PHYSICAL REVIEW B VOLUME 42, NUMBER 10 1 OCTOBER 1990

Hole-hole effective interaction in the two-dimensional Hubbard model

G. Fano and F. Ortolani
Dipartimento di Fisica and Sezione di Bologna, Istituto Nazionale di Fisica Nucleare, Universitá di Bologna via Irnerio 46, I-40126 Bologna, Italy

A. Parola
International School for Advanced Studies, Trieste, Italy

(Received 7 May 1990)

We present the first exact results of the ground-state energy in the two-dimensional Hubbard model on a 4×4 cluster for several values of U and fillings. The behavior of the binding energy of two holes as a function of U is discussed together with some analytical results in limiting cases. The analysis of the hole-hole correlation function allows one to determine the range of values of U where binding might be seen.

An open question in the field of strongly correlated electron systems is whether an effective attraction between quasiparticles can be induced by purely repulsive (Coulombic) interactions.[1] This problem has attracted more and more interest since the conjecture that the basic properties of high-temperature superconductors (HTSC) can be understood in terms of interacting electrons in a (rigid) two-dimensional (2D) lattice.[2] One of the simplest and most popular models which embodies such a picture is the Hubbard model (HM) on a square lattice, defined by the Hamiltonian

$$H=-t\sum_{\langle i,j\rangle,\sigma} c_j^{\sigma,\dagger}c_i^{\sigma}+U\sum_i n_i^{\uparrow}n_i^{\downarrow}\,, \tag{1}$$

where t ($t=1$ in the following) represents the nearest-neighbor hopping energy and $U>0$ the on-site Coulomb repulsion. This model has been extensively studied by analytical methods[3] and numerical simulations.[4] Both approaches have shown that the HM is a Mott insulator at half-filling (i.e., one electron per site) with antiferromagnetic ordering induced by the nesting property of the Fermi surface. More controversial is the behavior of the HM in the low-doping regime (i.e., at filling $\nu<1$) which is relevant to HTSC.[2] The main question is whether the holes, injected in the system upon doping, experience an effective attraction mediated by their interaction with the antiferromagnetic background. The tendency of holes to bind in pairs has been studied analytically by approximate methods[3,5] and numerically by exact diagonalization,[6] mainly in the strong-coupling limit of the HM (the so-called t-J model). Specifically, the binding energy Δ of two holes is defined as

$$\Delta=E_2+E_0-2E_1\,, \tag{2}$$

where E_n is the ground-state energy of the system with n holes. In the thermodynamic limit, the ground-state energy per site $E(N,N_s)/N_s$ depends on the number of electrons N and the number of sites N_s only through the filling $\nu=N/N_s$. If we neglect the O(1) finite-size corrections in the total [i.e., $O(N_s)$] energy of the system, we find that

$$\Delta\rightarrow\frac{1}{N_s}\frac{\partial^2(E/N_s)}{\partial\nu^2}\,. \tag{3}$$

Equation (3) would imply that the binding energy always vanishes in the thermodynamic limit and is asymptotically positive, being proportional to the bulk modulus, which is positive due to thermodynamic stability. This is, of course, the case at $U=0$. A finite (negative) value of Δ at infinite volume can only result if the O(1) corrections in the n-hole energies E_n do not cancel *exactly* in Eq. (2). At large volumes, these finite-size terms eventually overwhelm the bulk contributions which scales to zero according to Eq. (3).

In the t-J model, numerical results indicate that Δ is negative in a 4×4 lattice[6] for $J>0.1$. Nevertheless, this result is not conclusive since a finite-size scaling of the binding energy is hampered by the prohibitive difficulty of extending the diagonalization approach to larger systems. Should Δ approach a finite, negative value in the thermodynamic limit, it would imply the presence of an attractive effective interaction between holes. Such an attraction could, in turn, imply either the formation and uniform condensation of Cooper pairs, or else, phase separation between a hole-rich and a hole-deficient region. The Cooper pair regime is believed to occur in the negative U HM,[7] where a real attraction between electrons is present in the system. Conversely, recent speculations[8] suggest that phase separation is present in some region of the phase diagram of the t-J model. While the occurrence of phase separation can be proved rigorously[9] for a sufficiently large value of J/t, no proof is available for the more interesting $J\leq t$ case. Based on small-size energy studies, it has been impossible so far to argue unambiguously for either of these conclusions.

