Binding of holes in two-dimensional lattices with different boundary conditions

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Using exact diagonalization we compute the binding energy of two holes for the t-J model in lattices with different boundary conditions. We find that with periodic, antiperiodic, mixed, and other boundary conditions there is always negative binding energy in a certain range of J, for all the sizes studied. This is different from the behavior obtained in the one-dimensional case, suggesting that binding might survive in the thermodynamic limit in two dimensions.

The possibility of a superconducting state in a single-band model remains a central issue in the theoretical effort to understand high-T_c superconducting materials.[1]

In spite of intensive work over the past two years, it is still not clear whether two holes have a negative binding energy in single-band models of strongly correlated electrons on the square lattice. These models are the Hubbard model, the effective Hamiltonian obtained from it for large Coulomb repulsion, and a simplified version of this effective Hamiltonian called the t-J model.[2] The reason for this is that, due to difficulties in the analytical approaches, one has to resort to numerical work that has been limited to small lattice sizes.

Exact diagonalization studies of the Hubbard model, the full effective Hamiltonian, and the t-J Hamiltonian, performed for lattices up to 16 sizes[3-7] showed the existence of a negative binding energy for a certain interval of J, even in the presence of frustrating second-neighbor interactions.[7]

On the other hand, some earlier Monte Carlo calculations[8] suggested that the two-dimensional Hubbard model does not exhibit superconductivity. In a more recent study[9], using a new Monte Carlo method, a bound state of two holes in the Hubbard model on the 4×4 lattice at half filling was observed.

Since it is quite improbable that one will be able to study numerically much larger lattices in the near future, it has proven useful to study finite-size effects on lattices with different boundary conditions.[10] In particular, there are larger changes in the Fermi surface at different fillings by going from periodic to antiperiodic (or other) boundary conditions in one or both directions in the square lattice. Consequently, there are changes in the magnetic and kinetic energies that are reflected in the binding energy.

The role of different boundary conditions in finite lattices was stressed in a recent work by Fye, Martins, and Scalettar.[11] In this work, the binding energy of two holes is computed for the one-dimensional Hubbard model using the Bethe ansatz equations. By using periodic and antiperiodic boundary conditions, they generate two classes of lattices, depending on their size, which have degenerate or nondegenerate Fermi surfaces at half filling. It is shown that, for lattices with degenerate Fermi surfaces at half filling, the binding energy is negative for some lattice sizes, but the magnitude of this energy is reduced by going to larger lattices and eventually going to zero in the thermodynamic limit. Moreover, they found no binding for chains with no degeneracy at the Fermi level, and again, binding energy goes to zero in the thermodynamic limit. These results strongly suggest that there is no binding in the thermodynamic limit, for all values of U, for the one-dimensional Hubbard model.

In this report, following a suggestion made in Ref. 11, we compute the binding energy for the t-J model in small two-dimensional lattices with different boundary conditions (BC's) using exact diagonalization. Our purpose is to determine if the binding energy has a behavior similar to that observed in the one-dimensional case and, consequently, to determine if the binding found in the square lattice is merely a finite-size effect. In the opposite case, one could expect that the negative binding obtained for small two-dimensional clusters could survive in the thermodynamic limit.

The t-J model is defined by the Hamiltonian

$$H=-\sum_{\langle i,j\rangle,\sigma} t_{ij}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.}) + J\sum_{\langle i,j\rangle}\left[\mathbf{S}_i\cdot\mathbf{S}_j-\frac{n_i n_j}{4}\right], \tag{1}$$

where $\tilde{c}^{\dagger}_{i\sigma}$ is a creation operator of electrons with the constraint of no double occupied sites. $\tilde{c}^{\dagger}_{i\sigma}=(1-n_{i-\sigma})c^{\dagger}_{i\sigma}$, $n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}$, $n_i=n_{i\uparrow}+n_{i\downarrow}$, and S_i are the Heisenberg spin operators. For periodic BC's we put $t_{ij}=t=1$ in all the bonds.

We use a standard Lanczos algorithm[12] to obtain the ground-state energy for each lattice. For the 4×4 and 18-site tilted lattices, we implement translational symmetries to work in a reduced Hilbert space that corresponds to fixed momentum. For the tilted 8- and 10-site lattices, we put $t=-t$ on certain bonds in order to impose antiperiodic BC's in one ("mixed" BC's) or both ("antiperiodic" BC's) translational directions. For the 4×4 lattice, in order to preserve translational invariance while using nonperiodic boundary conditions in a given direction, we take the hopping constant for the bonds in that direction as $t\exp(i\theta/4)$, where $\theta=0$ (periodic), $\pi/2$, and π (antiperiodic).

