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Self-localization of holes in a lightly doped Mott insulator

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Abstract. We show that lightly doped holes will be self-trapped in an antiferromagnetic spin background at low-temperature, resulting in spontaneous translational symmetry breaking. The underlying Mott physics is responsible for such novel self-localization of charge carriers. Interesting transport and dielectric properties are found as the consequences, including large doping-dependent thermopower and dielectric constant, low-temperature variable-range-hopping resistivity, as well as high-temperature strange-metal-like resistivity, which are consistent with experimental measurements in the high-T_c cuprates. Disorder and impurities only play a minor and assistant role here.

PACS. 74.20.Mn Nonconventional mechanisms (spin fluctuations, polarons and bipolarons, resonating valence bond model, anyon mechanism, marginal Fermi liquid, Luttinger liquid, etc.) – 74.25.Ha Magnetic properties – 75.10.-b General theory and models of magnetic ordering

1 Introduction

There exist several types of electron localization in condensed matter physics. In the presence of disorder or impurities, waves can be localized due to quantum interference, which is generally known as the Anderson localization [1]. In a two-dimensional (2D) system carriers are expected [2] to be always localized with the resistance diverging either logarithmically ("weak localization") or exponentially ("strong localization") as $T \to 0$. A different kind of localization involves the self-trapping of small polarons in strong electron-phonon interacting systems. Both types of localization here mainly concern non-interacting or weakly correlated electrons.

In the high-T_c cuprates, the undoped system is a Mott insulator, in which the charge degree of freedom is totally frozen out by strong on-site Coulomb repulsion. The spins form an antiferromagnetic long range order (AFLRO) at low temperature, which quickly collapses upon hole-doping [3]. At small concentration, $\delta < 0.05$, the doped holes as charge carriers remain localized with the low-T resistivity well fit [4–7] by that of traditional variable-range-hopping (VRH) type, usually applicable to doped semiconductors. Only when the hole concentration exceeds 0.05 will the charge carriers be truly delocalized, where the ground state becomes a d-wave superconducting state.

But lightly doped high-T_c cuprates are of no conventional doped semiconductors. Here they are doped Mott insulators with the majority of the charge degree of freedom still remaining frozen. The strongly correlated effect should thus play a crucial role in the charge transport. The issue why doped holes should be always localized at small doping and how they eventually become delocalized with increasing doping is a very important question, which may also be relevant to understanding the microscopic mechanism of high-temperature superconductivity in the cuprates.

Recently, a new kind of self-localization, which can be particularly attributed to the Mott physics, has been proposed [8–10], in which the *pure* Coulomb interaction is responsible for the self-localization of electrons near half-filling. Here disorder or impurities is no longer as essential as in the Anderson localization, although they may be helpful to induce a true translational symmetry breaking at $T = 0$. Such a self-localization of holes is caused by the phase-string effect, referring to a stringlike defect left by the hopping of a hole which was previously identified [11] as an *irreparable* effect in the ground state of the $t-J$ model no matter whether there is an AFLRO or not at *arbitrary* doping [but some extra signs arising from the exchange between holes will reduce the singular phase string effect with the increase of doping (see Ref. [11])]. Furthermore, it has been also shown [8] that the charge localization does not contradict to the photoemission experiments [12] in which the observed "quasiparticle" dispersion in the single-particle spectral function can be well accounted for in terms of the "spinon dispersion".

In principle, it is not surprising that due to the separation [13] of spin and charge degrees of freedom in a

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doped Mott insulator, the charge carriers can get localized at low doping by scattering with fluctuations originated from an independent degree of freedom. In fact, in a different gauge-theory approach to the $t-J$ model, the localization of charge carriers has been also obtained [14], due to the scattering between the charge carriers and gauge fluctuations.

In this paper, we study such kind of self-localization phenomenon in a Mott insulator based on an effective model, known as the phase string model, which was obtained previously [11,15] as a low-energy description of the $t-J$ model. We shall focus on the spin ordered phase (not necessarily long-range ordered) at very low doping in this model and explore the unique charge self-localization behavior. As shown previously, a doped hole in such a model will induce [9,10] a dipole-like spin structure in the spin ordered phase, with the kinetic energy being severely frustrated by the phase string effect. In this work, we demonstrate that such a hole-dipole picture can be accurately described, based on the phase-string model, as each holon induces a topological "meron" distortion from the spinon degrees of freedom and two objects are bound together and self-trapped in real space. This is mathematically ensured by a dual Meissner effect and "flux-quantization" condition in the model. We then discuss the corresponding transport properties and show that the thermopower saturates to a Heikes-like formula as the result. While the resistivity exhibits a Mott-VRH-like behavior at low temperature, the collapse of the hole-dipole composites and the release of free "holons" at high-temperature will lead to a strange-metal-like behavior there. Furthermore, the existence of the hole dipolar structure predicts a large doping-dependent dielectric constant, which diverges at the deconfinement. All of these properties seem to paint a consistent picture for the complex transport and dielectric phenomena observed in the high-T_c cuprates.

The remainder of the paper is organized as follows. In Section 2, we discuss the self-localization of doped holes in the spin ordered phase at low doping by using the dual Meissner effect and "flux-quantization" condition based on the phase-string model. A renormalization group (RG) analysis will be used to determine the phase diagram. In Section 3, we discuss the experimental implications of the self-localization, including the thermopower, resistivity and dielectric constant, and make comparisons with experimental measurements. Finally, the conclusions are presented in Section 4.

2 Self-localization of holes in a doped Mott insulator

We shall adopt the phase-string model as the microscopic description of how doped holes move in an antiferromagnetic (AF) Mott insulator. This model is obtained [15] as a low-energy effective theory based on the $t-J$ model, which can accurately describe AF correlations at half-filling and possesses a d-wave superconducting ground state at doping concentrations larger than x_c ($\simeq$0.043 at $T=0$) [9]. What we will be interested in the following is the non-superconducting phase below the critical doping x_c, where an AFLRO or a spin glass state persists at low temperature.

The existence of such a non-superconducting phase is the consequence that the *long-range* AF correlations (not necessarily AFLRO) win in the competition with the kinetic energy of holes at sufficiently low doping. In the phase-string model, this phase will be characterized by the "spinon condensation". In the following, we shall analyze in detail the behavior of doped holes in this low-doping regime and demonstrate that the charge carriers must be self-localized in the ground state, resulting in spontaineous translational symmetry breaking.

