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Charge inhomogeneity in strongly correlated systems

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Recent scanning tunneling microscopy (STM) shows significant superconducting gap inhomogeneity in the bismuth–based high–temperature superconductors.[1] Moreover, there is a positive correlation between the magnitude of the superconducting gap and the position of dopant oxygen atoms.[2] It suggests that weakly screened electrostatic potentials of the dopants are responsible for the gap inhomogeneity. On the other hand, despite the presence of strong potentials the observed charge inhomogeneity is less than expected. Carrying out an exact diagonalization of finite systems we demonstrate how strong electron correlations can explain this discrepancy.

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1. Introduction

There is a broad ongoing discussion concerning the mechanism of high temperature superconductivity (HTSC). Despite twenty years of intensive investigations it still remains unclear. According to a commonly accepted view simple models of systems with strong electron correlation include most of the physics of HTSC. Consequently, the t–J or Hubbard models are most frequently used in theoretical investigations of HTSC. On the other hand, there is a community that believes that purely electronic models are insufficient to explain the mechanism of HTSC and, e.g., phonons have to be taken into account. Therefore, it is important to find out which of the experimental results can be explained within the framework of these simple models.

One of the experimental results that recently attracts a significant attention is the intrinsic inhomogeneity found in the bismuth–based high–temperature superconductors.[3] The questions arise whether this phenomenon is common to all the HTSC materials and whether it could say something about the underlying mechanism. This inhomogeneity has been found by many experimental groups with the help the scanning tunneling microscopy (STM). These experiments show a significant spatial modulation of the magnitude of the superconducting gap. The characteristic length of the modulation is of the order of the coherence length and the gap changes from about 25 meV to 75 meV. It has also been shown that there is positive correlation between the magnitude of the gap and the position of the out–of–plane dopant oxygen atoms. Therefore, a straightforward hypothesis has been postulated that the poorly screened electrostatic potential of a dopant repeals electrons from its neighborhood and the change of the concentration of carriers leads to the reduction of the gap.[4] However, the experiments show that the gap is enhanced close to the dopant atoms. At the same time the observed charge inhomogeneity is much smaller than that estimated from the analysis of the dopant's electrostatic potential. It seems that these results say against any simple model based on the purely electronic mechanisms. However, within the resonating–valence–bond mechanism of HTSC it has been shown that there exist a simple qualitatively explanation of the enhancement of the gap close to the dopants.[5] It will be briefly presented below.

However, in order to obtain a quantitative agreement with the experimental results the significant modulation of the gap should be accompanied by only a weak modulation of the charge concentration. The aim of the present paper is to show that strong Coulomb repulsion in a slightly doped Mott insulator strongly reduces the charge inhomogeneity induced by the dopant atoms. Using exact diagonalization approach we investigate how this effect depends on concentration of the dopants, the magnitude and screening of their electrostatic potential as well as on the concentration of the charge carriers.

1.1 Pairing interaction in the presence of dopant atoms

For the sake of completeness we briefly present the mechanism proposed in Ref. [5] that explains inhomogeneity–induced enhancement of the pairing interaction. Assuming that the exchange interaction is responsible for the pairing in the cuprates, we have derived the t–J model staring from the Hubbard one in the presence of diagonal disorder. It is known that in a clean system the virtual hopping between sites i and j leads to a spin–exchange interaction $J_{ij}=4t^2/\Delta E$, where t is the hopping integral and ΔE is the difference between the energy of the initial state with singly occupied sites i and j and the virtual state with empty site i and doubly occupied site j. In the absence of the disorder $\Delta E=U$, where U is the Coulomb interaction. However, diagonal disorder modifies the atomic energy levels ε_i, ΔE is no longer site independent and $J_{ij}=2t^2/\Delta E_{ij}+2t^2/\Delta E_{ji}$, where $\Delta E_{ij}=\varepsilon_i-\varepsilon_j+U$. It can easily be shown that in this case J_{ij} is always *larger* than in the homogeneous system independently of the spatial distribution of the energy levels.

