The formation and local symmetry breaking of Holstein polaron in t-J model

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Abstract

The polaron formation in t-J like model has been investigated on a 4 by 4 square lattice by using exact diagonalization method. Due to the competitions among magnetic energy, kinetic energy, electron-phonon interaction energy and lattice elastic energy, doped holes can either move freely or stay localized. While holes localize, the lattice distortion may result in the breaking of local symmetry. We further reveal the connections between polaron formation and local symmetry breaking. Since the formation of polaron may suppress antiferromagnetic correlation and even lead to the local ferromagnetic correlation, the localized state of polaron may favor the odd reflection symmetry around both x and y axes. Meanwhile we find that similar features show up in the Sz distribution of states with different reflection symmetry. Finally we make some predictions on the I-V relationship in the future scanning tunnel microscope experiments.

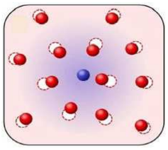
I. Motivation

The role of electron-lattice coupling has gained recent renewed interest. One reason is that the ARPES data in doped metallic cuprates revealed the energy dispersion strongly renormalized by *e*-ph interaction. Besides, the strong *e*-ph interaction is crucial for explanation of renormalization and line shapes of phonons observed in neutron scattering experiments. In addition, the large isotope effect on T_c for underdoped cuprates and on the superfluid density at the optimal doping suggests the vital role of *e*-ph coupling. Here we focus on the symmetry breaking of the ground state wave function by the formation of Holstein polaron in *t-J* like model.

II. Model Hamiltonian

Here we consider the Holstein *t-t'-J* model in adiabatic limit where the kinetic energy of the lattice can be neglected:

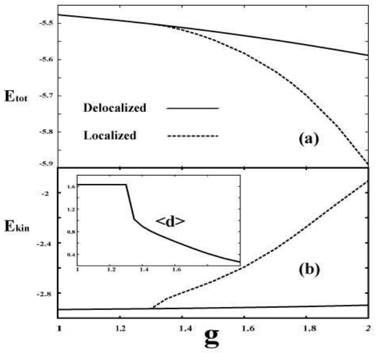
$$H=-t\sum_{\langle i,j\rangle\sigma}(c^+_{i\sigma}c_{j\sigma}+h.c.)-t'\sum_{\langle\langle i,j\rangle\rangle\sigma}(c^+_{i\sigma}c_{j\sigma}+h.c.)+J\sum_{\langle i,j\rangle}S_iS_j-g\sum_i u_i n_i^h+\frac{K}{2}\sum_i u_i^2$$



The first three terms are usual *t-t'-J* model, the fourth term describes the lattice potential proportional to the *e*-ph coupling constant *g*, the last term is the elastic energy with force constant K. In the adiabatic limit, displacement u_i can be treated classically and are determined by $u_i=(g/K)\langle n_i^h\rangle$, as shown in the right. In the following, we consider the *t-t'-J* model relevant to copper-based superconductors and the *t-t'-J-J'* model as a toy model relevant to iron-based superconductors.

III. Condition of polaron formation

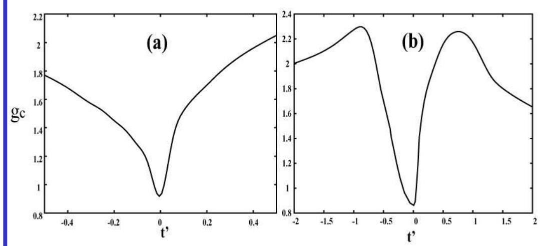
In well-known *t-t'-J* model, magnetic energy and kinetic energy are included. Adding electron-lattice interaction and lattice elastic energy, movement of doped holes is influenced by competition of these energies. The strength of electron-lattice interaction can be characterized by electron-lattice coupling constant *g*.



The lowest energy of delocalized and localized state as a function of *e*-ph coupling *g*.

A transition has been shown clearly for ground state in hole-doped system between delocalized state and localized state.

