PHYSICAL REVIEW B VOLUME 42, NUMBER 10 1 OCTOBER 1990

Binding of holes in one-dimensional Hubbard chains

R. M. Fye and M. J. Martins*
Department of Physics, University of California, Santa Barbara, California 93106

R. T. Scalettar
Department of Physics, University of California, Davis, California 95616

(Received 5 July 1990)

Using the Bethe ansatz, we calculate the binding energies of two holes just off half-filling in one-dimensional Hubbard chains. Somewhat surprisingly, we find binding comparable to that seen in two-dimensional systems in chains that have a degeneracy at the Fermi level in the noninteracting ($U=0$) limit. The binding initially *increases* with lattice size before beginning a slow decay to zero in the thermodynamic limit. We discuss the general implications of our results for binding energy and other numerical calculations of high-T_c models.

I. INTRODUCTION

A variety of studies has recently been made of the ground-state binding energy of two holes in various high-T_c models in order to determine whether the models might exhibit superconductivity. This binding energy is calculated using the formula

$$\Delta=[E(M-2)-E(M)]-2[E(M-1)-E(M)]\,, \qquad (1)$$

where $E(M)$ is the ground-state energy of the system studied for M electrons.

A negative Δ implies that the energy of two interacting holes is lower than that of two noninteracting holes; qualitatively, a net attraction is presumed to occur between holes leading to the observed "binding." Though this binding does not by itself guarantee the existence of superconductivity,[1] it is suggestive.

Such binding, or existence of a negative Δ, has been seen in two-dimensional CuO_2 clusters,[2,3] Hubbard[4,5] and extended Hubbard[6] models, and t-J models.[4,7-9] However, the calculations have all been limited to a small number of unit cells; the largest studied, to our knowledge, have been 4×4 Hubbard[5] and t-J (Refs. 4, 8, and 9) lattices. These systems are still sufficiently small that finite-size effects could play an important role, and it appears unlikely that calculations on high-T_c models can be performed on significantly larger lattices in the near future. Thus, it is of great interest to explore the general effect of finite system size on the calculation of binding energies.

In order to investigate this question, we have used the Bethe ansatz equations[10] to calculate binding energies Δ for the *one*-dimensional Hubbard model just off half-filling. The advantage of this technique is that we can get essentially exact results for very large systems, allowing us to understand the finite-size behavior in more detail than could be done otherwise.

In Sec. II, we discuss the model and our procedure. Section III contains our results. We close in Sec. IV with a summary and a discussion of the implications of these results for general binding energy and other calculations of high-T_c models.

II. MODEL AND PROCEDURE

The Hamiltonian which we consider is the one-dimensional Hubbard Hamiltonian on a closed chain of N sites,

$$H=(-t)\sum_{\sigma,j=1}^{N-1}(c_{j,\sigma}^{\dagger}c_{j+1,\sigma}+\text{H.c.})+(-t)\sum_{\sigma}(e^{i\theta}c_{N,\sigma}^{\dagger}c_{1,\sigma}+\text{H.c.})+U\sum_{j=1}^{N}n_{j\uparrow}n_{j\downarrow}\,. \qquad (2)$$

The first and second terms in the Hamiltonian "hop" electrons of the same spin σ between neighboring sites on a scale t set by the overlap of the on-site wave functions; the third term expresses the Coulomb repulsion U between two electrons of opposite spin at the same site. Different choices of θ reflect different boundary conditions. We will set $t=1$, giving a bandwidth of 4.

We consider periodic boundary conditions [$\theta=0$ in Eq. (2)] and antiperiodic boundary conditions ($\theta=\pi$). Chains of length $N=4j$ with periodic boundary conditions and chains of length $N=4j+2$ with antiperiodic boundary conditions have a degeneracy at the Fermi level in the noninteracting ($U=0$) limit in the half-filled case (total number of electrons $M=N$); we call such chains "degenerate" chains. Chains of length $N=4j$ with antiperiodic boundary conditions and chains of length $N=4j+2$ with periodic boundary conditions have no such degeneracy; we call such chains "nondegenerate" chains. We show this difference in Fig. 1 for $N=8$.

To calculate the binding energy $\Delta(N)$ for a chain of N sites just off half-filling, we solve the Bethe ansatz equations to obtain the ground-state energy of the half-filled case, and then the ground-state energies after one and two holes are introduced. $\Delta(N)$ is subsequently determined from Eq. (1).