2.1 Phase-string model

We start with the phase-string model $H_{\rm string}=H_h+H_s$, which is composed [15] of two terms: The charge degree of freedom as characterized by the "holon" term

$$H_h=-t_h\sum_{\langle ij\rangle}\left(e^{iA^s_{ij}}\right)h^\dagger_i h_j+H.c. \tag{1}$$

where $t_h\sim t$ and the "holon" operator, $h^\dagger_i$, is bosonic; the spin degrees of freedom as described by the "spinon" term

$$H_s=-J_s\sum_{\langle ij\rangle\sigma}\left(e^{i\sigma A^h_{ij}}\right)b^\dagger_{i\sigma}b^\dagger_{j-\sigma}+H.c. \tag{2}$$

where $J_s\sim J$ and the "spinon" operator, $b^\dagger_{i\sigma}$, is also bosonic.

Basic features of this model are as follows. At half filling, the gauge field A^h_{ij} can be set to zero in equation (2) and H_s reduces to the Schwinger-boson mean-field Hamiltonian [16], which describes both the long-range and short-range AF correlations fairly well. Upon doping, A^h_{ij} is no longer trivial as it satisfies a topological constraint: $\sum_C A^h_{ij}=\pi\sum_{l\in\Sigma_C}n^h_l$ (Σ_C denotes the area enclosed by C) with n^h_l denoting the "holon" number at site l, which is interpreted as that each "holon" behaves like a π-fluxoid as felt by the "spinons". Thus, A^h_{ij} will play the key role of frustrations introduced by holes that act on the spin degrees of freedom. Similarly, the "holons" are also subjected to frustrations from the spin background, through the gauge field A^s_{ij} in equation (1). Here A^s_{ij} satisfies a topological constraint: $\sum_C A^s_{ij}=\pi\sum_{l\in\Sigma_C}\left(n^b_{l\uparrow}-n^b_{l\downarrow}\right)$ with $n^b_{l\sigma}$ denoting the "spinon" (with index σ) number at site l, which can be interpreted as that each "spinon" behaves like a $\pm\pi$-fluxoid as perceived by the "holons".

The spin and charge degrees of freedom are thus mutually "entangled" in the phase-string model $H_{\rm string}$ based on two topological gauge fields, A^h_{ij} and A^s_{ij}. It has been shown [17] that if the holons (which are bosons) experience a Bose condensation at larger doping, the spinons, which behave as vortices according to A^s_{ij}, must be "confined" at low temperature. Such a "spinon confining phase" actually

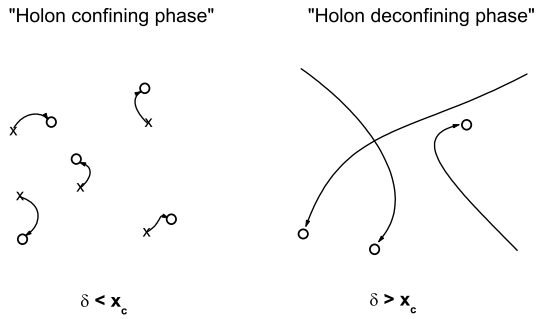

Fig. 1. Holes are self-trapped in real space at $\delta < x_c$ by the phase-string effect, carrying dipolar spin configurations. Holes become delocalized at $\delta > x_c$, with the critical doping concentration $x_c = 0.043$ (see text).

corresponds to the d-wave superconducting phase in the model. Here, the spinon confinement occurring in the *spin degree of freedom* is closely related to the superconducting phase coherence in the *charge degree of freedom*.

In contrast, if the spinons (which are also bosons) are Bose condensed at low doping, free holons as "vortices" cannot live alone either, and must be also "confined" [9,10]. Such a *spinon condensed phase* is thus also known as "holon confining phase", which constitutes a non-superconducting solution of the phase-string model in the lightly doped regime. In the following, we will demonstrate how holons will get self-trapped in real space in such a phase. The spin ordered phase as characterized by the spinon condensation is therefore intimately related to the charge self-localization (holon confining). Figure 1 schematically illustrates the above-mentioned two phases at different doping concentrations.

2.2 Antimerons induced by holons: "flux-quantization" condition

Let us recall that at half-filling, the Bose condensation of spinons,

$$\langle b_{i\sigma}\rangle \neq 0 \tag{3}$$

will naturally gives rise to an AFLRO lying in the x-y plane [18] with $\langle S_i^+\rangle = (-1)^i\langle b_{i\uparrow}\rangle\langle b_{i\downarrow}\rangle$. However, once a hole is added into such an ordered state, the energy cost associated with a *bare* holon, if the condensation (3) remains unchanged, would become *logarithmically divergent* in terms of H_s

$$\begin{aligned}\Delta E_s &\simeq \tilde{J}_s\int d^2\mathbf{r}\left[\mathbf{A}^h\right]^2\\ &\sim \frac{\pi}{2}\tilde{J}_s\ln(L/a)\to\infty,\end{aligned} \tag{4}$$

where $\tilde{J}_s \equiv J_s\langle b_{i\uparrow}\rangle\langle b_{i\downarrow}\rangle \sim 0.3J_s$, $\mathbf{A}^h$ is the continuum version of A^h_{ij}, L is the size of the sample and a is the lattice constant.

But this is not the correct physical picture. Note that equation (3) suggests that spinons are in a "superfluid" state. In reality, the two-component spinon "superfluid" in equation (3) can *response* to the presence of the vector potential $\mathbf{A}^h$ by forming *spin supercurrent,* like the Meissner effect in a superconductor. One may call it a dual Meissner effect here. Then the induced spin supercurrent can screen the effect of the "magnetic fluxes" introduced by A^h_{ij} in H_s in a similar fashion as the flux-quantization phenomenon in a superconductor, such that the resulting *renormalized* holon will acquire a finite self-energy. In the following, we demonstrate how this screening effect takes place in the phase-string model (2).

