What is the role of strong hole-lattice interaction in the hole-doped cuprate superconductivity?

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Abstract. We first present our molecular orbital cluster calculation results that indicate the presence of strong interaction between doped holes and the underlying lattice in the cuprate. It is also indicated that the naive Zhang-Rice singlet picture for the local electronic state needs to be revised: the doped hole is mainly concentrated in a single bridging oxygen, and the bridging oxygen p orbital and two nearby copper $d_{x^2-y^2}$ orbitals form a valence bond type bonding; this state is stabilized by local lattice distortions and the doped hole becomes a small polaron.

Next, we consider the current generation mechanism compatible with the above small polaron formation; actually, we present a new current generation mechanism that is effective even if all the doped holes become self-trapped small polarons. The current generation here reverses a long-standing belief that at half-filling the effective Hamiltonian for the $U \gg t$ Hubbard model is the Heisenberg model, thus, possible low energy excitations are those include spin degrees of freedom only. The new current generation mechanism yields the Fermi arc seen in the ARPES simulation; it also suggests that the phase of the superconductivity order parameter in underdoped cuprates arises without Cooper pair formation; i.e., the London current formula with effective charge $2e$ is realized without the Cooper pair formation.

The electric current here is generated by a fictitious magnetic field induced by spin vortices: because the presence of spin vortices causes a sign ambiguity of wave functions for electron hoping motion, a phase factor that ensures the single-valuedness of the wave function appears; and this phase factor gives rise to a vector potential for the fictitious magnetic field. The strong hole-lattice interaction stabilizes spin vortices by pinning each center at a polaron occupied site; thus, it will also stabilize the spin vortex induced current. Based on the new current generation mechanism, possibility of an artificial superconducting nano wire is presented. It is made in the Cu-O plane, and consists of pining centers of nonmagnetic atoms arranged in two parallel lines; here the nonmagnetic atoms play the role of lattice small polarons; and the region between the two arrays of vortex centers is a superconducting wire where a thermodynamically stable current flows.

1. Introduction
It is undeniable that strong interaction between doped holes and the underlying lattice exists in cuprates; abundant examples have been reported and some of them are presented in this symposium.

When the strong hole-lattice interaction in hole-doped curates is mentioned, the most often asked question is, “Is it the one responsible for Cooper pair formation?”. In the present work, however, we ask a different question: “Does it play any role in the appearance of the phase of the superconductivity order parameter?” , where the phase of the superconductivity order parameter
is the phase variable appears in the London current formula,

\[ J_{\text{London}} = C \left( \nabla \chi - \frac{2e}{c} A_{\text{em}} \right), \]  

(1)

where \( A_{\text{em}} \) is the vector potential; \( \chi \) is the phase of the superconductivity order parameter, which is multivalued with \( \chi \) and \( \chi + 2\pi \) being physically equivalent; it also satisfies the condition that the combination \( \nabla \chi - \frac{2e}{c} A_{\text{em}} \) is gauge invariant. It is well-known that the existence of thermodynamically stable \( \nabla \chi \) is enough for the persistent current generation and the occurrence of the Meissner effect [1]. The flux quantization in units \( ch/2e \) is derived from it; by considering the time dependence of \( \chi \), the ac Josephson effect with frequency \( 2eV/h \) (\( V \) is the applied voltage) is obtained. Therefore, in principle, even if Cooper pairs do not exit, superconductivity is realized if such a phase exists. In the standard theory, the phase \( \chi \) is believed to appear upon Cooper pair formation, thus, the above two questions are equivalent. However, when considering the superconductivity in underdoped cuprates they are better to be considered different. In the present work, we argue that \( \chi \) arises without the Cooper pair formation in underdoped cuprates [2].

A peculiar point of the cuprate is that in spite of the small lattice polaron formation, a significant electric conductivity is observed. The existing theory cannot explain this peculiarity; however, a new current generation mechanism we have recently constructed may be able to do it [3]. We will present this new mechanism in this work. Remarkably, this new mechanism gives rise to the London current formula in Eq. (1) without Cooper pairs, where the phase \( \chi \) arises as a Berry phase induced by spin vortices [3].