1.2 Fluctuations of the carrier concentration

Within the presented above scenario the superconducting gap inhomogeneity originates from the electrostatic potential of the dopant atoms. This potential, however, affects also the distribution of the electrons in the CuO_2 plane. In particular, the dopants attract holes introduced by the doping, what should lead to a significant increase of their concentration in the dopant's neighborhood. Such a strong charge inhomogeneity has been obtained within a mean–field–type approach. On the other hand, STM experiments indicate relatively weak modulation of the carrier concentration, much smaller than predicted by the mean–field calculations. In the present paper we attribute this discrepancy to the strong electronic correlations in the lightly doped Mott insulator. The idea behind this explanation is as follows: The number of electrons per lattice site in the cuprates is close to one. Since the electrostatic potential of a dopant atom repeals electrons from sites close to the dopant's position, the conservation of the number of electrons results in the increase of the concentration at sites away from the dopant. But the increase of concentration is limited by the strong correlations. In particular, the correlations prevent from exceeding the concentration of one electron per site. As a result, also the decrease of the electron concentration close to the dopants is limited and the charge inhomogeneity is much weaker, than predicted by calculations which do not correctly take into account the strong correlations. In the following section we present a quantitative analysis of this mechanism.

2. Model

We investigate a two dimensional Hubbard model with a diagonal disorder

$$\mathrm{H} = -\mathrm{t}\sum_{\langle \mathrm{i,j}\rangle,\sigma} \mathrm{c}^{+}_{\mathrm{i}\sigma}\mathrm{c}_{\mathrm{j}\sigma} + \mathrm{U}\sum_{\mathrm{i}} \hat{\mathrm{n}}_{\mathrm{i}\uparrow}\hat{\mathrm{n}}_{\mathrm{i}\downarrow} + \sum_{\mathrm{i},\sigma} \varepsilon_{\mathrm{i}}\hat{\mathrm{n}}_{\mathrm{i}\sigma} \quad (1)$$

where $c^{\dagger}_{i\sigma}$ creates an electron with spin σ at site i, $\hat{n}_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$, t is the nearest neighbor hopping integral, and U is the potential of the on–site Coulomb repulsion.

Following the experimental results, we assume that inhomogeneity is induced by the dopant oxygen atoms located approximately one and a half lattice constant above the copper oxygen plane. The impurity potential is screened by the carries that propagate in the CuO_2 plane. Therefore, the effectiveness of the screening should strongly depend on the occupation number. We assume that a single impurity located above the site m shifts the atomic level at site i by

$$V_i(m)=V_0\frac{\exp\left(\frac{-R_{mi}}{\lambda}\right)}{\sqrt{R_{mi}^2+z^2}}. \quad (2)$$

Here, z=1.5a is the distance between the CuO_2 plane and the dopant oxygen atoms, a is the lattice constant and R_{mi} is the distance between the sites i and m. As the value of λ is unknown, it will be considered as a free parameter. We will discuss the results obtained for $\lambda\in(a,\infty)$. In the presence of many impurities the atomic energy levels become

$$\varepsilon_i=\sum_m V_i(m), \quad (3)$$

where the summation runs over all the impurities.

3. Results and discussion

The Hamiltonian (1) has been diagonalized with the help of the Lanczös algorithm. Periodic boundary conditions have been assumed. In the presence of the dopant oxygen atoms $\varepsilon_i\neq$const and the total momentum of the electrons is not conserved.