Define $\langle b_{i\sigma}\rangle \equiv \sqrt{\rho_c^s a^2}z_{i\sigma}$, if $i \in A$ sublattice, and $\langle b_{i\sigma}\rangle \equiv \sqrt{\rho_c^s a^2}z^*_{i-\sigma}$, if $i \in B$ sublattice, with $|z_{i\uparrow}|^2 + |z_{i\downarrow}|^2 = 1$. Here ρ_c^s denotes the spinon "superfluid" density. Then the condensed part of H_s can be written as

$$\begin{aligned}H_s^{\rm cond} &= -J_s\sum_{\langle ij\rangle\sigma}\left(e^{i\sigma A^h_{ij}}\right)\langle b^\dagger_{i\sigma}\rangle\langle b^\dagger_{j-\sigma}\rangle + c.c.\\ &= -\tilde{J}_s\sum_{i\in A,j=NN(i)}\sum_\sigma\left(e^{i\sigma A^h_{ij}}\right)z^*_{i\sigma}z_{j\sigma} + c.c\\ &\simeq -\tilde{J}_s\sum_{i\in A,j=NN(i)}\sum_\sigma\left(1+i\sigma A^h_{ij}-\frac{1}{2}\left(A^h_{ij}\right)^2\right)\\ &\times z^*_{i\sigma}z_{j\sigma} + c.c\\ &\simeq E_s^0 + i\tilde{J}_s\int d^2\mathbf{r}\sum_\sigma\sigma\mathbf{A}^h\cdot(z^*_\sigma\boldsymbol{\nabla}z_\sigma - c.c.)\\ &+ \ \tilde{J}_s\int d^2\mathbf{r}\left(\mathbf{A}^h\right)^2\end{aligned} \tag{5}$$

in the continuum limit, where NN denotes the nearest neighboring sites, $\tilde{J}_s = J_s\rho_c^s a^2$, and $E_s^0 \equiv -4\tilde{J}_s N + 2\tilde{J}_s\int d^2\mathbf{r}\sum_\sigma|\boldsymbol{\nabla}z_\sigma|^2$. The spin "supercurrent", defined by $\mathbf{J}^s = -\partial H_s^{\rm cond}/\partial\mathbf{A}^h$, then reads

$$\mathbf{J}^s = 2\tilde{J}_s\left(\mathbf{v}^s - \mathbf{A}^h\right) \tag{6}$$

where

$$\mathbf{v}^s \equiv -\frac{i}{2}\sum_\sigma\sigma\left(z^*_\sigma\boldsymbol{\nabla}z_\sigma - c.c.\right). \tag{7}$$

Generally one expects a complicated distribution of the spin current nearby a holon. But in a distance far away from the holon, the supercurrent $\mathbf{J}^s$ should vanish in order to ensure the finiteness of the energy cost introduced by a holon. The same requirement has been used in a superconductor to realize the flux quantization. By contrast, here we are dealing with the "flux-quantization" in a two-component superfluid problem with an internal gauge freedom.

By requiring the spin supercurrent $\mathbf{J}^s$ vanish at the boundary C_∞ such that

$$\oint_{C_\infty} d\mathbf{r}\cdot\mathbf{J}^s = 0, \tag{8}$$

one arrives at

$$\oint_{C_\infty} d\mathbf{r}\cdot\mathbf{v}^s - \oint_{C_\infty} d\mathbf{r}\cdot\mathbf{A}^h = 0. \tag{9}$$

Note that $\oint_{C_\infty} d\mathbf{r}\cdot\mathbf{v}^s = \int d^2\mathbf{r}\,(\boldsymbol{\nabla}\times\mathbf{v}^s)\cdot\hat{\mathbf{z}}$. By introducing a unit vector

$$\mathbf{n} = \bar{z}\hat{\boldsymbol{\sigma}}z$$

where $\hat{\boldsymbol{\sigma}}$ is the Pauli matrix and $\bar{z} \equiv (z_\uparrow^*, z_\downarrow)$, one can straightforwardly show that

$$(\boldsymbol{\nabla}\times\mathbf{v}^s)\cdot\hat{\mathbf{z}} = \frac{1}{2}\mathbf{n}\cdot\partial_x\mathbf{n}\times\partial_y\mathbf{n}. \tag{10}$$

Thus, equation (8) finally reduces to the following "flux-quantization" condition

$$Q \equiv \int d^2\mathbf{r}\,\frac{1}{4\pi}(\mathbf{n}\cdot\partial_x\mathbf{n}\times\partial_y\mathbf{n}) = \frac{1}{2\pi}\oint_{C_\infty} d\mathbf{r}\cdot\mathbf{A}^h = \frac{1}{2}N^h \tag{11}$$

where N^h is the total number of doped holes.

Therefore, the spinon condensed phase in the phase-string model can be regarded as a (dual) Meissner state, in which each holon, due to its attachment to a π flux-oid, will always induce a "screening" response from the spinon condensate, which is of topological nature satisfying the "flux-quantization" condition (11), meaning that each holon will "nucleate" a spin "meron" configuration with a topological charge $Q = 1/2$. Such a meron configuration may be pictured as a spin vortex with the unit vector $\mathbf{n}$ lying in a spin x-y plane at a distance far away from the core, while, near the core, the unit vector $\mathbf{n}$ starts to tilt away from the x-y plane and points towards the z-axis at the core center, which covers one half of the unit sphere spanned by $\mathbf{n}$ once, in contrast to a skyrmion which covers the whole unit sphere exactly once with $Q = 1$.

Finally we note that such *holon-induced* merons are called *antimerons* in the earlier approach [9,10] because a holon itself also carries a meron (vortex) in the *original spin space*. To see this, let us recall that in the phase-string model, the spin operators are expressed in terms of spinon operators by [11]

$$S_i^+ = (-1)^i b_{i\uparrow}^\dagger b_{i\downarrow}\exp\left[i\Phi_i^h\right] \tag{12}$$

and $S_i^- = \left(S_i^+\right)^\dagger$, $S_i^z = \sum_\sigma \sigma b_{i\sigma}^\dagger b_{i\sigma}$. In the spinon condensed phase, one has

$$\left\langle S_i^+\right\rangle = (-1)^i\langle b_{i\uparrow}\rangle\langle b_{i\downarrow}\rangle\exp\left[i\Phi_i^h\right], \tag{13}$$

which is twisted away from an AFLRO lying in the x-y plane by the vortices centered at holons as determined by Φ_i^h. Here Φ_i^h is defined by

$$\Phi_i^h = \sum_{l\neq i}\mathrm{Im}\ln(z_i - z_l)n_l^h. \tag{14}$$

But equation (13) describes an *bare* holon effect which would result in a divergent self-energy of the holon as shown in equation (4). In order to compensate such a vortex configuration associated with a bare holon, the condensed spinon fields have to be twisted into

$$\langle b_{i\sigma}\rangle \to \langle b_{i\sigma}\rangle\exp\left[i\frac{\sigma}{2}\vartheta_i\right] \tag{15}$$

with an *antimeron* configuration ϑ_i[9,10], which is characterized just by $z_{i\sigma}$ in the present approach, satisfying the "flux-quantization" condition (11). Therefore, in the phase-string model, a renormalized holon is a composite with a bare holon bound to an induced antimeron as demonstrated above, while in the *original spin space*, it is an object composed of a meron (holon) and an antimeron, forming a *dipole* [9,10]. Two descriptions are equivalent.