If spin vortices are thermodynamically stable, the phase \( \chi \) is also thermodynamically stable; then, the current generated by spin vortices become a persistent current. In this respect, the strong hole-lattice interaction stabilizes spin vortices by pinning each core at a small polaron occupied site, and contributes to the generation of a persistent current.

In the following, we first present our theoretical result for the local lattice instability induced by the hole doping [4]; it provides a renewed view for the naive Zhang-Rice singlet state of the hole-doped local electronic state [5]. Actually, the lattice instability induced by the hole doping is significant; thus, the doped hole becomes self-trapped small polaron. The hopping probability of the small polaron is very small; the observed electric current cannot be explained by the polaron hopping; thus, it is necessary to construct a new current generation mechanism. In Section 3, we present a novel current generation mechanism that is effective even if doped holes become small polarons, and argue that the current expression in Eq. (1) is obtained from it. In Section 4 we conclude this work by proposing an artificial superconducting nano wire which utilizes the present new current generation mechanism.

### 2. Local lattice instability induced by hole-doping

In this section, we present our theoretical result on the local lattice instability brought about by hole-doping. In order to calculate the local electronic state we employ the molecular orbital cluster calculation. In this method part of a solid called “cluster” is embedded in a model potential that mimics the crystal environment; the electronic state of the embedded cluster is calculated using the quantum chemical molecular orbital method. One advantage of this method is that strong-electron correlation can be handled, systematically. However, the cluster size is not large enough; thus, the results are not converged bulk values; the accuracy of them has to be checked through the comparison with experimental values.

We have performed multiconfiguration molecular orbital calculation on the \((\text{Cu}_2\text{O}_11)_{18}^−\) and \((\text{Cu}_2\text{O}_11)_{17}^−\) clusters in \(\text{La}_{2−x}\text{Ba}_x\text{CuO}_4\), where the former is the parent undoped cluster and the latter is the one-hole-doped cluster. The details of the calculation are found in Ref. [4].
Figure 1. Potential energies for a local lattice deformation of \((\text{Cu}_2\text{O}_{11})^{18-}\) and \((\text{Cu}_2\text{O}_{11})^{17-}\). The deformation is the anti-phase combination of the breathing motion around the two Cu atoms, and labeled by R2. For unit R2 deformation, oxygen atoms move 1 (a.u.) in the directions indicated by the arrows. (a) Potential energy of R2 deformation for \((\text{Cu}_2\text{O}_{11})^{18-}\); solid, dashed, and dotted lines are used for the singlet ground, triplet ground, and singlet first excited states, respectively. (b) Potential energy of R2 deformation for \((\text{Cu}_2\text{O}_{11})^{17-}\); solid and dashed lines are used for the doublet ground and first excited states, respectively.

In Fig. 1, potential energy curves for the deformation R2 (definition is depicted in Fig. 1(a)) are shown. The parent cluster does not show any lattice instability, but the hole doped cluster does. The ground state potential minimum is at R2=0.14 and the stabilization energy by the deformation is 0.21 eV. This is close to a peak value observed in the photoinduced absorption spectra [6]; thus, present results support the argument that the peak is the evidence that doped holes become small polarons.

Cu-O bond length fluctuations in \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) \((x = 0.15)\) are measured by the EXAFS experiment [7]; the peaks of the short and long Cu-O lengths in the CuO2 plane are around 1.87Å and 1.96Å, respectively. These values are comparable with those for R2=0.14 deformation in which the short and long Cu-O lengths are 1.82Å and 1.96Å, respectively. Also the peaks of the short and long apical Cu-O lengths observed in the experiment are around 2.29Å and 2.43Å, respectively, which are close to the R2=0.14 values, 2.34Å and 2.49Å, respectively. The agreement between the calculated and experimental results strongly suggests that the doped holes become small polarons.

The energy difference between the ground and first excited states in the parent cluster is about 1.6 eV, which is close to the energy gap observed in the optical absorption measurement in undoped cuprates [8]; this energy gap was assigned to the charge transfer gap, and the present result supports this assignment. The excitation energy from the ground state to the first excited state in the hole doped cluster is 0.97 eV at R2=0.14; this energy is close to the peak value in the energy loss function observed in the optical measurement of \(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4\) [8].

Overall, the above mentioned agreements between the present calculations and the experimental results indicate that the present cluster calculation is a reasonably good one.

