume that all the phonon modes are dispersionless with frequency ω and that the electrons do not interact with displacements of their own atoms, $g_{\alpha}(0) \equiv 0$. We also use $\hbar = 1$ throughout the Letter.

In the limit of strong el–ph interaction, it is convenient to perform the Lang–Firsov canonical transformation [22]. Introducing $S = \sum_{\mathbf{mn}\alpha} g_{\alpha}(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}})c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}}(d^{\dagger}_{\mathbf{m}\alpha}-d_{\mathbf{m}\alpha})$ one obtains a transformed Hamiltonian without an explicit el–ph term:

$$\begin{aligned} \tilde{H} &= e^{-S}He^{S} \\ &= -\sum_{\mathbf{n}\neq\mathbf{n}'} \hat{\sigma}_{\mathbf{nn}'}c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}'} + \omega\sum_{\mathbf{m}\alpha}\left(d^{\dagger}_{\mathbf{m}\alpha}d_{\mathbf{m}\alpha}+\frac{1}{2}\right) \\ &\quad + \sum_{\mathbf{n}\neq\mathbf{n}'} v(\mathbf{n}-\mathbf{n}')c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}}c^{\dagger}_{\mathbf{n}'}c_{\mathbf{n}'} - E_p\sum_{\mathbf{n}} c^{\dagger}_{\mathbf{n}}c_{\mathbf{n}}. \end{aligned} \tag{2}$$

The last term describes the energy which polarons gain due to el–ph interaction. E_p is the familiar polaron (Franck–Condon) shift,

$$E_p = \omega\sum_{\mathbf{m}\alpha} g^2_{\alpha}(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}})^2, \tag{3}$$

which we assume to be independent of $\mathbf{n}$. E_p is a natural measure of the strength of the el–ph interaction. The third term in Eq. (2) is the polaron–polaron interaction:

$$v(\mathbf{n}-\mathbf{n}') = V_c(\mathbf{n}-\mathbf{n}') - V_{\mathrm{pa}}(\mathbf{n}-\mathbf{n}'), \tag{4}$$

$$\begin{aligned} V_{\mathrm{pa}}(\mathbf{n}-\mathbf{n}') = 2\omega\sum_{\mathbf{m}\alpha} &g_{\alpha}(\mathbf{m}-\mathbf{n})g_{\alpha}(\mathbf{m}-\mathbf{n}') \\ &\times (\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}'}), \end{aligned} \tag{5}$$

where V_{pa} is the inter-polaron *attraction* due to joint interaction with the same vibrating atoms. Finally, the first term in Eq. (2) contains the transformed hopping operator $\hat{\sigma}_{\mathbf{nn}'}$:

$$\begin{aligned} \hat{\sigma}_{\mathbf{nn}'} = T(\mathbf{n}-\mathbf{n}')\exp\Bigg[&\sum_{\mathbf{m}\alpha}\big[g_{\alpha}(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}}) \\ &- g_{\alpha}(\mathbf{m}-\mathbf{n}')(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}'})\big] \\ &\times \left(d^{\dagger}_{\mathbf{m}\alpha}-d_{\mathbf{m}\alpha}\right)\Bigg]. \end{aligned} \tag{6}$$

At large $E_p/T(\mathbf{n}-\mathbf{n}')$ this term is a perturbation. In the first order of the strong coupling perturbation theory [6], $\hat{\sigma}_{\mathbf{nn}'}$ should be averaged over phonons

because there is no coupling between polarons and phonons in the unperturbed Hamiltonian (the last three terms in Eq. (2)). For temperatures lower than ω, the result is

$$t(\mathbf{n}-\mathbf{n}') \equiv \langle \hat{\sigma}_{\mathbf{n}\mathbf{n}'} \rangle_{\rm ph} = T(\mathbf{n}-\mathbf{n}') \exp\bigl[-G^2(\mathbf{n}-\mathbf{n}')\bigr], \tag{7}$$

$$G^2(\mathbf{n}-\mathbf{n}') = \sum_{\mathbf{m}\alpha} g_\alpha(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}}) \times \bigl[g_\alpha(\mathbf{m}-\mathbf{n})(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}}) - g_\alpha(\mathbf{m}-\mathbf{n}')(\mathbf{e}_{\mathbf{m}\alpha}\cdot\mathbf{u}_{\mathbf{m}-\mathbf{n}'})\bigr]. \tag{8}$$