Another independent probe of possible binding between holes is the hole-hole correlation function

$$1+h(R)=\frac{\langle m_0 m_R\rangle}{\mu^2}\,, \tag{4}$$

where $m_R=[1-n^{\uparrow}(R)][1-n^{\downarrow}(R)]$ is the hole density operator, and μ^2 is the uncorrelated value of $\langle m_0 m_R\rangle$ corresponding to the same number of holes, defined by the requirement that $\sum_{R\neq 0}h(R)=0$.

The aim of this Rapid Communication is threefold: (i) to present the first exact results of the binding energy $\Delta(U)$ in the HM on a 4×4 lattice; (ii) to discuss its

asymptotic behavior for larger systems in the two limiting cases $U=0$ and $U=\infty$; and (iii) to compare the physical picture emerging from the study of the binding energy to that coming from the hole-hole correlation function $h(R)$.

Exact diagonalization in small clusters has shown that in the parameter region of the t-J model where binding seems to be present (i.e., where $\Delta<0$) the hole-hole correlation function $h(R)$ is monotonic and positive at short distance,[6] supporting the presence of an effective attraction between holes. However, a previous analysis[10] of the HM in a 4×4 lattice at intermediate coupling ($U=4$) suggests repulsive hole correlations, even if an independent estimate[11] of the binding energy Δ shows attraction. In order to analyze this apparent contradiction in more depth, we have investigated the dependence of Δ on the coupling U by exact diagonalization of the HM on a 4×4 cluster. Since, in weak coupling, the typical magnetic correlation length[3(b)] $\xi=\hbar v_F/E_{\mathrm{SDW}}$ (where v_F is the Fermi velocity and $E_{\mathrm{SDW}}\sim U/2$ is the spin-density-wave gap) decreases roughly as $1/U$, a study of Δ as a function of U may give some information on the size dependence of the binding energy.[12]

Exact diagonalization of the Hamiltonian (1) has been carried out by fully exploiting the symmetries of the lattice,[13] thereby reducing the dimension of the Hilbert space from about 165×10^6 to a few million. Such a reduction of the Hilbert space allows the implementation of the standard Lanczos method on a supercomputer in order to obtain the lowest eigenstate. Independent runs have been carried out in each of the 20 irreducible representations of the symmetry point group[13] of the 4×4 lattice with periodic boundary conditions. In such a way we have identified the representations which provide the lowest energy. A full description of the method, together with an extensive survey of the results will be published elsewhere.

In Table I the ground-state energies of the 4×4 lattice at $\nu=\frac{16}{16}$, $\frac{15}{16}$, and $\frac{14}{16}$ are given for values of U up to $U=50$. At half-filling the ground state is totally symmetric for all U in agreement with a theorem by Lieb.[14] The one-hole state is sixfold degenerate with total momenta $(\pm\pi/2,\pm\pi/2)$, $(0,\pi)$, $(\pi,0)$, respectively, in agreement with previous findings in the t-J model. The two-hole system presents a level crossing of states of different symmetry. For $U<U_0\sim3$ the ground state is sixfold degenerate: A doublet of states of momentum (π,π) and p rotational symmetry, and a quartet of states with momentum $(\pm\pi/2,\pm\pi/2)$. For $U>U_0$ the ground state is threefold degenerate: a state of momentum (0,0) and $d_{x^2-y^2}$ symmetry and a doublet of states with momentum $(0,\pi)$ and $(\pi,0)$. This confirms the results of an independent calculation[10] where an almost degeneracy was found at $U=4$.

TABLE I. Ground-state energy of the Hubbard model in the 4×4 cluster for several values of U and fillings $\nu=\frac{16}{16}$, $\frac{15}{16}$, and $\frac{14}{16}$. The binding energy Δ [see Eq. (2)] is also quoted. The estimated error is, at most, in the last figure.

U	$\frac{16}{16}$	$\frac{15}{16}$	$\frac{14}{16}$	Δ
1	−20.79272	−21.08996	−21.39283	-5.63×10^{-3}
2	−18.01757	−18.58505	−19.17135	-1.88×10^{-2}
3	−15.63666	−16.45364	−17.30003	-2.94×10^{-2}
4	−13.62185	−14.66524	−15.74459	-3.60×10^{-2}
6	−10.55222	−11.96700	−13.42123	-3.94×10^{-2}
8	−8.46887	−10.14724	−11.86883	-4.32×10^{-2}
10	−7.02900	−8.89301	−10.80701	-5.00×10^{-2}
12	−5.99222	−7.99376	−10.05147	-5.62×10^{-2}
16	−4.61186	−6.80729	−9.06557	-6.28×10^{-2}
20	−3.73990	−6.06801	−8.46144	-6.53×10^{-2}
24	−3.14144	−5.56692	−8.05975	-6.73×10^{-2}
28	−2.70618	−5.20647	−7.77669	-6.99×10^{-2}
32	−2.37589	−4.93556	−7.56832	-7.31×10^{-2}
40	−1.90842	−4.55695	−7.28588	-8.04×10^{-2}
50	−1.53078	−4.25663	−7.07718	-9.47×10^{-2}