2.3 Self-localization of holes: RG analysis

According to the above analysis, the infinite self-energy of a *bare* holon in the spinon condensed phase can be removed by "nucleating" a topological spin antimeron configuration and bound to the latter. This picture is precisely ensured by the "flux-quantization" condition as shown above. Since the induced antimeron is an infinite-size semiclassical object which has no kinetic energy and cannot propagate, the "confinement" of a holon to it then means that the holon will be self-trapped in space. Due to the translational symmetry, these induced antimerons can be located anywhere in space and therefore will result in *spontaneous translational symmetry breaking* in the spinon condensed phase.

Physically, such a self-localization of charge carriers in the low-doping regime can be attributed to the irreparable phase-string effect created by the motion of holes, as discussed in reference [10]. The phase-string model provides a mathematical framework to conveniently handle this effect. In this description, the locations of the antimeron and the holon inside a dipole constitute the starting and ending points of the motion of a holon, and the phase-string connecting such two points has relaxed into a dipolar picture, with a remaining branch-cut connecting two poles [10].

If one tries to spatially separate the holon from the induced antimeron, the uncompensated spin supercurrent $\mathbf{J}^s$ will increase the self-energy, representing an attractive potential which binds the bare holon to the antimeron. According to equation (5), such a potential can be estimated by

$$V \simeq q^2\ln\frac{|\mathbf{r}|}{a} \tag{16}$$

at $|\mathbf{r}| > a$, where $q^2 = \pi\tilde{J}_s$, and $\mathbf{r}$ is the distance between the holon and antimeron. At $|\mathbf{r}|\to\infty$, V diverges in consistency with equation (4). The same result was also obtained in references [9,10].

When there are many holon-antimeron dipoles, one expects to see a *screening effect* on the confining potential by reducing V to $V_{\mathrm{eff}} = \frac{1}{\kappa}V$, where κ denotes the dielectric constant. Previously it has been shown [9] that with the increase of doping concentration, eventually a transition at $T = 0$ takes place, as $\kappa\to\infty$ or $V_{\mathrm{eff}}\to 0$, from the holon self-localization (confining) phase to a delocalization (deconfining) phase at $\delta = x_c \simeq 0.043$ (see Fig. 1). On the other hand, with the increase of temperature, neutral vortex-antivortex pairs like those in the XY model can also be thermally excited, leading to a conventional

contribution to the screening effect. To distinguish such two kinds of vortex-antivortex pairs, we shall call a dipole associated with a holon as a charged pair and the other kind as a neutral pair. In the following, we shall treat the screening effect due to both charged and neutral dipoles on an equal footing based on an RG treatment [9,19]. In contrast to the conventional Kosterlitz-Thouless (KT) theory [20], here the number of vortex-antivortex pairs remains finite even at $T = 0$, where it is equal to δN (i.e., the number of holons).

The probability for the neutral dipoles with two poles separated by a distance r is controlled by the neutral pair fugacity $y_n^2(r)$. In the conventional KT theory [20], the initial $y_n^2(a) = e^{-\beta E_c^n}$, (where $\beta = \frac{1}{k_B T}$ and the core energy $E_c^n \sim q^2$). But since the charged dipole number will be always fixed at δ per site, the probability for the charged dipoles is no longer governed by the fugacity $y_h^2(a) = e^{-\beta E_c^h}$, (where E_c^h denotes its core energy). Instead, the initial fugacity must be adjusted accordingly and E_c^h will turn out to be no longer so important [9,19].

In an RG procedure, the contributions from the dipoles with the sizes between r and $r + dr$ will be integrated out, starting from $r = a$. The renormalization effect is then represented by three renormalized quantities, $X(r) \equiv \frac{2\pi\kappa}{\beta q^2}$, $y_n^2(r)$, and $y_h^2(r)$, which satisfy the following famous recursion relations [20,21]

$$dy_h/dl = (2 - \frac{\pi}{X})\, y_h, \tag{17}$$

$$dy_n/dl = (2 - \frac{\pi}{X})\, y_n, \tag{18}$$

$$dX/dl = 4\pi^3(y_n^2 + y_h^2), \tag{19}$$

where $r = ae^l$.

Define $Y^2(l) = y_h^2(l) + y_n^2(l)$, with $Y_0^2 = y_h^2(l = 0) + y_n^2(l = 0)$. From equations (17–19), we find

$$Y^2 = Y_0^2 + \frac{1}{\pi^3}(X - X_0) - \frac{1}{2\pi^2}\ln\frac{X}{X_0} \tag{20}$$

where $X_0 \equiv X(l = 0) = \frac{2\pi}{\beta q^2}$ (with $\kappa(l = 0) = 1$). The RG flow is then obtained from equation (19) by

$$l = \int_{X_0}^{X} \frac{dX'}{4\pi^3 Y_0^2 + 4(X' - X_0) - 2\pi\ln(X'/X_0)}. \tag{21}$$

The neutral pair fugacity can be determined by $y_n^2(l) = e^{-2\int_0^l (2-\frac{\pi}{X})dl'}$, which will show a similar behavior as in the conventional KT theory.