By comparing Eqs. (3), (5), and (8), the mass renormalization exponents can be expressed via E_p and $V_{\rm pa}$ as follows:

$$G^2(\mathbf{n}-\mathbf{n}') = \frac{1}{\omega}\left(E_p - \frac{1}{2}V_{\rm pa}(\mathbf{n}-\mathbf{n}')\right). \tag{9}$$

This is the simplest way to calculate G^2 and (bi)polaron masses once the 'static' parameters E_p and $V_{\rm pa}$ are known.

It is easy to see from the above equations that the long-range el–ph interaction increases E_p and $V_{\rm pa}$ but *reduces* G^2 (when measured in natural units of E_p/ω). Thus polarons get tighter and at the same time lighter. Bipolarons form when $V_{\rm pa}$ exceeds V_c and they are relatively light too. We note that the Holstein model is the limiting case with the highest possible $G^2 = E_p/\omega$. In this respect, the Holstein model is *not* a typical el–ph model.

To obtain analytical description of the *multi*-polaron system we restrict our consideration to the strong coupling case $|v| \geqslant t$. In this regime the polaron kinetic energy is the smallest energy and thus can be treated as a perturbation. The system is adequately described by a purely polaronic model:

$$H_p = H_0 + H_{\rm pert}, \tag{10}$$

$$H_0 = -E_p \sum_{\mathbf{n}} c^\dagger_{\mathbf{n}} c_{\mathbf{n}} + \sum_{\mathbf{n}\neq\mathbf{n}'} v(\mathbf{n}-\mathbf{n}') c^\dagger_{\mathbf{n}} c_{\mathbf{n}} c^\dagger_{\mathbf{n}'} c_{\mathbf{n}'}, \tag{11}$$

$$H_{\rm pert} = -\sum_{\mathbf{n}\neq\mathbf{n}'} t(\mathbf{n}-\mathbf{n}') c^\dagger_{\mathbf{n}} c_{\mathbf{n}'}. \tag{12}$$

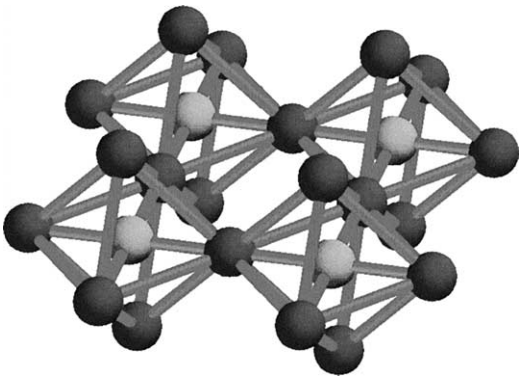

Fig. 1. Four octahedra of the copper–oxygen perovskite layer. Holes reside on the in-plane oxygens but interact with apical oxygens.

The many-particle ground state of H_0 depends on the sign of the polaron–polaron interaction, the carrier density, and the lattice geometry. Here we consider a two-dimensional lattice of ideal octahedra that can be regarded as a simplified model of the copper–oxygen perovskite layer, see Fig. 1. The lattice period is $a = 1$ and the distance between the apical sites and the central plane is $h = a/2 = 0.5$. The hole degrees of freedom in the cuprates are the oxygen p-states. We assume that all in-plane atoms, both copper and oxygen, are static but apical oxygens are independent three-dimensional isotropic harmonic oscillators. Thus there are six lattice degrees of freedom per cell. Because of poor screening the hole–apical interaction is purely Coulombic,

$$g_\alpha(\mathbf{m}-\mathbf{n}) = \kappa_\alpha/|\mathbf{m}-\mathbf{n}|^2, \quad \alpha = x, y, z.$$

To account for the experimental fact that the holes couple stronger to z-polarized phonons than to the others [3], we choose $\kappa_x = \kappa_y = \kappa_z/\sqrt{2}$. The direct hole–hole repulsion is

$$V_c(\mathbf{n}-\mathbf{n}') = \frac{V_c/\sqrt{2}}{|\mathbf{n}-\mathbf{n}'|}$$

so that the repulsion between two holes in the NN configuration is V_c. We also include the bare nearest neighbor (NN) hopping $T_{\rm NN}$, the next nearest neighbor (NNN) hopping across copper $T_{\rm NNN}$, and the NNN hopping between octahedra $T'_{\rm NNN}$.