Let us investigate the local electronic state by examining the natural orbitals, \(\{\chi_{i\sigma}\}\), which diagonalize the spin-specified first-order reduced density matrix as

\[
\rho_{\sigma}(x,x') = \sum_{i,\sigma} n_{i\sigma} \chi_{i\sigma}(x)\chi_{i\sigma}^*(x'),
\]

where \(n_{i\sigma}\) is the occupation number for the natural orbital \(\chi_{i\sigma}\).

In Table 1, occupation numbers and main characteristics of active natural orbitals are tabulated, and in Fig. 2 some of them are plotted. In the undeformed cluster, two holes reside...
Table 1. Main characteristics, and spin-up and spin-down electron occupation numbers of natural orbitals for the (Cu₂O₁₁)¹⁷⁻ cluster. Results for active natural orbitals of the ground states with no deformation and R₂=0.14 are tabulated. Natural orbitals for up and down spin are different for each orbital number but very similar.

| Orb. | Main characteristics | Up (Down) | Main characteristics | Up (Down) |
|------|----------------------|-----------|----------------------|-----------|
| 80   | Cu A 3dₓ²−ᵧ²; O(1b) 2px | 0.92 (0.80) | Cu(b) 3dₓ²−ᵧ²O(1b) 2px | 0.95 (0.95) |
| 82   | Cu S 3dₓ²−ᵧ²; O(1b) 2s  | 0.88 (0.12) | Cu(a) 3dₓ²−ᵧ² | 1.00 (0.00) |
| 83   | Cu A 3dₓ²−ᵧ²; O(1b) 2px | 0.20 (0.08) | Cu(b)3dₓ²−ᵧ²O(1b,2b) 2px | 0.06 (0.06) |

Figure 2. Contour plots of natural orbitals for the ground state with no deformation and R₂=0.14 of the (Cu₂O₁₁)¹⁷⁻ cluster in the CuO plane. (a) the 80th down-spin orbital; (b) the 82nd down-spin orbital; (c) the down-spin 83rd orbital; (d) the 83rd up-spin orbital (doped hole orbital) for the ground state with R₂=0.14.

in the three orbitals tabulated in Table 1, in which the 80th and 83rd are oxygen rich orbitals and the 82nd is a copper orbital. It can be deduced that one of the holes is in the 82nd orbital and the other is in the combination of the 80th and 83rd orbitals. The fractional occupation numbers in Table 1 indicate that two holes are in a highly-correlated electronic state constructed by these three orbitals. This electronic state seems to have the valence bond character assumed by Zhang and Rice [5] and explains the photoemission measurement result that the doped hole is mainly in oxygen orbitals [9]. However, this state is unstable against lattice deformation; the photo-created hole will eventually become a lattice small polaron. The doped hole containing orbital in the deformed cluster is plotted in Fig. 2(d); it is a linear combination of Cu(b) 3dₓ²−ᵧ² and in-plane oxygen p orbitals surrounding it; this hole containing orbital is a single molecular orbital in contrast to the valence-bond-electronic state assumed in the Zhang Rice singlet state.

3. A new electric current generation mechanism in doped Mott insulators
The result in the previous section indicates that doped holes in cuprates become self-trapped small polarons. Then, they are not good charge carriers for electric current, especially at low temperatures. In this situation, existing theories cannot explain the observed electric
conductivity and superconductivity. We have recently presented a new electric current generation mechanism that works in this situation. In this section, we briefly explain it; the details are found in Ref. [3].

A standard model for Mott insulators is the $U \gg t$ Hubbard model given by

$$H = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_j c_{j\uparrow}^\dagger c_{j\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow}.$$  (3)

In order to take into account the effect of small polaron formation in this model, we consider the extreme case, i.e., we consider the case where all the doped holes become immobile self-trapped small polarons. In this case the small polaron effect is incorporated simply by eliminating hole occupied sites from accessible electron hopping sites. Then, the system is effectively half-filled even after the hole-dpoint; we only consider this situation in the following.