What makes the present approach different from the conventional KT theory is the presence of a finite density of the charged dipoles (holon-antimeron pairs). Here, by noting $\frac{y_h^2(r)}{r^4} d^2\mathbf{r}$ as the areal density of charged pairs of sizes between r and $r + dr$ [20], we have the following constraint

$$\delta/a^2 = \int_a^\infty dr\, 2\pi r\, \frac{y_h^2(r)}{r^4}, \tag{22}$$

or

$$\delta/a^2 = \int_a^\infty dr\, 2\pi r\, \frac{Y^2(r)}{r^4} - \frac{1}{2\pi^2 a^2}\int_0^\infty dl e^{-2l}\, y_n^2$$
$$= \frac{1}{2\pi^2 a^2}\int_0^\infty dl e^{-2l}\frac{dX}{dl} - \frac{1}{2\pi^2 a^2}\int_0^\infty dl e^{-2l}\, y_n^2. \tag{23}$$

After an integral transformation, such a constraint can be rewritten as

$$2\pi^2\delta + \frac{2\pi k_B T}{q^2} + \frac{1}{2\pi^2 a^2}\int_0^\infty dl e^{-2l}\, y_n^2 = 2\int_0^\infty e^{-2l}\, X\ dl. \tag{24}$$

For $\beta q^2 \gg 1$, $y_n^2 < y_n^2(0) \sim \exp(-\beta q^2) \to 0$, the probability for neutral pairs remains a small number and can be neglected.

The RG flow diagram of equations (17–19) is as follows: the two basins of attraction are separated by the initial values which flow to $X^* \to \frac{\pi}{2}$ and $y_h^* \to 0$, $y_n^* \to 0$ in the limit $l \to \infty$. In terms of equation (21), the separatrix of the RG flows is given by

$$l = \int_{X_0}^{X} \frac{dX'}{4(X' - \frac{\pi}{2}) - 2\pi\ln(2X'/\pi)}. \tag{25}$$

"Deconfining" temperature $T_{\rm de}$. Based on the RG equations of (24) and (25), one can determine the critical hole density $\delta_{\rm de} = \delta_{\rm de}(T)$ or temperature $T_{\rm de} = T_{\rm de}(\delta)$ at which the charged dipoles collapse and holons are "deconfined" from the bound state with the antimerons and become delocalized.

We first consider the case at $T = 0$. Since neutral vortices do not exist at $T \to 0$, equation (24) reduces to

$$2\pi^2\delta_{\rm de} = 2\int_0^\infty e^{-2l}\, X\ dl = \int_0^{\pi/2} e^{-2l}\, dX. \tag{26}$$

The critical doping $\delta_{\rm de}$ at $T = 0$ is then numerically determined by $\delta_{\rm de}(0) \simeq 0.043$, which was previously obtained in reference [9] as denoted by x_c. Now consider the limit at $\delta \to 0$, where we approximately have $X(l) \simeq X_0 \simeq X(l \to \infty) = \frac{\pi}{2}$, and equation (24) becomes

$$2\pi^2\delta + \frac{2\pi k_B T_{\rm de}}{q^2} \simeq \frac{\pi}{2}, \tag{27}$$

which gives rise to $T_{\rm de}(\delta = 0) \simeq \frac{q^2}{4k_B} = \frac{\pi\tilde{J}_s}{4k_B}$ and $T_{\rm de}(\delta) \simeq T_{\rm de}(0) - \delta\pi q^2/k_B$ at $\delta \ll 1$.

The holon "confining" and "deconfining" phases are separated by $T_{\rm de}(\delta)$ in the $T-\delta$ phase diagram as shown in Figure 2. In the "confining" phase, holons are self-trapped by binding to the induced antimerons. In the original spin space, each renormalized holon can be regarded as a dipolar object. In this regime, AFLRO or short-ranged AF ordering (spin glass) can still form, if the interlayer coupling is introduced: the Néel transition temperature is obtained as $T_N(\delta) \approx -\frac{\pi J}{k_B \ln\alpha} - 3\delta J/k_B$, with $\alpha \sim 10^{-5}$ representing the ratio of the interlayer coupling $J_\perp/J$[9], which is schematically illustrated in Figure 2 by the dashed curve.

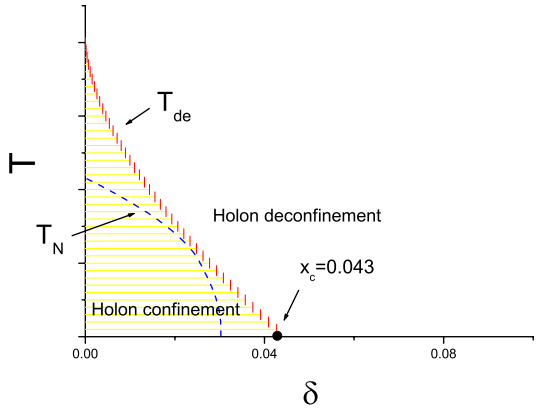

Fig. 2. The low-doping phase diagram determined by the RG analysis. The boundary set by $T_{\rm de}(\delta)$ separates the holon confining and deconfining phases with $T_{\rm de}(\delta = 0) \simeq \frac{\pi \tilde{J}_s}{4k_B}$ (see text). The Néel temperature $T_{\rm N}$ is determined by introducing an interlayer coupling.

Previously we have also shown that a superconducting phase will set in beyond $\delta > x_c$, where delocalized bosonic holons will experience a Bose condensation at low temperatures.

3 Experimental implications

3.1 Thermopower

The spontaneous translational symmetry breaking in a lightly doped Mott insulator has very unique experimental consequences. In such a system, since each doped hole can be self-trapped anywhere in space, due to the translational symmetry of the original Hamiltonian, there will be a *large* and *doping-dependent entropy* associated with the energetically degenerate configurations of holes in real-space distribution. Such an anomalous entropy associated with the charge carriers can be directly probed in a thermopower measurement.

It has been previously known [22,23] that for charge carriers in a narrow band, when the temperature is raised to exceed the bandwidth, the thermopower will be saturated to a T-independent constant, which is entirely determined by the entropy change per added carrier. Namely, the thermopower S_e at high-T will reduce to

$$S_e \to \frac{\mu}{eT} = -\frac{1}{e}\left(\frac{\partial S}{\partial N_e}\right) \qquad (28)$$

where μ denotes the chemical potential, S the entropy, and N_e the total electron number.

The self-localization of doped holes means a vanishing bandwidth of the charge carriers and a spontaneous translational symmetry breaking with a lot of degenerate real-space configurations in the distribution of holes. The formula (28) can be directly applied in such a case based on a general thermodynamic consideration.

