Conducting Electron Strings in Oxides

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Abstract

We investigate a formation of electron strings due to short and long-range electron-phonon and electron-electron interactions. We found that insulating and conducting electron strings may arise in materials with not very wide bands, like HTSC. We estimate the string length and the number of particles self-trapped into a single string taking into account the typical parameters of cuprates, like La_2CuO_4. The conducting strings have typically a small doping ($n < 0.3$) and are created mostly due to the long-range electron-phonon interaction although short-ranged anti-ferromagnetic and electron phonon interactions such as a deformation potential, an interaction with Jahn-Teller deformations and with Holstein optical phonons may play also an important role. Probably such strings play an important role in the creation of stripe phase observed in HTSC.

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There is a growing body of experimental evidences[1–4] and theoretical arguments[5,6] indicating on existence of complex inhomogeneous mesoscopic structures forming from holes and spins in HTSC and other oxides. Such inhomogeneous structures were conventionally ascribed to *a stripe phase*, have been anticipated in theoretical papers[8–12] and have been originally observed in HTSC by Biancone, Thurston, Tranquada, et al[13–18] et al. In the most recent papers the one dimensional character of charge and spin fluctuations[17] and an importance of the lattice distortions in the creation of the mesoscopic stripe structures[3,2] have been clearly demonstrated.

The stripe structure has been also observed in other oxides, manganites[4], where the important role of the lattice effects has been also indicated. All these experiments show that the stripe phenomenon is generic and the lattice deformations may play an important role in the stripe formation and the stripe behavior.

Independently from these experiments, we have recently suggested that the lattice plays an important role in a self-creation of such mesoscopic structures of the stripe phase[5,6]. We have proposed that in materials with narrow bands there may arise a many-particle self-trapping in the form of a long cigar shaped object named as *strings*. The string's phenomen is

a many-particle generalization of a conventional self-trapping effect which usually leads to a formation of fluctuons, deformons, polarons and other single and two particle objects studied very intensively in the past (see, for example, the review[7] and references in). The electron strings may be created both by a long- and by a short-range electron-phonon interaction. In the limit of very narrow bands studied in Refs[5,6] the electron hopping vanishes and strings are insulating defects. On the other hand the observed stripes are highly conducting or superconducting[13–18,3,1].

In the present work we have extended our studies, taking into account the finite bandwidth and treat the kinetic energy of electrons on equal footing with their potential energy. We found that with the increase of the bandwidth when the contribution of electron kinetic energy increases there may arise a new type of strings - *conducting strings*. The appearence of electronic strings may have a strong influence on the low energy physics. Since the creation of strings is related to atomic displacements they may be detected by all sorts of experiments which may detect such displacements. They primarily must include Scanning Tunneling Microscopy (STM) experiments. The X-ray and neutron scattering, photoemission experiments may be also very useful although a mesoscopic size of the strings may create an obstacle. The strong lattice fluctuations, which may be associated with a highly conducting string proposed in the present paper, has been detected by MeV helium ion channeling, an ultrafast real-space probe of atomic displacements[2].

In general such strings may correspond to either a ground state or a metastable state. For a short range electron phonon interaction the strings are mostly insulating and typically correspond to a metastable state. However in a doped antiferromagnet the criterion for the strings formation (for both conducting and insulating) is strongly improved. Both types of strings may arise in a ground state. At the very low doping such conducting strings are probably ordered into a Wigner crystal. The strings forming a Wigner crystal may have no an orientational order. With the increase of the doping the orientational order must definitely arise and the Wigner crystal or an analogous nematic liquid crystal should be seen in the experiments as some kind of mesoscopic superstructures. The stripe phase may correspond to the liquid crystal consisting of these highly conducting electron strings. Depending on the distance between these strings the liquid crystal may also be in two states insulating and conducting. The conducting state arises due to a percolation through these strings. In other words the conducting phase is formed when a conducting percolative path of an infinite length will arise.