The first step toward the construction of the new current generation mechanism is to include the itineracy of electrons brought about by the destruction of the antiferromagnetic order. For this purpose, we define new annihilation operators $a_j$ and $b_j$ (and creation operators $a_j^\dagger$ and $b_j^\dagger$); they are defined as

$$(a_j \ b_j) = e^{i \frac{\xi_j}{2}} \begin{pmatrix} e^{i \frac{\xi_j}{2} \cos \frac{\theta_j}{2}} & e^{-i \frac{\xi_j}{2} \sin \frac{\theta_j}{2}} \\ -e^{i \frac{\xi_j}{2} \sin \frac{\theta_j}{2}} & e^{-i \frac{\xi_j}{2} \cos \frac{\theta_j}{2}} \end{pmatrix} \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix},$$  (4)

where the angles $\xi_j$ and $\theta_j$ are azimuth and polar angles of the spin direction at the $j$th site.

Note that a phase factor $e^{i \frac{\xi_j}{2}}$ is added in Eq. (4) so that the transformation matrix is single-valued; without it, sign ambiguity occurs with respect to the phase shift $\xi_j \rightarrow \xi_j + 2\pi$ although $\xi_j$ and $\xi_j + 2\pi$ are physically equivalent. The added phase factor $e^{i \frac{\xi_j}{2}}$ compensates the sign change of $e^{i \frac{\xi_j}{2}}$ by its sign change $e^{i \frac{\chi_j+\pi}{2}} = -e^{i \frac{\chi_j}{2}}$. An example for $\chi$ is $\chi = \xi$ but many other choices are possible. A similar phase factor is known to appear in the context of the Berry phase effect [10]. The inclusion of this phase factor is the crucial point for the current generation; as is shown later, it gives rise to the vector potential for a fictitious magnetic field; this filed acts as the effective magnetic field for electron hopping motion, and generates current.

Using the new operators, the electron hopping term in Eq. (3) becomes $K_a + K_b + K_{ab}$, where $K_a$, $K_b$, and $K_{ab}$ are, respectively, given by

$$K_a = - \sum_{k,j} t_{kj} e^{i (\chi_k - \chi_j)} \left(e^{i \frac{\xi_k - \xi_j}{2} \cos \frac{\theta_k}{2} \cos \frac{\theta_j}{2}} + e^{-i \frac{\xi_k - \xi_j}{2} \sin \frac{\theta_k}{2} \sin \frac{\theta_j}{2}}\right) a_k^\dagger a_j,$$  (5)

$$K_b = - \sum_{k,j} t_{kj} e^{i (\chi_k - \chi_j)} \left(e^{i \frac{\xi_k - \xi_j}{2} \sin \frac{\theta_k}{2} \sin \frac{\theta_j}{2}} + e^{-i \frac{\xi_k - \xi_j}{2} \cos \frac{\theta_k}{2} \cos \frac{\theta_j}{2}}\right) b_k^\dagger b_j,$$  (6)

$$K_{ab} = \sum_{k,j} t_{kj} e^{i (\chi_k - \chi_j)} \left(e^{i \frac{\xi_k - \xi_j}{2} \cos \frac{\theta_k}{2} \cos \frac{\theta_j}{2}} - e^{-i \frac{\xi_k - \xi_j}{2} \sin \frac{\theta_k}{2} \sin \frac{\theta_j}{2}}\right) a_k^\dagger b_j + \sum_{k,j} t_{kj} e^{i (\chi_k - \chi_j)} \left(e^{i \frac{\xi_k - \xi_j}{2} \sin \frac{\theta_k}{2} \sin \frac{\theta_j}{2}} - e^{-i \frac{\xi_k - \xi_j}{2} \cos \frac{\theta_k}{2} \cos \frac{\theta_j}{2}}\right) b_k^\dagger a_j.$$  (7)

The optimal spin arrangement is the antiferromagnetic one given by conditions:

$$\xi_i - \xi_j = \pi, \quad \theta_i + \theta_j = \pi, \quad i \text{ and } j \text{ are nearest neighbors.}$$  (8)

We retain the latter condition in Eq. (8); $\theta$ is so chosen that it maximizes the amplitude of the matrix elements for $K_a$ and $K_b$, which leads to $\theta = \frac{\pi}{2}$ for all sites. Taking the $z$-axis normal to
the CuO plane, this means the polarization of spin is confined in the CuO plane; this is actually, what is seen in the parent compound of the cuprate.