For the Bethe ansatz prescription for Hubbard chains with general boundary conditions, including the two considered in this paper, we refer the interested reader to Refs. 11 and 12. To check that our procedure was working correctly, we made extensive comparisons with exact

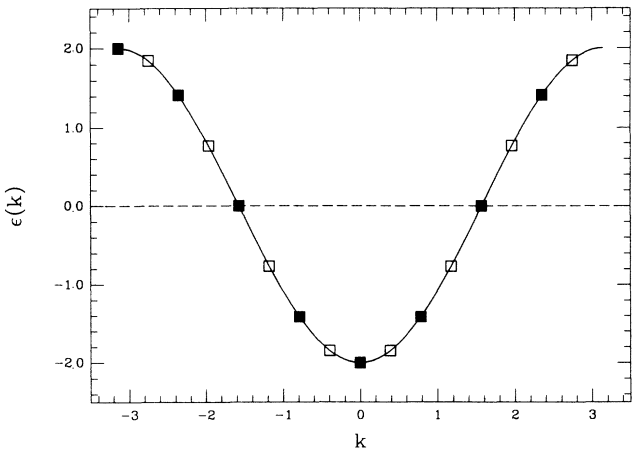

FIG. 1. Single-particle energies $\epsilon(k)$ vs k for $t=1$ and $U=0$. Solid line: $N=\infty$; solid squares: $N=8$, periodic boundary conditions; open squares: $N=8$, antiperiodic boundary conditions. Note degeneracy at the Fermi level [$\epsilon(k)=0$] for periodic boundary conditions.

diagonalization and Lanczös results for systems of 2, 4, 6, 8, and 10 sites.

III. RESULTS

In Fig. 2, we show the binding energy $\Delta(N)$ vs N with $t=1$ and $U=4$ for nondegenerate chains (top) and degenerate chains (bottom). We note the existence of binding (negative Δ) in the degenerate chains but not in the nondegenerate ones.

Treating first the nondegenerate case, we observe the decay of (positive) $\Delta(N)$ to zero in the thermodynamic limit. This decay is expected,[4] as two repulsive holes can move infinitely far apart in an infinite system. All values of U studied, from $U=\frac{1}{4}$ to $U=32$, showed nondegenerate binding behavior qualitatively similar to that shown for $U=4$. On that basis, we conjecture that binding *never* occurs in nondegenerate chains for any U or N.

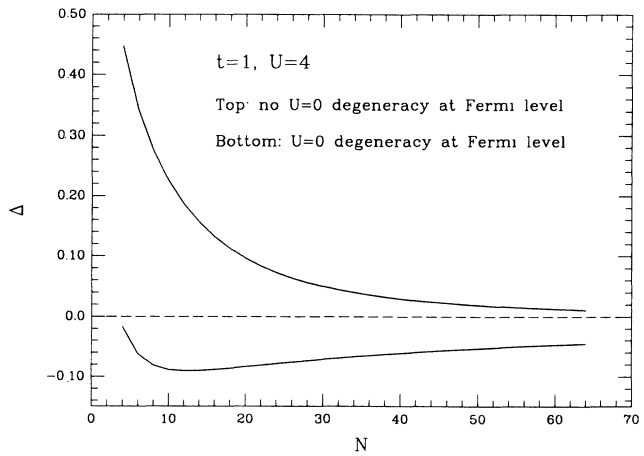

FIG. 2. Binding energy Δ vs lattice size N for $t=1$ and $U=4$. Top: nondegenerate lattices. Bottom: degenerate lattices. Note initial increase of binding-energy magnitude with N in degenerate sequence, followed by slow decay.

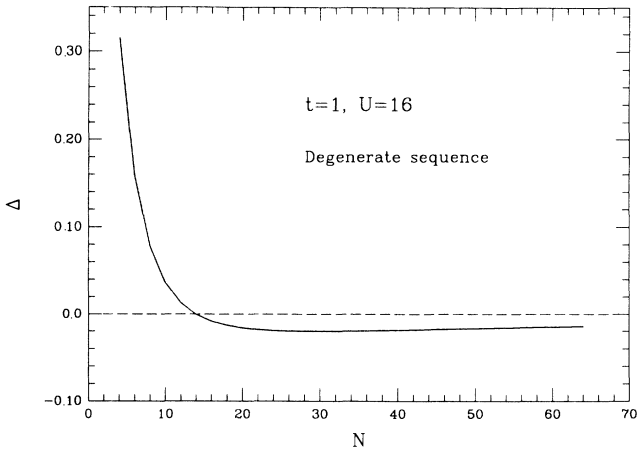

FIG. 3. Binding energy Δ vs lattice size N with $t=1$ and $U=16$ for degenerate sequence. Note lack of binding for small lattices.

In the degenerate sequence with $t=1$ and $U=4$, however, binding is seen to occur for all N. $\Delta(N)$ initially increases dramatically with lattice size, plateauing when $N=12$ at the value $\Delta=-0.090$.[13] It then begins a slow decay as N increases further. This decay is expected when compared with the nondegenerate results, as binding should be independent of boundary conditions in the thermodynamic limit.