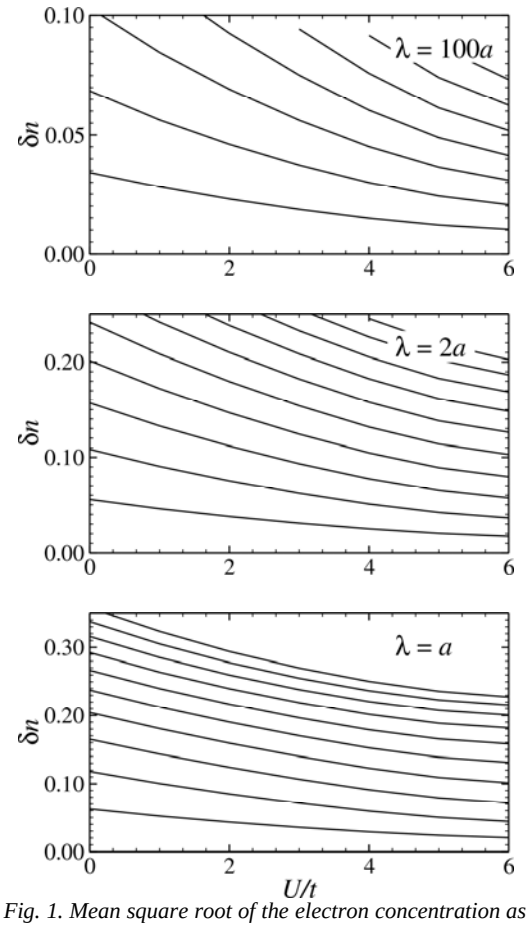

Fig. 1. Mean square root of the electron concentration as a function of the Coulomb interaction for a 12–site cluster with one impurity and 11 electrons. Successive lines, starting from the lowest one correspond to $V_0 = t, 2t, 3t, etc.$ Different panels correspond to different values of the screening length.

The lack of the translational invariance puts limits on the accessible sizes of the clusters. We have carried out numerical calculations for a 12–site cluster with one, two and three impurities and assumed that each dopant atom introduces one hole into the CuO_2 plane.

In order to compare the numerical results with the experimental data we have calculated the mean square root of the electron concentration $\delta n=\sqrt{\frac{1}{N}\sum_i (n_i-\bar{n})^2}$, where $n_i=\langle \hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}\rangle$ and $\bar{n}=\frac{1}{N}\sum_i n_i$.

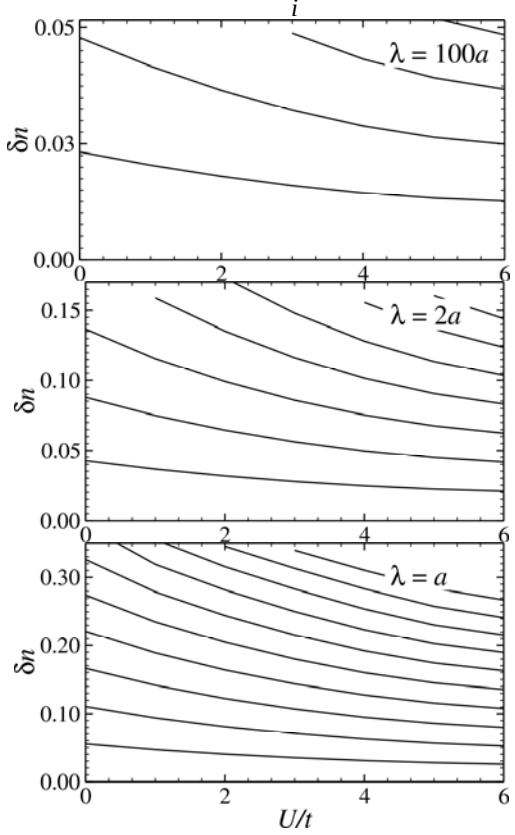

Fig. 2. The same as in Figure 1, but for a cluster with 2 impurities and 10 electrons.

Figs. 1,2, and 3 show δn as a function of the Coulomb potential for one, two and three impurities, respectively. As expected, the electron–electron correlations reduce the charge inhomogeneity. However, the effectiveness of this mechanism depends on the remaining model parameters. Namely, in the absence of the screening ($\lambda\to\infty$), and for a large doping the atomic levels are weakly modulated

As a consequence, the charge inhomogeneity is relatively weak even in the absence of the Coulomb repulsion. Although the electronic correlations lead to a reduction of δn, this reduction does change the physical picture in a sense that the charge inhomogeneity fulfills the experimental requirement $\delta n<0.1$ [2]. However, for a strongly screened impurity potential ($\lambda\sim a$) there is a significant charge inhomogeneity in the uncorrelated systems. In this case Coulomb repulsion strongly reduces δn.