In Fig. 1 we show the binding energy Δ as a function of U for both the 4×4 lattice (●) and the 2×2 "lattice" (○). These results show that binding of holes is present in both systems. In the 4×4 case, it actually increases with U up to $U=50$. However, at very large U, $\Delta(U)$ changes its sign and, at $U=\infty$, it saturates at the value[6] $\Delta_\infty\sim-1.32$, while $\Delta_\infty=4(2-\sqrt{2})\sim2.34$ for the 2×2 cluster. Comparing our results with previous Monte Carlo calculations on the same system,[11] we find a binding energy at $U=4$ which is three times smaller. Therefore, we conclude that the statistical error was underestimated in Ref. 11.

A distinctive feature of the curves shown in Fig. 1 is the presence of an abrupt change in the trend of $\Delta(U)$ between the "small-coupling regime," where Δ is negative, and the "large-U" region, where Δ quickly becomes large and positive. The characteristic value of U where this transition occurs is strongly dependent on the size of the system. It is tempting to relate this behavior to the early saturation of the one-hole energy towards the value $E_1=-4$ implied by the Nagaoka theorem.[15] A rough estimate of the magnitude of the coupling U above which the one-hole ground state becomes ferromagnetic, shows that it is asymptotically proportional to the number of sites N_s. In fact, a variational bound in the spin-$\frac{1}{2}$ subspace can be obtained by means of the state

$$|\psi\rangle=c_{\mathbf{Q}}^{\dagger}|\psi_H\rangle,$$

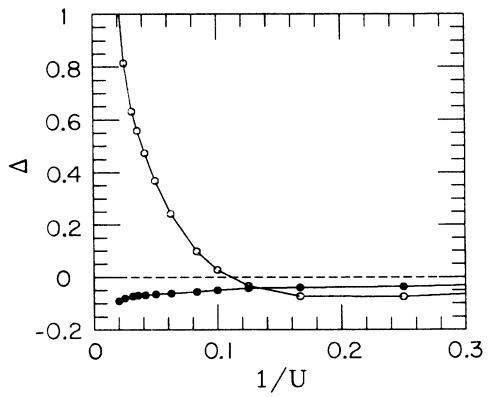

FIG. 1. Binding energy Δ [see Eq. (2)] as a function of $1/U$. The lines are only guides to the eye.

where $|\psi_H\rangle$ is the ground state of the Heisenberg model and $\mathbf{Q}$ is the largest momentum in the Brillouin zone, i.e., (π,π). A straightforward calculation shows that, for sufficiently large systems, the energy of the ferromagnetic state is variationally worse than that of $|\psi\rangle$ for $U < U_c = \alpha N_s$, where α is of order unity. Therefore, the Nagaoka mechanism which dominates the structure of the one-hole ground state in the $U \to \infty$ limit becomes rapidly irrelevant at fixed U for increasing lattice size. At $U=\infty$, where double occupations are strictly forbidden, it is possible to analyze in detail how the binding energy scales with the size of the system. In this limit, from strong coupling expansion, it is known that the ground-state energy at half-filling E_0 vanishes as $1/U$, while the energy of one hole approaches the Nagaoka limit $E_1 = -4$. Let us now evaluate the energy E_2 of two holes for $U=\infty$. Let us consider a spin-polarized state of the kind

$$|\psi_{SF}\rangle = c^{\dagger}_{k_1} c^{\dagger}_{k_2} \prod_k c^{\dagger\uparrow}_k |0\rangle .$$

Choosing k_1 and k_2 at the corner of the Brillouin zone, we have the "spinless fermions" variational bound

$$E_2 \le E_{SF} = -8 + O(1/N_s) .$$

In order to obtain a lower bound, let us write the exact ground state $|\psi_2\rangle$ as a linear superposition of states $|R_1,R_2\rangle$ characterized by the position R_1,R_2 of the two holes: $|\psi_2\rangle = \sum_{R_1,R_2} \phi(R_1,R_2)|R_1,R_2\rangle$. The matrix elements $\langle R_1,R_2|H|R_3,R_4\rangle$ vanish unless the pairs (R_1,R_2) (R_3,R_4) have one coincident site and the others are nearest neighbors. Overestimating all the nonvanishing matrix elements by one, we obtain the matrix elements of a Hamiltonian H_{HCB} describing a system of two hard-core bosons. Hence we can write

$$-E_2 \le \sum_{R_1,R_2,R_3,R_4} |\phi(R_1,R_2)||\phi(R_3,R_4)|\langle R_1,R_2|H_{HCB}|R_3,R_4\rangle \le -E_{HCB} = 8 + O(1/N_s) ,$$

where E_{HCB} is the ground-state energy of H_{HCB}.