Substituting $\theta = \frac{\pi}{2}$, the hopping terms are rewritten as

$$K_a = -\sum_{k,j} t_{kj} e^{\frac{i\pi(\chi_{k-k})}{2}} a_k^\dagger a_j, \quad K_b = -\sum_{k,j} t_{kj} e^{\frac{i\pi(\chi_{k-k})}{2}} \cos \frac{\xi_k - \xi_j}{2} b_k^\dagger b_j,$$

$$K_{ab} = i\sum_{k,j} t_{kj} e^{\frac{i\pi(\chi_{k-k})}{2}} \sin \frac{\xi_k - \xi_j}{2} (a_k^\dagger b_j + b_k^\dagger a_j).$$  

Then, it is seen that if the antiferromagnetic order is destroyed, i.e. $\xi_j - \xi_j \neq \pi$, the hopping matrix elements for $K_a$ and $K_b$ are not all zero; in this case, electrons in these bands become itinerant to some extent. From now on, we call the “$K_a$ band” the lower band, and “$K_b$ band” the upper band.

The zeroth order Hamiltonian we employ is given by

$$H_0 = K_b + H_U, \quad H_U = U \sum_j e_j^\dagger c_j c_j^\dagger c_j^\dagger e_j^\dagger = U \sum_j a_j^\dagger b_j^\dagger b_j.$$  

Usually, $H_U$ is taken as the zeroth order Hamiltonian, but $K_b$ is added to the present zeroth order Hamiltonian. Since $K_b$ can be rewritten using the “Bloch state” creation and annihilation operators denoted by $\hat{b}_a^\dagger$ and $\hat{b}_a$, respectively, as

$$K_b = \sum_a \epsilon_a \hat{b}_a^\dagger \hat{b}_a; \quad \hat{b}_a = \sum_j U_{a,j} b_j,$$  

inclusion of $K_b$ means that the electron itineracy in the upper band is taken into account in the zeroth order.

Let us consider the promotion of electrons from the lower to the upper band by the perturbation $K_{ab}$. If $K_b$ is not included in the zeroth order, the second order perturbation gives only the antiferromagnetic spin exchange interaction. However, if $K_b$ is included, itineracy of electrons are also included by the same perturbation. The energy cost for the retrieval of local electron itineracy is in the order of $t^2/U$, in the same order as the local destruction of the antiferromagnetic order.

Actually, it can be shown that if $\nabla \chi$ is not zero, electric current flow occurs thanks to the itineracy of electrons in the upper band [3]. Note that this reverses a long-standing belief that at half-filling the effective Hamiltonian for the $U \gg t$ Hubbard model is the Heisenberg model, thus, possible low energy excitations are those include spin degrees of freedom only. Although the Heisenberg model correctly describes excitation energies, the mapping from the Hubbard model to the Heisenberg one is incomplete; the latter fails to take into account the spreading of wave functions through the itinerant upper band which is possible in the former.

After a suitable approximation, it can be shown that the $x$ component of the current density at the $l$th site is given by

$$j(l)_x[A_{em}] \approx \sum_{n, \alpha, (k, k') = (l, l \pm x)} t_{nk'} \sin \frac{\xi_k - \xi_j}{2} \sin \frac{\xi_{n-k} - \xi_{k'}}{2} |U_{n\alpha}^\dagger U_{a\alpha}| \cos \beta_{kn} \sin \left(\frac{\chi_{k-k'}}{2} - \frac{q}{2}\right) A_{kn}$$

$$U + \epsilon_{\alpha}$$

where the only nearest neighbor hopping is taken into account (i.e., $t_{nk'}$ is $t$ if $n$ and $k'$ are nearest neighbor sites; zero otherwise); and $A_{kn}$ is given by

$$A_{kn} = \int_n^k A_{em} \cdot r,$$
Figure 3. (Color online) Plots of spin texture and current distribution for an effectively half-filled state of the $U \gg t$ Hubbard model (the second nearest neighbor hopping is also included). Calculations are performed for a two dimensional $16 \times 16$ square lattice with open boundary conditions. Parameters used are $U = 8t$ and $t' = -0.2t$. The number of doped holes is 8; half of them are centers of merons and the rest are centers of antimerons. (a) Plot for spin configuration. Centers of spin vortices are indicated as “M” for meron (winding number $+1$ spin vortex) and “A” for antimeron (winding number $-1$ spin vortex), respectively. (b) Plot for current density $\mathbf{j}$ (short black arrows) and $\mathbf{\nabla} \chi$ (long orange arrows). “M” and “A” here indicate centers of counterclockwise and clockwise loop currents, respectively.