Putting N_h hole on N lattice sites with no-double-occupancy would give rise to an entropy $S = k_B \ln N!/N_h!\,(N-N_h)!$, which then leads to the Heikes formula [22,23] $S_e^H = \frac{k_B}{e} \ln \frac{(1-\delta)}{\delta}$, by noting $N_e = N - N_h$ in equation (28) and using the Sterlings approximation at $N \to \infty$ with $N_h = N\delta$. But since each doped hole is actually a dipolar composite composed of a meron and an antimeron located at two poles, which do not coincide with each other as wall as with other hole dipoles, the total entropy should be reduced by this fact. One can determine the entropy by assuming that two poles of each hole dipole are loosely bound such that it becomes a problem with a total number of $2N_h$ poles, instead of N_h, being put on N lattice sites without double occupancy. Correspondingly one obtains the following modified Heikes formula

$$S_e^{mH} = \frac{k_B}{e} \ln \frac{(1-2\delta)}{2\delta}. \qquad (29)$$

This formula has no other fitting parameters and is a universal function of the doping concentration δ.

The Heikes-type formula (29) is plotted in Figure 3, as the solid curve, together with the experimental data obtained at room temperature in the Sr and Ba doped La_2CuO_{4-y} compounds [24] (full square and bigger circle), $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+y}$ system [25] (cross), and from the recent measurement by Wang and Ong [26] in $La_2Sr_xCuO_{4-y}$ (small full circle). Figure 3 shows that equation (29) agrees qualitatively and quantitatively well with the experimental measurements in the insulating regime, where the experimental thermopower is sharply reduced from 300 μV/K near half-filling to around 0 in the metallic regime. The agreement of the theory and experiment quickly deviates in the metallic regime, where the experimental thermopower remains within a narrow range of $\sim\pm 10$ μV/K in the optimal and overdoped regimes of the metallic phase and with a much prominent temperature dependence. We also caution that in Figure 3, the doping concentrations in the data for $Bi_2Sr_2Ca_{1-x}Y_xCu_2O_{8+y}$ [25] were indirectly determined by the method involving the Hall effect which may be not as reliable as the hole density obtained in LSCO and LBCO compounds.

Note that some modified Heikes formulae have been used [24,25] phenomenologically to fit the magnitude and doping-dependence of the experimental data in the same low doping regime. However, it has long been a puzzling question why the hole bandwidth should be shrunk to an order of magnitude smaller than the temperature scale $\sim$100 K in order to explain the experiment. The self-localization of doped holes in the present theory, on the other hand, naturally explains this. It is particularly interesting to note that the doping-dependent thermopower calculated numerically [27] based on the $t-J$ model has also shown the same qualitative behavior with a comparable magnitude. Furthermore, such thermopower behavior is also related to the anomalous entropy property according to the numerical result [27]. Finally, we would like to point out that the self-localization of the doped holes will break down when the temperature is raised beyond the

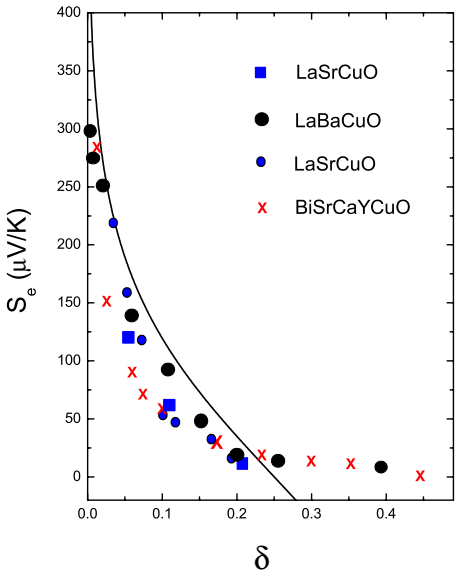

Fig. 3. The thermopower determined by equation (29) as a function of doping concentration (solid curve). Experimental data are from references [24–26] (see text).

"confining" temperature T_{de} where the thermopower behavior of (29) is no longer valid, as to be discussed later.

An another important experimental fact is that S_e has been generally found [28,24,25] to decrease continuously to zero as T is reduced below 100 K . Such a phenomenon can be easily understood in our theory as follows. Since the holes are self-trapped in space, any impurities, no matter how weak, can easily *pin down* them in space at sufficiently low temperatures, truly breaking the translational invariance, and therefore causing the diminishing of the degeneracy (and thus the entropy). The thermopower should then quickly deviate its high-temperature saturation value and vanish as $T \to 0$. In this regime, the Mott VRH will dominate the charge transport, as to be discussed below.

3.2 Resistivity

3.2.1 Mott variable range hopping at low temperature

Experimentally, the cuprate superconductors have universally exhibited the localization of charge carriers at low temperatures, in the low-doping regime of $\delta < 0.05$. The resistivity can be well fit [4–7] by the following Mott VRH formula

$$\rho_M \sim e^{\left(\frac{T_0}{T}\right)^{1/\gamma}} \tag{30}$$

with $\gamma \sim 3-4$ and $T_0 \sim 10^6$ K at $T \to 0$, usually applicable to a doped semiconductor. This implies a strong localization of the doped holes in this regime. But lightly doped cuprates by no means resemble a doped semiconductor. The strong Coulomb interaction makes it a doped Mott insulator, in which the doped holes interact *strongly* with the spin background. As the result, they can be self-trapped at low doping even without any disorder as described before.

So the self-localization of the doped holes in the lightly doped Mott insulator will provide an intrinsic mechanism to explain the localization phenomenon generally observed in the cuprates. Disorder or impurities, on the other hand, should only play a minor role in such a system. As noted above, in the presence of disorder, the spontaneous translational symmetry breaking of the lightly doped Mott insulator (with a lot of degeneracies) can easily become truly translational breaking, as the self-localized holes, without the penalty from the kinetic energy, can be easily pinned down by the impurities. Therefore, the low-doping phase can also be regarded as a strong Anderson localization system at low temperatures, even though the presence of disorder or impurities may not be really strong. In other words, *the impurity effect will get "amplified" by the Mott physics at low doping.*

Recall that a holon has its own bare hopping term, governed by H_h in equation (1), which in the continuum limit reduces to

$$H_h \simeq \int d^2\mathbf{r} \frac{(-i\nabla + \mathbf{A}^s)^2}{2m_h}, \tag{31}$$

with an effective mass $m_h = \frac{1}{2t_h a^2}$ and $\mathbf{A}^s$ as the continuum version of the gauge field A^s_{ij}. So the holon is expected to hop around based on H_h and is bound to the induced antimeron by the attractive potential (16). At low temperature, $\mathbf{A}^s$ may be neglected as spinons are in RVB pairing [15]. Then the Schrödinger equation for a hole-dipole can be written down by

$$-\frac{1}{2m_h}\boldsymbol{\nabla}^2\psi + V\psi = E^h\psi. \tag{32}$$

Define $\psi(\mathbf{r}) \equiv \psi(r,\phi)$. To compute the radial component of the wave function we note that asymptotically at large r the Schrödinger equation reduces to a form whose (radial) solutions can be expressed as

$$\psi(r,\phi) \sim e^{-\sqrt{\ln\frac{r}{a_0}}\frac{r}{a_0}} \tag{33}$$

where $a_0 = \frac{1}{\sqrt{2m_h q^2}} = \sqrt{\frac{t_h}{\pi J_s}}a$.