In conclusion, we have obtained two bounds ($E_{HCB} \le E_2 \le E_{SF}$) which tend to a common value: $E_{HCB} = E_{SF} = -8$, implying $\Delta \to 0$ at $U=\infty$ for infinite volume. In the case of the 4×4 lattice, the previous inequalities give[16] $-7.57 \le E_2 \le -6$, consistently with the exact result[6] $E_2 = -6.678$. Note that E_2 is strictly larger than the theoretical lower bound, implying that the spin configuration is not able to optimize the phases of the hole hopping. The above analysis shows that the large positive value of Δ at $U=\infty$ in the 4×4 lattice is a finite-size effect which scales to zero for larger systems. Unfortunately, the previous analysis cannot be generalized to finite U where the problem of finite-size corrections is still open.

It is interesting to compare our findings with the results of the exact diagonalization of the ten-site cluster by Ogata and Shiba.[17] The overall behavior of the binding energy as a function of U is quite similar to the one we find, being characterized by a large positive value at $U=\infty$ ($\Delta_\infty = 2$) and a vanishing limit for $U \to 0$. The main difference in $\Delta(U)$ is related to the weak coupling regime where the ten-site cluster shows a *positive* Δ, probably related to the closed-shell nature of the $U=0$ half-filled system. However, also in the ten-site cluster, $\Delta(U)$ attains *negative* (i.e., attractive) values in a range of couplings about $U \sim 10$. Notice that, in moving from the smaller (2×2) to the larger (4×4) systems, the position of the minimum of $\Delta(U)$ shifts towards the strong-coupling limit.

In the regime where the physical properties of the HM are faithfully represented by the t-J Hamiltonian, a simple argument suggests the formation of domains around the hole where the antiferromagnetism is frustrated,[8] e.g., a Nagaoka ferromagnetic polaron. The size ξ of these domains can be estimated by minimizing the sum of the magnetic energy due to frustration ($\sim \xi^2/U$) and the kinetic energy due to confinement ($\sim 1/\xi^2$). The resulting size ξ is of the order of $U^{1/4}$. Therefore, we expect that finite-size effect are relevant both in the weak-coupling regime (where $\xi \sim 1/U$) and in strong coupling (where $\xi \sim U^{1/4}$), in agreement with our previous analysis of these two limits.

In Fig. 2 we plot the hole-hole correlations $h(R)$ as a function of the distance for the ground state of the two-hole system at different values of the interaction U. Since $h(\mathbf{R})$ is not necessarily isotropic, we take an "angular"

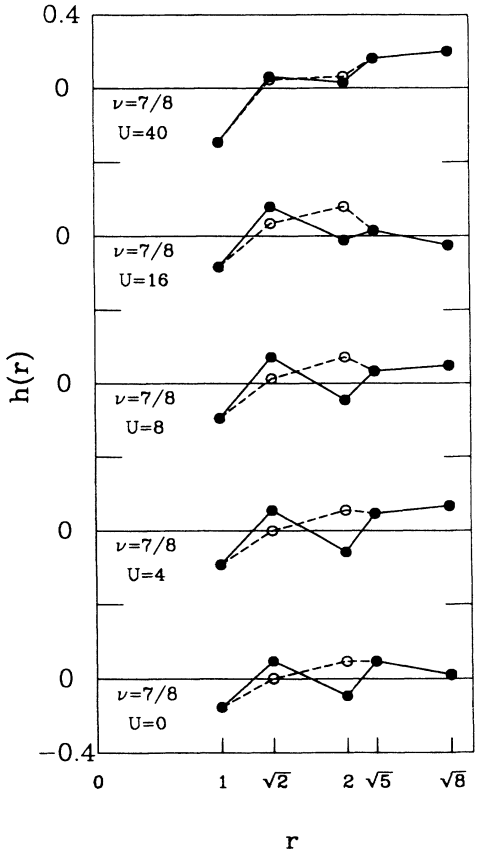

FIG. 2. Hole-hole correlations [see Eq. (4)] in the ground state of the HM at $\nu = \frac{14}{16}$. The solid line refers to the state of zero momentum, while the dashed line corresponds to the state of momentum $(\pi,0)$.

average over all sites with the same distance $|\mathbf{R}|$. In Fig. 2 the correlations in the state of total momentum (0,0) are shown (solid line) together with those of the states of momenta $(0,\pi)$ and $(\pi,0)$ (dashed line). This is the ground state only for $U > U_0 \sim 3$.