where $\mathbf{A}_{\text{em}}$ is the vector potential, and $\beta_{kn}^a$ is the phase of $U_{na}^{-1}U_{ak} = |U_{na}^{-1}U_{ak}| e^{i \beta_{kn}^a}$. Note that it can be shown that $\left( \frac{A_{kn}}{2} - \frac{\xi_j}{c} A_{kn} \right)$ is gauge invariant, thus, $j(l)_x$ is also gauge invariant [3].

The current generation explained here is most likely to be realized as a collection of loop currents since the energy cost for the destruction of the antiferromagnetic order is minimized by the collective creation of spin vortices with total winding number zero [11]. Actually, the minimal energy spin vortex excitation is a creation of a nearby meron-antimeron pair [11], where “meron” is a spin vortex with winding number $+1$, and “antimeron” is that with winding number $-1$.

The collection of loop currents generated by spin vortices are expected to be fairly stable, since spin vortices are characterized by integral topological numbers (winding numbers); if each center of a spin vortex is located at a hole occupied site, an additional stabilization will be obtained due to the pinning of the spin vortices. It will also contribute to the reduction of the spin vortex creation energy because it decreases the core energy by increasing the core size.

Let us examine the current generated by spin vortices, and calculate the ARPES spectra. We use the following mean field Hamiltonian for this purpose:

$$\hat{H} = K_a + K_b + K_{ab} + \hat{H}_U; \quad \hat{H}_U = U \sum_j \left( \langle a_j^\dagger a_j \rangle b_j^\dagger b_j + \langle b_j^\dagger b_j \rangle a_j^\dagger a_j - \langle a_j^\dagger a_j \rangle \langle b_j^\dagger b_j \rangle \right). \quad (15)$$

In the $U \gg t$ limit, it can be shown that the ARPES spectrum calculated using the above Hamiltonian agrees with that calculated by degenerate perturbation theory in the effectively half-filled case.

For $\xi_j$ in the hopping terms, we choose the following:

$$\xi_j = \pi(j_x + j_y) + \sum_M W(j, M) - \sum_A W(j, A) \quad (16)$$
where the function $W(j, M)$ is given by

$$W(j, M) = \tan^{-1} \frac{j_x-M_x}{j_y-M_y};$$  \hspace{1cm} (17)

$j, M,$ and $A$ indicate two dimensional coordinates for the $j$th site, center of meron, and center of antimeron, respectively; they are expressed using their components as $j = (j_x, j_y)$, $M = (M_x, M_y)$, and $A = (A_x, A_y)$, respectively.

$\chi_j$ is chosen as follow:

$$\chi_j = \xi_j - 2\sum_{M'} W(j, M') - 2\sum_{A'} W(j, A').$$  \hspace{1cm} (18)

Usually, a site with a meron center creates a counterclockwise loop current (winding number +1 loop current) due to the phase $W(j, M)$ in $\xi$ (see Eq. (16)). If the same site is also included in the sum over $M'$ in $\chi$, clockwise loop current (winding number −1 loop current) arises, instead, due to the phase $W(j, M) - 2W(j, M) = -W(j, M)$; namely, the term with sum over $M'$ in Eq. (18) reverses the current direction from that is expected from the $\chi = \xi$ choice. The term with the sum over $A'$ in Eq. (18) does the same thing for antimeron centers.

In Fig. 3, an example of a collection of loop currents generated by spin vortices is displayed. Loop currents arise around spin vortices. It is also seen that the current density is almost proportional to $\nabla\chi$. Actually, it can be demonstrated that the current density is given by

$$j = C\nabla\chi$$  \hspace{1cm} (19)

in numerical results [3]; this relation is shown to hold to a good accuracy irrespective of the inclusion of the second nearest neighbor hopping matrix element $t'$; it also holds even if different current distributions are chosen by choosing different $\chi$’s in Eq. (18).