We will classify the lattices according to their degen-

eracy in the noninteracting limit ($U=0$) as has been done previously for the one-dimensional Anderson model.[18]

Let us consider the tight-binding model obtained from the Hubbard model by taking the Coulomb repulsion $U=0$. In this case, the up and down electrons move around in the lattice independently of each other. At $U=\infty$, or $J=0$ in the t-J Hamiltonian, we obtain again a tight-binding model with the constraint of no double occupancy. In this case, the magnetic ordering becomes a highly nontrivial problem, and, for finite-size lattices, it is strongly dependent on the imposed boundary conditions.[10]

Taking the Hubbard model as the starting point, we consider, as in Ref. 11, two series of lattices, one with a degenerate Fermi surface at half filling, the z component of the total spin S_z equal to zero, and $U=0$, and the other with a degenerate Fermi surface under the same conditions.

For lattices with length side L equal to $(l_x^2+l_y^2)^{1/2}$, where l_x and l_y are integers with l_x+l_y even, the single-particle energies are given by

$$\varepsilon(\mathbf{k})=-2[\cos(k_x-\varphi_x)+\cos(k_y-\varphi_y)] , \tag{2}$$

where

$$\boldsymbol{\varphi}=\frac{\pi}{N}(0,0), \quad \text{periodic BC} ,$$

$$\boldsymbol{\varphi}=\frac{\pi}{N}(l_x,l_y), \quad \text{mixed BC} ,$$

$$\boldsymbol{\varphi}=\frac{\pi}{N}(l_x-l_y,\, l_x+l_y), \quad \text{antiperiodic BC} ,$$

and $N=L^2$ is the number of sites of the cluster. The allowed momenta $\mathbf{k}=(k_x,k_y)$ are given by

$$k_x=\frac{2\pi}{N}(l_x n_x+l_y n_y) ,$$

$$k_y=\frac{2\pi}{N}(-l_y n_x+l_x n_y) .$$

Then, taking into account Eq. (2), in the case of degenerate Fermi surface, we study the following lattices: (i) $\sqrt{8}\times\sqrt{8}$, with periodic BC, (ii) 4×4, with periodic BC, and (iii) 4×4, with antiperiodic BC, while in the series of nondegenerate clusters, we include (i) $\sqrt{10}\times\sqrt{10}$, with periodic BC, (ii) 4×4 with, mixed BC, and (iii) $\sqrt{18}\times\sqrt{18}$, with periodic BC.

TABLE I. Binding energies for the degenerate clusters for the t-J model.

J	$\sqrt{8}\times\sqrt{8}$ Periodic	4×4 Periodic	4×4 Antiperiodic
0.000	3.1010	1.3225	0.6075
0.100	1.7200	−0.1219	0.1006
0.200	0.3385	−0.1693	0.0542
0.400	−0.6828	−0.3481	−0.1897
0.600	−1.1540	−0.5268	−0.4842
0.800	−1.6722	−0.7063	−0.7271
1.000	−2.1803	−0.8873	−0.9587

TABLE II. Binding energies for the nondegenerate clusters for the t-J model.

J	$\sqrt{10}\times\sqrt{10}$ Periodic	4×4 Mixed	$\sqrt{18}\times\sqrt{18}$ Periodic
0.000	2.0000	0.7064	1.3866
0.100	0.3847	−0.0371	0.0178
0.200	−0.5324	−0.1836	−0.1927
0.400	−0.9015	−0.3813	−0.4333
0.600	−1.2114	−0.5540	
0.800	−1.6190	−0.7273	−0.7950
1.000	−2.0661	−1.0000	

The binding energy is defined as usual as

$$\Delta(N_e)=[E(N_e-2)-E(N_e)]-2[E(N_e-1)-E(N_e)] , \tag{3}$$

where $E(N_e)$ is the ground-state energy of the system with N_e electrons. The results for $\Delta(N_e)$ with $N_e=N$ (half filling) for the degenerate series are shown in Table I for various values of J, and for the nondegenerate series in Table II.[14]