Then one may estimate the transition probability Γ_{ij} of the holon between any two adjacent antimerons ("impurities"), located at i and j, based on equation (33). It is given by

$$\Gamma_{ij} \sim \exp\left(-\frac{2r_{ij}\sqrt{\ln\frac{r_{ij}}{a_0}}}{a_0} - \frac{\epsilon_{ij}}{T}\right) \tag{34}$$

where r_{ij} is the distance and ϵ_{ij} is the on-site energy difference between two "impurity" sites. Except for the factor $\sqrt{\ln\frac{r_{ij}}{a_0}}$, this formula is essentially the same as in the original Mott theory. As the temperature is lowered, the motion between neighboring sites becomes more difficult due to the lack of appropriate energy differences. Consequently, it is more likely for the carriers to hop to a more distant site if this means that the energy difference is less.

It is known [29–31] as the Mott VRH. Except for a logarithmic correction, the resistivity for the 2D Mott VRH can be determined according to equation (34) by the following expression

$$\rho(T) \sim e^{\left(\frac{T_0}{T}\right)^{1/3}\sqrt{\frac{1}{3}\ln\frac{T_0}{T}}} \tag{35}$$

where T_0 is a characteristic temperature given by $T_0 = \frac{13.8}{D_0 a_0^2}$. Here D_0 is the energy density of the impurity states, which is assumed to be constant in the VRH regime.

It has been well known that once the anisotropic 3D is considered, the exponent γ in the Mott VRH conductivity generally will be changed from 3 to 4, with a modified T_0[32]. Furthermore, the interacting effect between the holons, given by $V_{12} = -\pi\tilde{J}_s \ln\frac{|\mathbf{r}_1-\mathbf{r}_2|}{a}$, has been ignored here, which can also modify the exponent in the VRH theory.

3.2.2 Crossover to deconfinement at high-temperature

The "deconfining" temperature $T_{\rm de}$ will represent a characteristic temperature beyond which holons are deconfined from the antimerons. Once the holons are unbound from their antimeron partners and move freely at $T > T_{\rm de}$, their transport will be solely governed by the hopping term of the phase-string model (31). Here the interaction between holons and antimerons becomes irrelevant as $V \to 0$ in the above RG analysis. Instead we must consider the contribution from the gauge fluctuations of $\mathbf{A}^s$ in equation (31), which will play an essential role for scattering at high temperatures.

Note that $\mathbf{A}^s$ satisfies the following condition:

$$\oint_C d\mathbf{r}\cdot\mathbf{A}^s = \pm\pi\sum_{l\in\Sigma_C}\left(n^b_{l\uparrow}-n^b_{l\downarrow}\right) \equiv \Phi_C. \tag{36}$$

We can estimate the strength of the fluctuations of $\mathbf{A}^s$ by defining

$$\varpi = \sqrt{\langle\Delta\Phi^2_\square\rangle}, \tag{37}$$

where $\Phi_\square$ denotes the flux per plaquette:

$$\Phi_\square = \pm 2\pi\frac{1}{4}\sum_\square S^z_l \tag{38}$$

according to equation (36). At very high-temperature limit, one may neglect the NN spin-spin correlations such that

$$\begin{aligned}\varpi &\sim 2\pi\sqrt{\langle(S^z_l)^2\rangle}\\ &= \pi\sqrt{1-\delta}\sim\pi,\end{aligned} \tag{39}$$

which implies very strong flux fluctuations per plaquette in the high-T limit.

As a matter of fact, if the fluctuations of $\mathbf{A}^s$ is treated in the quasistatic limit with an annealed average over static flux distributions in equation (31), the transport properties are the same as those studied in reference [33]. In particular, the scattering rate has been found [33]

$$\frac{1}{\tau} \simeq 2k_{\rm B}T,$$

if $\varpi > \pi/2$, which is satisfied in our case according to equation (39) in the high-T limit. Corresponding, the resistivity is

$$\rho \sim T \qquad \text{at } T \gg 1. \tag{40}$$

Namely, the charge transport in high-T "deconfining phase" will generally follow a strange-metal behavior due to the scattering between the holons and gauge field $\mathbf{A}^s$ in equation (31).

In the crossover from the low-T VRH behavior (35) to the high-T linear temperature behavior (40), one expects to see a minimal resistivity $\rho_{\rm min}$. We point out that generally the "deconfining temperature" $T_{\rm de}$ does not necessarily coincide with the characteristic temperature of $\rho_{\rm min}$. The latter may occur at a lower temperature as the fluctuations in $\mathbf{A}^s$ can already become important when the Néel temperature T_N is approached from below. In the above discussion of the VRH resistivity, such a scattering effect has been neglected at low-T, which should lead to the enhancement of the resistivity once it becomes important. Another possibility is that the holon induced antimerons may start to move with the increase of temperature, resembling the "flux-flow" in a superconducting phase, which also may lead to a qualitative change of the resistivity. These possibilities in the intermediate temperature regime are beyond the scope of the present work.

3.3 Dielectric constant

Another interesting prediction of the self-localization of doped holes is the existence of a *large* and *doping-dependent dielectric constant* as each hole is a dipolar object of a bound state of a holon and a localized antimeron. One thus expects that the dielectric constant increases linearly with doping initially and finally diverges as the deconfining point is approached with increasing doping concentration.