According to Eq. (3), the polaron shift is given by the lattice sum (after summation over polarizations):

$$E_p = 2\kappa_x^2\omega \sum_{\mathbf{m}} \left(\frac{1}{|\mathbf{m}-\mathbf{n}|^4} + \frac{h^2}{|\mathbf{m}-\mathbf{n}|^6} \right) = 31.15\kappa_x^2\omega, \tag{13}$$

where the factor 2 accounts for the two layers of apical sites. (For reference, Cartesian coordinates are $\mathbf{n} = (n_x + 1/2, n_y + 1/2, 0)$, $\mathbf{m} = (m_x, m_y, h)$, n_x, n_y, m_x, m_y being integers.) The polaron–polaron attraction is

$$V_{\rm pa}(\mathbf{n}-\mathbf{n}') = 4\omega\kappa_x^2 \sum_{\mathbf{m}} \frac{h^2 + (\mathbf{m}-\mathbf{n}')\cdot(\mathbf{m}-\mathbf{n})}{|\mathbf{m}-\mathbf{n}'|^3|\mathbf{m}-\mathbf{n}|^3}. \tag{14}$$

Performing lattice summations for the NN, NNN, and NNN′ configurations one finds $V_{\rm pa} = 1.23E_p$, $0.80E_p$, and $0.82E_p$, respectively. Substituting these results in Eqs. (4) and (9) we obtain the full inter-polaron interaction: $v_{\rm NN} = V_c - 1.23E_p$, $v_{\rm NNN} = V_c/\sqrt{2} - 0.80E_p$, $v'_{\rm NNN} = V_c/\sqrt{2} - 0.82E_p$, and the mass renormalization exponents: $G^2_{\rm NN} = 0.38(E_p/\omega)$, $G^2_{\rm NNN} = 0.60(E_p/\omega)$, $G'^2_{\rm NNN} = 0.59(E_p/\omega)$.

Let us now discuss different regimes of the model. At $V_c > 1.23E_p$, no bipolarons are formed and the systems is a polaronic Fermi liquid. The polarons tunnel in the *square* lattice with NN hopping $t = T_{\rm NN}\exp(-0.38E_p/\omega)$ and NNN hopping $t' = T_{\rm NNN} \times \exp(-0.60E_p/\omega)$. (Since $G^2_{\rm NNN} \approx G'^2_{\rm NNN}$ one can neglect the difference between NNN hoppings within and between the octahedra.) The single-polaron spectrum is therefore

$$E_1(\mathbf{k}) = -E_p - 2t'[\cos k_x + \cos k_y] \pm 4t\cos(k_x/2)\cos(k_y/2). \tag{15}$$

The polaron mass is $m^* = 1/(t+2t')$. Since in general $t > t'$, the mass is mostly determined by the NN hopping amplitude t.

While the infinite Hubbard U prevents the simplest on-site bipolaron the coupling to apical oxygens allows an inter-site NN bipolaron if $V_c < 1.23E_p$. The inter-site bipolarons tunnel in the plane via four resonating (degenerate) configurations A, B, C, and D, see Fig. 2. In the first order in $H_{\rm pert}$, one should retain only these lowest energy configurations and discard all the processes that involve configurations with higher energies. The result of such a projection is the bipolaronic Hamiltonian

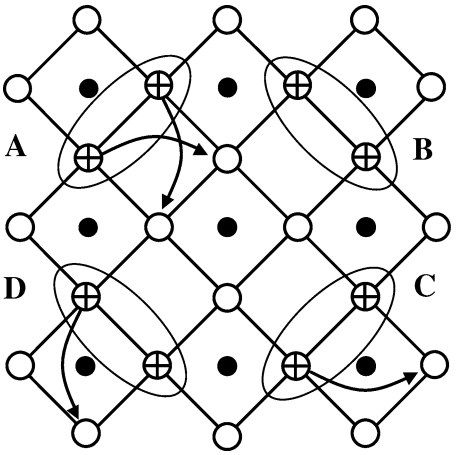

Fig. 2. Top view on the perovskite layer. The apical sites are not shown. The four bipolaron configurations A, B, C, and D all have the same energy. Some possible single-polaron hoppings t' are indicated by arrows. Note that the bipolaron movement is first-order in t'.