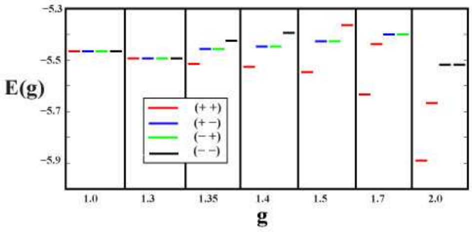
Obviously, g_c goes up with increasing $|t'|$. That is to say, if doped carrier has more kinetic energy, then need more lattice attraction to be localized. The asymmetry between $t'>0$ and $t'<0$ caused by the kind of carrier, hole or electron. It is harder for two electrons, than one hole, to be localized. Therefore the $t'<0$ part for hole-doped cuprates has smaller g_c than $t'>0$ part for electron-doped cuprates.



t-t'-J model. *t-t'-J-J'* model

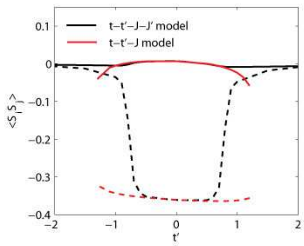
The added J' term bring system frustration to antiferromagnetic order. Holes prefer to stay localized because of J term, however, J' term is on the contrary. Small J' weaken the localization of holes. Big J' would restrict holes again.

IV. Properties of state with polaron formation



Four states occupy lowest energy level with different parity are displayed as a function of *e*-ph coupling *g*.

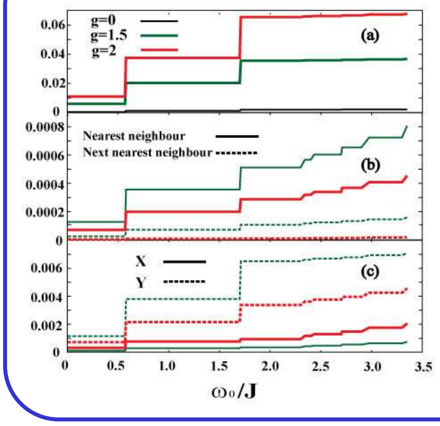
When *g* is quite small, the ground state is the same as that of *t-t'-J* model and it has 4-fold degeneracy. We identify these 4 states by reflection symmetries with respect to *x* and *y* axes, which is denoted as (++), (+-), (-+), (- -), respectively. Figure in the left shows that the strong electron-lattice interaction may lead to strongly localized states as ground state. Its corresponding parity symmetry is (++). However, (+-), (-+), (- -) states are excited states with weak hole localization.



For *t-t'-J* model, small ferromagnetic (FM) correlation appears at where holes gather. Antiferromagnetic (AFM) correlation stays at where no lattice distortion exist. FM correlation would be weaken by increasing kinetic energy *t'*, even AFM correlation caused. From the curves for *t-t'-J-J'* model, there is an apparent transition in spin correlation function at bond between NN site of the location where hole stays and NNN site. That is to say, large *t'* would restrict holes at where surrounded by its NN site.

Spin correlation function of bond connecting where hole localized and its NN site (solid line), NN site and NNN site (dash line) in ground state with polaron formation.

V. Connection with experiment measurement



Integrated differential conductance at holes location (solid line), its NN site (dash line) and its NNN site (dot line) for different e-ph coupling g as a function of the cutoff energy ω.

Local density of state at hole location is much more than that at its NN or NNN site. And the difference of LDOS between hole occupied site and other sites increases as electron-lattice interaction magnifies.

VI. Conclusions

In conclusion, the existence of *e*-ph interaction makes it reasonable to calculate the change on the properties of correlated electron system caused by this interaction. In the correlated electron system, scattering by this interaction results in momentum non-conservation of the whole system. In other words, the local translational symmetry of states has been broken by *e*-ph interaction. And momentum is not a good quantum number to characterize states any longer. So the localized states due to *e*-ph interaction would be denoted by their parity symmetry as a good quantum number. The exploration reveals that at where strong correlated, polaron would suppress AFM correlation and even induce local FM correlation which strengthen the stability of localized state and promote formation of polaron conversely. This affect results in the strong localized state is always with (++) parity symmetry. In the calculation of quantity which can be measured experimentally, rotational symmetry may change while cutoff-voltage scan. Therefore, this kind of symmetry breaking indicates the existence of polaron resulting from *e*-ph interaction. Maybe, in the future, STM and NMR experiment will give some evidences to confirm the existence of localized states due to *e*-ph interaction.

References

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