However in the present paper we limit ourself by studies of a single highly conducting string. We have employed the Hartree-Fock many body-wave function as a variational wave function to describe fermions self-trapped by a string potential well. Outside the self-trapped potential well the wave function is vanishing reflecting the fact that these electrons are self-trapped. We have performed calculations of the number of particles and the length of the string having a lowest energy per particle for the narrow band materials with short- and long-ranged electron phonon interactions also taking into account finite values of the bandwidth.

We consider the general Hamiltonian of spinless fermions interacting via a strong long-range electron-electron repulsion and with different types of phonons on a $d-$ dimensional hypercubic lattice:

$$H = -t \sum_{<i,j>} a_i^\dagger a_j \quad + \sum_{q,i} \omega(q) n_i [u_i(q) b_q + h.c.] + \sum_q \omega(q) b_q^\dagger b_q + \sum_{i<j} V(i-j) n_i n_j, \tag{1}$$

where t is the electron hopping-integral, the operator $a_i^\dagger(a_i)$ creates (destroys) a fermion at a lattice site i , n_i is the occupation number operator $a_i^+ a_i$ and the operator $b_q^\dagger(b_q)$ is an operator of the creation (destruction) of a phonon. The summations in eq.(1) extend over the lattice sites i and -as indicated by $< i, j >$ -over the associated next nearest sites j. The matrix element of the electron-phonon interaction is equal to

$$u_n(q) = \frac{\gamma(q) \exp(iqn)}{\sqrt{2N}} \tag{2}$$

The function $\gamma(q)$ and the phonon dispersion relation $\omega(q)$ are different for different types of the electron-phonon interaction. For example, for optical longitudinal phonons (Pekar-Frölich interaction[19]) in continuum limit the product $\gamma^2(q)\omega(q) = 4\pi e^2/(\epsilon^* q^2)$ with $1/\epsilon^* = 1/\epsilon_\infty - 1/\epsilon_0$. For the Holstein phonons of the fixed frequency $\hbar\omega_0$ the function $\gamma(q)$ is a $q-$ independent function $\gamma(q) = \gamma$. In general for the short-range electron phonon interaction the $\gamma^2(q)\omega(q) = const = c$. The long-range part of the Coulomb interaction has a conventional type[5]:

$$V(i-j) = \frac{e^2}{\bar{\epsilon} \mid i-j \mid} \tag{3}$$

where it is plausible to assume that for spinless fermions the effective dielectric constant $\bar{\epsilon}$ may be taken as $\bar{\epsilon} = \epsilon_\infty$. Such Hamiltonian, we believe, may correctly describe both the strong electron-electron repulsion and the effect of an electron-phonon interaction which effectively creates an attraction, i.e. two dominant interactions which competition together with a competition of kinetic electron energy leads to a formation of highly conducting electron strings.

The Hartree-Fock many-body wave function of the M self-trapped particles $\Psi(1, 2, ..., M)$ which we employ to calculate an expectation value of the Hamiltonian, eq.(1) has a form of a Slater determinant

$$\Psi(1, 2, ..., M) = \frac{1}{\sqrt{M!}} \det \mid\mid \psi_i(k_j) \mid\mid \tag{4}$$

consisting of single particle wave functions:

$$\psi_n(k_x) = \begin{cases} \frac{1}{\sqrt{N}} \exp(ik_x n_x) & \text{if} \quad 1 \leq \mathrm{n_x} \leq \mathrm{N} \\ \equiv 0, & \text{otherwise} \end{cases} \tag{5}$$

Each of these wave functions describes the electron(hole) trapped by N neighboring sites (string potential well) with equal probability, $1/N$. If string is oriented in the **x** direction and is located on the sites $n_x = 1, ..., N$ the particle quasi-momentum k_x is determined by boundary conditions at the ends of the string. For next simplicity we use periodical boundary conditions. As a first example we consider a short-ranged electron-phonon interaction.