$$\begin{aligned} H_b = {} & (V_c - 3.23E_p) \times \sum_{\mathbf{l}} \left[A^\dagger_{\mathbf{l}} A_{\mathbf{l}} + B^\dagger_{\mathbf{l}} B_{\mathbf{l}} + C^\dagger_{\mathbf{l}} C_{\mathbf{l}} + D^\dagger_{\mathbf{l}} D_{\mathbf{l}} \right] \\ & - t' \sum_{\mathbf{l}} \left[A^\dagger_{\mathbf{l}} B_{\mathbf{l}} + B^\dagger_{\mathbf{l}} C_{\mathbf{l}} + C^\dagger_{\mathbf{l}} D_{\mathbf{l}} + D^\dagger_{\mathbf{l}} A_{\mathbf{l}} + \text{h.c.} \right] \\ & - t' \sum_{\mathbf{n}} \left[A^\dagger_{\mathbf{l}-\mathbf{x}} B_{\mathbf{l}} + B^\dagger_{\mathbf{l}+\mathbf{y}} C_{\mathbf{l}} + C^\dagger_{\mathbf{l}+\mathbf{x}} D_{\mathbf{l}} + D^\dagger_{\mathbf{l}-\mathbf{y}} A_{\mathbf{l}} + \text{h.c.} \right], \end{aligned} \tag{16}$$

where $\mathbf{l}$ numbers octahedra rather than individual sites, $\mathbf{x} = (1,0)$, and $\mathbf{y} = (0,1)$. A Fourier transformation and diagonalization of a 4×4 matrix yields the bipolaron spectrum:

$$E_2(\mathbf{k}) = V_c - 3.23E_p \pm 2t'\left[\cos(k_x/2) \pm \cos(k_y/2)\right]. \tag{17}$$

There are four bipolaronic subbands combined in a band of width $8t'$. The effective mass of the lowest band is $m^{**} = 2/t'$. The bipolaron binding energy is $\Delta = 2E_1(0) - E_2(0) = 1.23E_p - V_c - 8t - 4t'$. Because of an infinite Hubbard repulsion, the energy splitting between the singlet and triplet inter-site bipolaron states is zero.

We would like to emphasize that the inter-site bipolaron moves already in the *first* order in polaron hopping. This remarkable property is entirely due to the strong on-site repulsion and long-range electron–phonon interaction that leads to a nontrivial connectivity of the lattice. This situation is unlike all other models studied previously. (Usually the bipolaron moves only in the second order in polaron hopping and therefore is very heavy.) In our model, this fact combines with a weak renormalization of t' yielding a *superlight* bipolaron with mass $m^{**} \propto \exp(0.60E_p/\omega)$. We recall that in the Holstein model $m^{**} \propto \exp(2E_p/\omega)$. Thus the mass of the Fröhlich inter-site bipolaron scales approximately as *cubic root* of that of the Holstein on-site bipolaron.

At even stronger el–ph interaction, $V_c < 1.16E_p$, NNN bipolarons become stable. More importantly, holes can now form 3- and 4-particle clusters. The dominance of the potential energy over kinetic in Hamiltonian (10) enables us to readily investigate these many-polaron cases. Three holes placed within one oxygen square have four degenerate states with energy $2(V_c - 1.23E_p) + V_c/\sqrt{2} - 0.80E_p$. The first-order polaron hopping processes mix the states resulting in a ground state linear combination with energy $E_3 = 2.71V_c - 3.26E_p - \sqrt{4t^2 + t'^2}$. It is essential that between the squares such triads could move only in higher orders in polaron hopping. In the first order, they are immobile. A cluster of four holes has only one state within a square of oxygen atoms. Its energy is

$$E_4 = 4(V_c - 1.23E_p) + 2\left(\frac{V_c}{\sqrt{2}} - 0.80E_p\right) = 5.41V_c - 6.52E_p.$$

This cluster, as well as all the bigger ones, is also immobile in the first order of polaron hopping. We conclude that at $V_c < 1.16E_p$ the system becomes a charge segregated insulator within the first-order perturbation theory with respect to the kinetic energy. A more accurate characterization of the charge segregated state and the phase boundary requires higher-order corrections.