From these data we notice the presence of a repulsive core around the hole for every U. This is not the case of the t-J model where, for $J > 0.1$, a nearest-neighbor attractive correlation has been found.[6] The repulsive core is likely to be of kinematic origin, being present also in the free electron limit. At large coupling ($U = 40$) the behavior of $h(R)$ suggests repulsion between holes, notwithstanding that the binding energy at the same U is negative ($\Delta \sim -0.08$) and relatively large. In this regime, however, the calculation of the antiferromagnetic order parameter shows that antiferromagnetism is considerably frustrated by the presence of the holes suggesting that the whole 4×4 cluster has to be identified with a single bag. At intermediate coupling ($U = 8$–16) the hole-hole correlations in Fig. 2 show some attractive feature at next-nearest-neighbor distance. This is, in fact, the most promising range of couplings for the occurrence of binding, as previously discussed. In the weak-coupling limit the correlation function still shows a hump at next-nearest-neighbor distance. Note, however, that a similar trend can be found also in the "uncorrelated" $U = 0$ case, suggesting that the positiveness of the correlation function is not a direct consequence of an effective attractive interaction between holes.

In conclusion, we have reported the first exact data on two different probes of binding between holes in the HM. Although our results show some evidence in favor of an effective attraction, one should keep in mind that finite-size effects can be relevant in a small lattice. The most favorable range of the coupling constant for the occurrence of binding seems to be $U \sim 16$–20. Further analysis of this region would be quite valuable for a clarification of this issue. A proper finite-size scaling based on accurate Monte Carlo data on larger lattices would definitively indicate whether the binding we find is a genuine effect which persists in the thermodynamic limit.

The authors are greatly indebted to Professor E. Tosatti for enlightening discussions. One of us (A.P.) acknowledges support from the International School for Advanced Studies (Trieste, Italy) Centro di Calcolo Interuniversitario dell'Italia Nord-Orientale collaborative project.

[1] J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985).

[2] See, for instance, *Proceedings of the Adriatico Conference Towards the Theoretical Understanding of the Mechanisms of High T_c Superconductors,* edited by G. Baskaran, S. Lundqvist, E. Tosatti, M. P. Tosi, and Yu Lu (World Scientific, Singapore, 1988).

[3] (a) N. E. Bikers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **62**, 961, (1989); (b) J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11 633 (1989).

[4] S. R. White *et al.*, Phys. Rev. B **40**, 506 (1989); S. Sorella *et al.*, in *Proceedings of the Adriatico Conference Towards the Theoretical Understanding of the Mechanisms of High T_c Superconductors* (Ref. 2).

[5] See, for instance, *Proceedings of the Conference on Dynamics of Spin Fluctuations in High Temperature Superconductors,* edited by G. Reiter, NATO Advanced Study Institutes (Plenum, New York, to be published).

[6] J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B **39**, 7074 (1989); Y. Hasegawa and D. Poilblanc (unpublished); E. Dagotto, J. R. Schrieffer, A. Moreo, and T. Barnes (unpublished).

[7] R. T. Scalettar *et al.*, Phys. Rev. Lett. **62**, 1407 (1989).

[8] V. J. Emery, S. A. Kivelson, and Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).

[9] S. Sorella (private communication).

[10] A. Parola *et al.* (unpublished).

[11] E. Dagotto, A. Moreo, R. L. Sugar, and D. Touissant, Phys. Rev. B **41**, 811 (1990).

[12] One of us (A.P.) thanks Professor R. Schrieffer for a discussion on this point.

[13] G. Fano, F. Ortolani, and F. Semeria, Int. J. Mod. Phys. B **3**, 1845 (1989); G. Fano, F. Ortolani, and A. Parola (unpublished).

[14] H. E. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[15] Y. Nagaoka, Phys. Rev. **147**, 392 (1966); Y. Fang, A. Ruckenstein, E. Dagotto, and S. Schmitt-Rink, Phys. Rev. B **40**, 7406 (1990).

[16] A. Parola *et al.*, in *Proceedings of the Conference on Dynamics of Spin Fluctuations in High Temperature Superconductors* (Ref. 5).

[17] M. Ogata and H. Shiba, J. Phys. Soc. Jpn. (to be published).