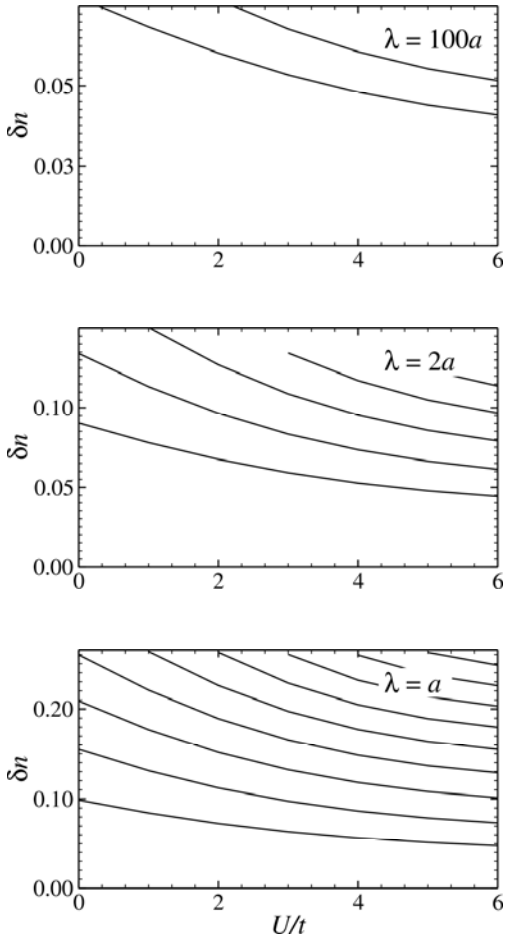

Fig. 3. The same as in Figure 1, but for a cluster with 3 impurities and 9 electrons.

The above results clearly show that strong electronic correlations are responsible for the significant reduction of the impurity–induced charge inhomogeneity. This statement holds true in a wide range of model parameters. In the following we confirm that the underlying physical mechanism is directly related to the vicinity to the Mott–Hubbard insulator. For this sake we relax the assumption that each dopant atom introduces one hole into the copper–oxide plane.

Fig. 4 shows δn as a function of the Coulomb potential for $\lambda=2$ and various concentrations of electrons. In order to compare the influence of the Coulomb potential on density fluctuations for different average electron concentrations, rather than the magnitude of the fluctuations itself, the fluctuations have been scaled, so that they all are the same in the absence of the electronic correlations (δn is unmodified for $n=1$).

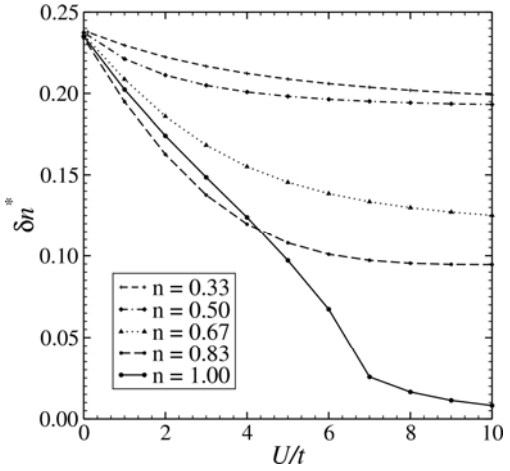

Fig. 4. Renormalized mean square root of the electron concentration as a function of the Coulomb interaction for a 12–site cluster with one impurity of V_0=5t for various electron concentrations. The electron density fluctuations for concentration n≠1 are scaled so that their mean square root for U=0 is equal to that for n=1.

In the case of half–filling, strong Coulomb repulsion prevents from developing of the charge inhomogeneity despite strong impurity potential. Contrary to this case, for low electron concentration, the mean root square of the electron distribution is almost correlation independent. This result clearly supports the proposed concept of the reduced charge inhomogeneity in the doped Mott insulators.

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