The superconductivity window that we have found, $1.16E_p < V_c < 1.23E_p$, is quite narrow. The fact, that within this window there are no three or higher polaron bound states, implies that bipolarons repel each other. The system is effectively the charged Bose gas, which is a well known superconductor (for a review, see Ref. [6]). It follows from our model that superconductivity in cuprates should be very sensitive to any external factor that affects the balance between V_c and E_p. For instance, pressure changes the octahedra geometry and hence E_p and $V_{\rm pa}$. Chemical doping enhances internal screening and consequently reduces E_p.

We now assume that the superconductivity condition is satisfied and show that our 'Fröhlich–Coulomb' model possesses many key properties of the underdoped cuprates. The bipolaron binding energy Δ should manifest itself as a normal state pseudogap with size of approximately half of Δ [6]. Such a pseudogap has indeed been observed in many cuprates. There should be a strong isotope effect on the (bi)polaron mass because $t, t' \propto \exp(-\text{const}\sqrt{M})$. Therefore the replacement of O^{16} by O^{18} increases the carrier mass [24]. Such an effect has been observed in the London penetration depth of the isotope-substituted samples [1]. The mass isotope exponent, $\alpha_m = d\ln m^{**}/d\ln M$, was found to be as large as $\alpha_m = 0.8$ in $La_{1.895}Sr_{0.105}CuO_4$. Our theoretical exponent is $\alpha_m = 0.3E_p/\omega$, so that the bipolaron mass enhancement factor is $\exp(0.6E_p/\omega) \simeq 5$ in this material. With the bare hopping integral $T_{\rm NNN} = 0.2$ eV we obtain the in-plane bipolaron mass $m^{**} \simeq 10m_e$. Calculated with this value the in-plane London penetration depth,

$$\lambda_{ab} = \left[m^{**}/8\pi ne^2\right]^{1/2} \simeq 316 \text{ nm}$$

(n is the hole density), agrees well with the measured one $\lambda_{ab} \simeq 320$ nm. Taking into account the c-axis tunneling of bipolarons, the critical temperature of their Bose–Einstein condensation can be expressed in terms of the experimentally measured in-plane and c-axis penetration depths, and the in-plane Hall constant R_H as

$$T_c = 1.64f\left(eR_H/\lambda_{ab}^4\lambda_c^2\right)^{1/3}.$$

Here $f \approx 1$, and T_c, eR_H and λ are measured in K, cm^3 and cm, respectively [25]. This expression neglects both the hard-core and long-range electrostatic repulsion of bipolarons. The relevant atomic density of bipolarons is well below 1, and the static lattice di-

electric constant is very large in the cuprates, which justifies the ideal Bose-gas approximation for T_c [6]. Using the experimental $\lambda_{ab} = 320$ nm, $\lambda_c = 4160$ nm, and $R_H = 4 \times 10^{-3}$ cm^3/C (just above T_c) one obtains $T_c = 31$ K in striking agreement with the experimental value $T_c = 30$ K. The recent observation of the normal state diamagnetism in $La_{2-x}Sr_xCuO_4$ [26] also confirms the prediction of the bipolaron theory [27]. In this Letter we have not addressed the important issue of the symmetry of the superconducting order parameter. In the bipolaron theory the symmetry of the pseudogap may be different from that of the superconducting order parameter. The latter could be d-wave [23]. Many other features of the bipolaronic (super)conductor, e.g., the unusual upper critical field, electronic specific heat, optical and tunneling spectra match those of the cuprates (for a recent review, see Ref. [28]).

In conclusion, we have studied a many-polaron model with strong long-range electron–phonon and Coulomb interactions. The model shows a rich phase diagram depending on the ratio of the inter-site Coulomb repulsion and the polaronic (Franck–Condon) level shift. The ground state is a polaronic Fermi liquid at large Coulomb repulsion, a bipolaronic high-temperature superconductor at intermediate Coulomb repulsion, and a charge-segregated insulator at weak repulsion. In the superconducting phase, inter-site bipolarons are remarkably light leading to a high critical temperature. The model describes many properties of the underdoped cuprates.

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