The dielectric constant defined in the RG analysis in Section 2.3 can be written by $\kappa(l) = X(l)\beta q^2/2\pi$. We can determine $\kappa = \kappa(l=\infty) = X(l=\infty)\beta q^2/2\pi$ by equation (24) numerically (taking $\kappa(l=0)=1$). Figure 4 and the inset show the results for $\kappa - 1$ at $T = 0.1\frac{q^2}{2\pi}$ and $T = \frac{q^2}{2\pi}$, respectively. At half-filling, $\kappa = 1$, as no contribution from the hole-dipoles. We see that with the increase of the hole concentration, the dielectric constant grows linearly with δ at first, then deviates the linearity shown by the dashed line, indicating the increase of the dipole size. Eventually it diverges at a critical doping concentration $\delta_{\rm de} = \delta_{\rm de}(T)$, beyond which the dipoles will collapse and free holons will be released.

The general trend of the calculated in-plane dielectric constant, shown in Figure 4, qualitatively agrees [34] with the experimental measurements [5,6] in the low-doping

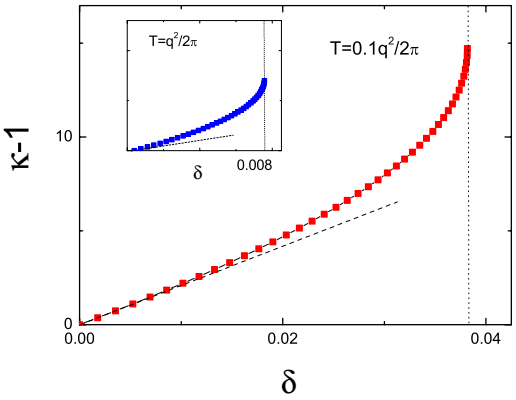

Fig. 4. The dielectric constant κ as a function of doping calculated at different temperatures. $\kappa = 1$ at half-filling, and the dashed lines indicate the linear dependence of the doping concentration. In the main panel, κ diverges at $\delta_{\rm de} = 0.038$ and in the inset $\delta_{\rm de} = 0.008$.

cuprates. Indeed, for the lightly-doped cuprates, a large, doping-dependent dielectric constant has been observed in the *ab*-plane, which increases with the hole concentration δ, initially linearly then becoming divergent at some higher concentrations [5,6]. In contrast, the out-plane (*c*-axis) dielectric constant shows no essential change as a function of δ.

In a doped-semiconductor picture, a dielectric constant contributed by the doped holes can only be significant when the holes are bound to impurities, which is in the localized regime at low temperature. But such a dielectric constant should be usually anisotropic 3D-like rather than pure 2D-like as the experiment revealed. Especially it is difficult to explain why the dielectric constant should diverge in the *ab*-plane while remains constant in the c-axis. Furthermore, if the majority of the holes remains bound to impurities, it is hard to reconcile with the large *saturated* thermopower observed at $T \gtrsim 100$ K.

In contrast, the dipolar structure of the doped holes in the present framework can naturally lead to a *large* dielectric constant *in the ab-plane*, no matter whether the hole-dipoles are pinned down by impurities or not, as long as the hole dipole composites remain stable. The hole dipoles are presumably de-pinned from impurities at $T \gtrsim 100$ K in our theory, since a large thermopower has been seen in experiment. With further increasing temperature, the dipolar structure will eventually collapse and the holon will become *deconfined* from its antimeron partner. Consequently the large dielectric constant and thermopower should be both quickly reduced above $T_{\rm de}$, where the resistivity also starts to behave like a strange-metal as T becomes sufficiently high.

4 Conclusions

In this paper, we studied the motion of doped holes in a spin ordered background at low doping. Based on the phase-string model, we demonstrated that the holes will get self-localized in space, leading to spontaneous translational symmetry breaking without the presence of disorder or impurities.

This novel property is an important consequence of the Mott insulator at low doping, described by the phase-string model as the low-energy effective description of the $t-J$ Hamiltonian. The doping effect and the interplay between charge and spin degrees of freedom are characterized by a unique gauge structure with a mutual duality. At low doping, the spinon condensation forces a "confinement" on the holons, making the latter self-localized and resulting in an insulator with AFLRO or spin glass. This is in contrast to the higher-doping phase, where the holon condensation forces a "confinement" on the spinon part, resulting in a superconducting phase coherence [17].

We found strong experimental implications based on the self-localization of holes. Large and doping-dependent thermopower can naturally explain the experimental data which had been very hard to understand by conventional theories. A large and doping-dependent in-plane dielectric constant indicates a composite structure of the holes and provides a unique explanation of the experimental observations, which otherwise are very difficult to comprehend. Furthermore, the low-T VRH resistivity observed experimentally was interpreted as the direct consequence of the self-localization with disorders playing a minor role, which explains why the critical doping of the delocalization in the cuprates is universally around $\delta_c \sim 0.05$ at $T = 0$, not very sensitive to the density of disorders in the samples. The phase-string model also naturally shows how the resistivity evolves into a strange-metallic linear-T behavior at sufficiently high temperatures above the delocalization temperature. Most importantly, we wish to emphasize that all these peculiar experimental properties were shown to be explained consistently within a single theoretical framework.

It should be noted that many results in this paper are correct only for a homogeneous phase. There may exist another possibility, namely, the stripe instability [10] in the phase string model, which can result in an inhomogeneous phase. Since holes are self-localized, their kinetic energies are suppressed such that the potential energy will become predominant. The dipole-dipole interaction might cause stripe instability at low temperatures, with hole-dipoles collapsing into a one-dimensional line-up (stripe) [10]. The pinning effect of disorders may stabilize the homogeneous phase at low-T, so does the long-range Coulomb interaction. But it would be very interesting to incorporate the inhomogeneous tendency in various dynamic properties at low doping in future investigations.

Finally we comment on the problem of a single-hole doped into the half-filling antiferromagnetic ground state, which has been extensively studied based on the finite-size exact diagonalization as well as the self-consistent Born approximation, both of which suggesting a finite quaiparticle spectral weight [35–37]. However, the phase string effect shows [11] that the spectral weight must be vanishing if the hole is mobile. In fact, the doped hole is always localized by the phase string effect as discussed in reference [8]. This discrepancy with the aforementioned numerical results has been attributed [8] to the fact the localization lengths are usually relatively larger than the sample size

(in order to properly determine such a localization length, the kinetic energy of the hole must be considered). In the present approach for the dilute but finite density of holes, the effect of screening on the potential energy has been taken into account by the RG method. But the kinetic energy of doped holes is not included since they are confined to the immobile merons, whose effect may affect the critical value of x_c and $T_{\rm de}$, but not the qualitative behavior of the holon confinement at low doping.

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