Although for any type of the short-ranged interaction the results obtained are similar, at the first stage we discuss only an interaction with acoustical phonons, i.e. with the lattice deformations. As in Refs[5,6] we employ an adiabatic approximation considering a very slow motion of the lattice(see, for example in Refs[5,6]). With the use of this many body wave function we have estimated an expectation value of Hamiltonian H, eq.(1). These calculations have been done into two steps. Using this many-body wave function, first, we have calculated the one body and the pair correlation functions. Then with the use of adiabatic approximation we have excluded slow (classical) phonon variables to get an expression for adiabatic potential (see, for details, Refs[5,6]) which is a total energy including the Coulomb and exchange energies. The calculated expression of the total energy per particle has the form:

$$\frac{E_S}{M} = 2dt - 2t\frac{\sin \pi n}{\pi n} + 2t\frac{\sin \pi n}{\pi M} - \frac{cn}{2} + 2\epsilon_c n \log M \tag{6}$$

where d is a dimension of the hypercubic lattice, the value n is an electron(hole) doping inside the string: $n = M/N$. For the short range interaction of interest the coupling constant in the Hamiltonian(1) (note that we consider an interaction with acoustical phonons) $\gamma^2(q)\omega(q) = c = D^2/K$ with D is a deformational potential and K is an elastic modulus (see, for example, in Ref.[5]). This estimation of the total energy has been obtained on the basis of an exact solution[5] found in the limit of the very strong coupling $c/t \gg 1$. This expression, eq.(6), represents a variational estimation of the total energy of M particles self-trapped into the string of the length N valid for a wide range of values c/t. Therefore in the framework of the variational approach we may get a reliable estimation of a number of particles, a length and the energy of electron string valid for a wide range of the parameters of the Hamiltonian such as a coupling constant c, the bandwidth t and the characteristic Coulomb energy ϵ_c. Here the values M and n are variational parameters. The optimal number of particles trapped into the string of fixed length N is determined by a minimization of E_S/M with respect to M and it is given by the eq.:

$$M = \frac{2t \sin \pi n}{\epsilon_c \pi n} \tag{7}$$

After the substitution of this expression into the eq.(6) for E_S we get the dependence $E_S = E_S(n)$ on the doping of the string $n = M/N$. Depending on the relation between values t, c and ϵ_c there may exists one or two types of solutions which correspond to two different types of strings: insulating[5], when $n = 1$ and conducting, when $n < 1$. When $c \sim t \gg \epsilon_c$ the string may have a conducting state as a ground state. The small ratio ϵ_c/t may arise when there is a strong screening between carrent carriers. This usually occurs for mobile polarons where we have to put into the effective Coulomb energy ϵ_c (which is effectively a value of an intersite Coulomb repulsion) instead of the high-frequency dielectric constant ϵ_∞ the static dielectric constant ϵ_0[20]. Then the number of particles trapped into the string is described by eq.(7). In the latter case the string state is indeed a ground state, while the polaron states correspond to excited states. When the coupling constant c is very large ($c \gg t$ and $c > \epsilon_c$) the eq. (7) is not applicable, since the associated solution describing a conducting string disappears while the other solution associated with the marginal extremum $n = 1$ and describing insulating strings still exists. Thus, in extreme strong coupling lomit the string

is always insulating with $N = M$ and the number of particles in such a string is defined as (see, for comparison, ref.[5])

$$M = \exp(\frac{c}{2\epsilon_c} - 1) \tag{8}$$

The minimum energy E_S associated with an insulating string which has been calculated with the use of the relation $N = M$, the eq.(8) and the expression for E_S, eq.(6), is simplified to the form(see, for comparion, in the ref.[5]):

$$E_{S-min} = (2dt - \frac{\epsilon_c}{2})M \tag{9}$$

The comparison of eq.(9) and with the energy of M single polarons equal to $M(2dt - c/2)$ indicates that an insulating string with M trapped charged particles may have a lower energy than the total energy of M separated self-trapped particles if $\epsilon_c > c$. That is the insulating string with $M > 1$ (these values of M correspond to the inequality $\epsilon_c < c$, see, eq.(8)) is associated with a metastable minumum. This metastable minimum may become an absolute minimum in the doped antiferromagnet. For a single hole in the antiferromagnet there is an increase in the exchange energy equal to $2dJ$, where J is an exchange constant. For M separated holes this energy increase is equal to $2dMJ$. On the other hand for M holes trapped in a string such increase in exchange energy is equal to $J(2dM - M + 1)$. Therefore, the absolute minimum of the total energy of the deformational string in a doped antiferromagnet is described by the eq.:

$$E_{S-min} = \left[2dt - \frac{\epsilon_c}{2} + (2d-1)J\right] M + J \tag{10}$$

where the value M is defined by eq.(8). The comparison of this expression with the total energy of M separated self-trapped particles indicates that the strings may have a lower energy if the following inequality holds:

$$\epsilon_c \leq c \leq (\epsilon_c + 2J) \tag{11}$$

Thus, the exchange interaction between anti-ferromagnetic spins significantly improves the physical conditions required for a string formation in doped antiferromagnets. Therefore, at low temperatures, if this condition holds the M separated particles will condense into a string configuration.

All these string solutions found for deformational type of strings arise also in the case when the electron is interacting with Jahn-Teller phonons. In this case the electron(hole) Hamiltonian and the Hamiltonian of electron-phonon coupling is very different from the discussed case since there are two symmetry different orbitals which are associated with different hopping integrals and with two competing, symmetry different, deformations (see, a detailed discussion of the Jahn-Teller Hamiltonian in Ref.[21]). In spite on this fact when these orbitals are degenerate the problem of the string formation may be simplified and, after estimation of expectation values for the Jahn-Teller Hamiltonian, can be effectively reduced to the equations presented above, eqs(6,7,8,11) (see, for details in Ref.[22]). That is, for the Jahn-Teller deformations there may arise two type of electron strings, insulating and

highly conducting. For the conducting strings the number of particles self-trapped into a single string is determined with the aid of the equation(7) while for the insulting Jahn Teller string (when $N = M$) the number of particles M self-trapped into the string is determined by eq.(8) with the change of the constant c by

$$c \to \frac{\lambda^2}{c_{11} - c_{12}} \tag{12}$$

where λ is a constant of the Jahn-Teller electron-phonon coupling and c_{11}, c_{12} are conventional elastic modulus for a crystal with a cubic symmetry. In general for, any short-range type of electron-phonon interaction as, for example, with Holstein phonons in Holstein model there may arise the described electron strings. The number of particle in the string is defined by eqs(7, 8) while the string length depends on the type of the string and must be estimated by a minimization $E_S(n)$ with respect to the values n, numerically. For each type of phonons which have a short-range interaction with electrons(holes) the coupling constant in eqs.(7, 8) must be defined, respectively, while the main eqs.(7,8,6) remain the same.

The case when a single electron or a hole is interacting with polar phonons,.i.e with longitudinal optical phonons with the frequency ω_0 is relevant to most of oxides having a considerable ionic bonding and may be considered analogously. In this case the constant of the electron- phonon interaction $\gamma^2(q) = 4\pi e^2/(q^2\epsilon^*\hbar\omega_0)$. We adopt the Pekar formalism[19] to the tight-binding model where all Pekar equations decribing electronic and phonon degrees of freedom must be treated in a form of discrete equations (see, for example in Ref.[6]).

Then the value of total energy including the Coulomb and exchange contributions from the long-range Coulomb forces between fermions may be calculated analogously to the case of short-range electron-phonon interaction presented above (see, also for example, in the Refs[5,6]). That is, first, with the aid of the Hartree-Fock many-body wave function of the M self-trapped particles $\Psi(1, 2, ..., M)$ (see, eq.(4)) we have calculated the pair and off-diagonal correlation functions, and then with the use of these functions the dependence of the total energy on n and M having the form:

$$\frac{E_S}{tM} = 2d + E_c n\,(0.6 + \log(M)) \; - E_p n\,(1.4 - \log(n) + \log(M)) - \\ - \frac{2\;(M-n)\;\sin(\pi\, n)}{M^2 \sin(\frac{\pi n}{M})} \tag{13}$$

where we introduced the notations $E_c = 2\epsilon_c/t$ and $E_p = 2\epsilon_c\alpha/t$ and $\alpha = (1 - \epsilon_\infty/\epsilon_0)$