Since the term

$$\nabla\chi - \frac{2e}{c} A_{em}$$  \hspace{1cm} (20)

is gauge invariant [3], the relation in Eq. (19) should be considered as the $c^{-1}A_{em} \to 0$ limit of the gauge invariant current density given by

$$j = C \left( \nabla\chi - \frac{2e}{c} A_{em} \right).$$  \hspace{1cm} (21)

This current expression is equivalent to the one in Eq. (1). It is remarkable that it is obtained without mentioning Cooper pairs.

In Fig. 4, an example of the simulation of the ARPES spectrum is shown. It exhibits the Fermi arc-like feature. It can be shown that this feature is related to the existence of an extended current flow region. In such a region, the hopping matrix elements are nonzero due to the destruction of the antiferromagnetic order; thus, wave functions spread over the lattice to some extent, and give rise to the Fermi-arc feature. Note that this feature is obtained without the itinerary of the doped holes.

Now we present an spin vortex arrangement that may lead to a macroscopic current; it consists of linear arrays of spin vortices as is shown in Fig. 5. In Fig. 5(b), the current distribution that exhibits a river-like current flow region is displayed. In this figure, the current produced by the spin vortices has a correspondence with a magnetic field produced in a solenoid: the current between the lines of vortex centers in the figure corresponds to a magnetic field inside the solenoid, and each loop current center marked “M” or “A” in the figure corresponds to a section of a wire that carries electric current. It is suggested from this figure that a macroscopic current may be created if the current flow through an macroscopic region; in order that this is possible, the spin vortices that generate the current must be thermodynamically stable.
Figure 4. The same as Fig. 3, but with a different spin configuration and a different current distribution. The number of holes are 32 of which 8 are centers of spin vortices. (a) Plot for spin configuration. (b) Plot for ARPRS profile. It is calculated using the orbitals obtained by the self-consistent diagonalization of $\bar{H}$ in Eq. (15) to $\bar{H} = \sum_s \varepsilon_s \bar{d}_s \bar{d}_s - U \sum_j \langle a_j^\dagger a_j \rangle \langle b_j^\dagger b_j \rangle$. The intensity is calculated as $\int_{\omega_1}^{\omega_2} d\omega \sum_{s, \sigma} |\langle 0 | \bar{d}_s^\dagger c_{k\sigma} | 0 \rangle|^2 \delta(\omega + \varepsilon_s)$, where $|0\rangle$ is the ground state, and the integration is performed from the energy of the highest occupied level (the 224th level, $\omega_2 = 0.50t$) to that of an arbitrary chosen lower level (the 210th level, $\omega_1 = 0.29t$).

Figure 5. The same as Fig. 3, but with a different spin configuration and a different current distribution. The number of holes are 32 of which 8 are centers of spin vortices. (a) Plot for spin configuration. (b) Plot for current density that exhibits a charge flowing river.

4. Artificial superconducting nano wire
It is remarkable that the phase variable that may serve as the phase of the superconductivity order parameter is obtained without Cooper pair formation. In order that it can produce a persistent current, it has to be thermodynamically stable. For the macroscopic current generation, the macroscopic extension of the parameter $C$ in Eq. (21) must be considered; it should depend on both the stability and amplitude of the current. The stability will depend on the stability of the spin vortex, which is brought about by the strong hole-lattice interaction. The amplitude of the current will be proportional to the number of stable spin vortex centers, thus, will be proportional to the number of doped holes. In order for the current to be a
macroscopic one, the number of spin vortices has to be large enough so that the overlap of the current flow regions around each spin vortices covers the whole sample; therefore, the minimal doping concentration should exist.

The present work suggests that an artificial superconducting nano wire may be constructed by artificially creating centers of spin vortices in cuprates CuO plane, where the centers are arrange in two parallel lines as in Fig. 5. One way to create stable vortex centers at specified points is to replace some of copper atoms by non-magnetic atoms such as Zn. In this way, spin vortices are pinned by the substituted atoms instead of by small polarons. Once an electric current is forced to flow in the region between the two lines of artificially placed non-magnetic atoms, spin vortices will be created due to the condition of “minimal dissipation of current flow”. If the created spin vortices are thermodynamically stable, the generated current is also thermodynamically stable. The stability of spin vortex centers may be increased by the use of non-magnetic atoms. If this is the case, a higher operation temperature of persistent current will be achieved. In this respect, it may be worth noting that the lattice defect is known to increase the superconducting transition temperature for some materials [12].

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