We see from Tables I and II that, in all the cases, there are intervals of J where the binding energies take negative values. Moreover, for the 4×4 lattice, we have studied all the possible BC's obtained by taking θ_x, $\theta_y=0$, $\pi/2$, and π, and in all cases we find binding of holes for certain intervals of J

In the t-J model one has to worry about phase separation. To determine this possibility, we compute the binding energy between pairs of holes defined by

$$\Delta_{\text{pair}}(N_e)=[E(N_e-4)-E(N_e)] -2[E(N_e-2)-E(N_e)] . \tag{4}$$

To prevent phase separation, it is necessary that this quantity takes positive values. We found that for the 4×4 lattice with mixed BC's, the binding energy Δ is negative, while the binding of pairs Δ_{pair} is positive for $0.15\lesssim J\lesssim0.6$. This result is similar to that previously found with periodic BC's.

Binding of holes can also be detected through the hole-hole correlation functions, which are defined by

$$C(\mathbf{r})=\frac{1}{N_h}\sum_i \langle(1-n_i)(1-n_{i+r})\rangle , \tag{5}$$

TABLE III. Hole-hole correlation functions for the 4×4 lattice with mixed boundary conditions. The position r is indicated by its coordinates in lattice spacing units.

J	(0.1)	(1.1)	(2.0)	(2.1)	(2.2)
0.0	0.031 862	0.062 800	0.062 795	0.093 138	0.123 212
0.1	0.044 585	0.067 833	0.070 573	0.080 577	0.086 872
0.2	0.051 622	0.070 518	0.072 998	0.073 796	0.070 258
0.4	0.066 289	0.072 979	0.079 384	0.060 165	0.043 503
0.8	0.094 541	0.069 494	0.088 733	0.037 535	0.016 252

TABLE IV. Binding energies for the Hubbard model on the $\sqrt{8}\times\sqrt{8}$ tilted lattice with various boundary conditions.

U	Periodic	Mixed	Antiperiodic
20.0	0.728 287 7	0.659 139 7	0.320 171 6
10.0	0.078 120 8	0.102 623 5	0.256 034 3
5.0	−0.125 909 9	0.003 855 2	0.031 503 5
2.0	−0.065 758 5	−0.020 249 7	−0.028 428 4
0.0	0.000 000 0	0.000 000 0	0.000 000 0

where N_h is the number of holes and n_i is the occupation number of electrons at site i, which gives the probability that there is a hole at site $\mathbf{r}$ given that there is one at the origin.

From Table III we infer that, for mixed BC's those holes that for $J=0$ try to stay as far apart from one another as possible, tend to get closer together as J increases. However, only for $J \gtrsim 0.8$ are the holes predominantly in nearest-neighbors sites, but, as stated before, for these values of J, one surely has phase separation. This behavior of the hole-hole correlation functions is not as clearly consistent with the notion of binding of holes as for periodic BC's.

Finally we present some results for the one-band Hubbard model:

$$H = -\sum_{\langle i,j\rangle,\sigma} (c_{i\sigma}^{\dagger} c_{i\sigma} + \text{H.c.}) + \text{U} \sum_{i} n_{i\uparrow} n_{i\downarrow} , \tag{6}$$

where $c_{i\sigma}^{\dagger}$ are creation operators of electrons. We recall that the t-J model is an approximation of the Hubbard model for large U, with $J = 4t^2/U$.[4,5] One should notice that for the Hubbard model negative binding energies have already been obtained[7] for the $\sqrt{8}\times\sqrt{8}$ and $\sqrt{10}\times\sqrt{10}$ lattices with periodic BC's that correspond to a degenerate Fermi surface and a nondegenerate Fermi surface, respectively. In Table IV, we see that for the $\sqrt{8}\times\sqrt{8}$ lattice with different BC's there are always values of U for which the binding energy is negative.

From these results, we conclude that for the t-J model and, presumably, also for the Hubbard model, there is binding of holes in finite lattices irrespective of the imposed boundary conditions. This behavior is strikingly different from that found for the Hubbard model in one-dimensional clusters, where, for nondegenerate clusters, the binding energy is positive for all lattice sizes. This difference between one- and two-dimensional finite systems lends support to the idea that the binding found in the latter case is not merely an artifact of the finite-size lattices considered, and it could survive in the thermodynamic limit. Of course the behavior of the binding energy versus N is quite nonmonotonic, so we are unable to attempt any extrapolation, and we cannot rule out the possibility of its vanishing in the thermodynamic limit.

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