A minimization of this expression with respect to M and n gives an estimation for the length of the string N and the number of particles M trapped into the string. For the value of M one may get an analityc expression in the form:

$$M = \frac{2\sin(\pi n)}{(E_c - E_p)\pi n} \tag{14}$$

The value of the doping n may be calculated numerically after the next substitution of eq. (14) into eq.(13) and next minimization with respect to only one variable, n. In the limit when the string has a very low density $n \ll 1$ the values of M and N may be presented by analityc formula:

$$M \approx \frac{\epsilon_0 a t}{e^2} \tag{15}$$

$$N \approx M^{1/\alpha} \exp(1.6/\alpha - 1.4) \tag{16}$$

The total energy of the string per electron equals $j_{string} = 2d - 2 + 2/N - nE_c$. To be in a ground state this string energy must be smaller than the energy of an individual polaron j_p equal to $2d - E_p$. The comparison of these two energies gives the precise criterion for the string formation. The conducting string corresponds to the ground state iff

$$E_p < 2 - 2/N + nE_c, \tag{17}$$

which is roughly means that the polaron shift must be smaller than the string bandwidth $2t$.

Thus, we arrive at the conclusion that in oxide compounds having ionic character of the bonding the formation of highly conducting electron strings created by a polarization potential is possible. The string length is typically much larger than the number of self-trapped holes, which is determined by the dielectric constants of the solid.

Our findings are probably relevant to stripe formation observed in HTSC[13–18,1–3] To check if this criterion, eq.(17) is satisfied for the HTSC and to estimate the length of the string we choose the typical parameters of HTSC (for example, for La_2CuO_4, $\epsilon_0 = 30$, $\epsilon_\infty = 5$, the interatomic distance $a = 3.8\mathring{A}$ and the hopping integral $t = 1eV$). Then by a minimization of eq.(13) we obtain that 7 holes will be trapped into the string with the length equal to $N = 40$ interatomic distances or $\sim 150\mathring{A}$. The value of M may be also estimated with the use of eq.(16) which approximately gives the same number. Note that this cigar-shape 7−particle string has a lower energy than 7 separated polarons and this string is highly conducting which is in contrast with an insulating string created by strong short-range electron-phonon interaction[5]. It is probable that in other HTSC undoped materials the size of the strings is not that much different.

Thus, we arrive at the conclusions that in polar oxide materials, like HTSC there may arise electronic strings which are linear multi-particle "electronic molecules". At low temperatures the electron strings may be ordered in CuO planes creating a nematic liquid crystal. The striped phase in HTSC observed in numerous experiments may correspond to such a liquid crystal of strings. It seems that our conclusion about the important contribution of the phonons into the origin of the stripe phase is confirmed in recent experiments which discover a huge influence of isotope effect on the critical temperature of the stripe ordering[3] and strong lattice fluctuations in YBCO[2] which may be associated with the string's dynamics.

The observed stripes may be related to the hole strings arising for a small hole doping. Such strings may well form a Wigner crystal. In the limit of the very small doping the localized strings have no orientational order. It will take very long time to equilibrate to establish the orientational order. With the next increase of the doping, the inter-string interaction increases and at some critical value of doping there arises a transition into a Wigner crystal where there is an orientational order. It is also possible that instead of the transition there will be a crossover to an orientational order. At the next increase of the doping, at the some next critical value, such Wigner crystal is melted and the new phase *a liquid* crystal forming from these conducting strings does arise. With next increase of the hole doping the concentration of these strings increases and they may form either a nematic

or smectic liquid crystal which probably constitutes a stripe phase observed in Refs[13–18,1–3]. Note that in all these transitions or in the crossover arising with the change of the doping the only change occurs is that the change in the distance between the strings while the strings structure (like, a doping or a length)) is not changed. With the isotope changes[3] the structure of individual strings is changed and, therefore, the critical temperature of the stripe ordering must be changed.

In summary, we found that in oxides HTSC there may arise *highly-conducting* electron strings which are linear electronic molecules. Note that to find such molecules we have to treat the kinetic and potential energies of electrons on equal footing. A single electronic molecule has a cigar shape with the length of the order of 10-20 nanometers and consisting of 7-10 holes. For other oxides the string parameters will not be changed as much. It is also very natural that such "polymeric" electron molecules may form a liquid crystal which may be associated with the stripe phase of HTSC[23].

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