We have found that this general behavior, an initial increase in binding-energy magnitude followed by a slow decay, holds for all $U/t<4.5$ in degenerate chains. Also, the lattice size N at which *maximum* binding occurs for a given U appears to increase monotonically with U.

An additional feature appears, however, when $U/t>4.5$, as illustrated in Fig. 3 for $U=16$. Here, we see that no binding occurs until a critical lattice size is reached. The binding-energy magnitude then increases, plateaus (here, at $N=30$), and begins to decay as before.

As U/t increases beyond 4.5, it becomes necessary to go to larger and larger lattices before binding occurs; for ex-

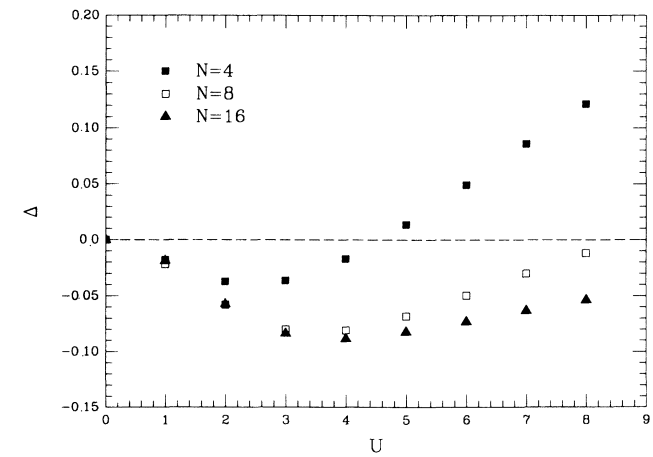

FIG. 4. Binding energy Δ vs U, with $t=1$, for $N=4$ sites (top, solid squares); $N=8$ sites (middle, open squares); and $N=16$ sites (bottom, solid triangles). Note general increase of binding with increasing lattice size.

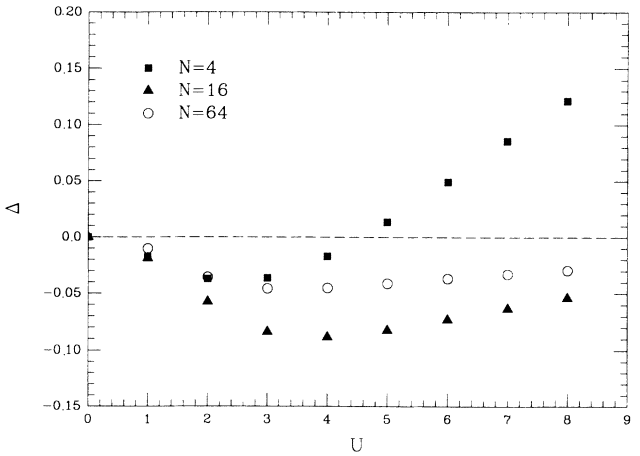

FIG. 5. Binding energy Δ vs U, with $t=1$, for $N=4$ sites (solid squares); $N=16$ sites (solid triangles); and $N=64$ sites (bottom, open circles). Note general *decrease* of binding in going from $N=16$ to $N=64$, following the *increase* in going from $N=4$ to $N=16$.

ample, there is no binding for $U/t=48$ until $N=40$. However, once binding sets in, it appears that it never completely vanishes as finite N is further increased. This leads us to the somewhat nonintuitive conjecture that, although binding will eventually decrease with lattice size for any U, the *range* of U/t over which binding occurs will actually *increase* monotonically with lattice size.

We note that the general nonmonotonic behavior of $\Delta(N)$ with N in degenerate chains could be very misleading if one were restricted to small lattices. For example, in Fig. 4 we show Δ vs U ($t=1$) for $N=4$, 8, and 16. As N increases, both the magnitude of Δ *and* the range of U over which Δ is negative increase. These results could easily lead one to suspect that binding persisted in the thermodynamic limit.

However, in Fig. 5, we again show Δ vs U, but for $N=4$, 16, and 64. After an initial increase in the magnitude of Δ from $N=4$ to $N=16$, we now see a general *decrease*[14] going from $N=16$ to $N=64$. In fact, as expected[10] in the one-dimensional repulsive-U Hubbard model, our results suggest very strongly that Δ is zero in the thermodynamic limit for all values of U.

IV. CONCLUSIONS

Using the Bethe ansatz equations, we calculated the binding energies $\Delta(N)$ of two holes just off half-filling in one-dimensional Hubbard chains of varying lengths N. Our main purpose was to investigate the general effect of finite size on such calculations. We found no binding in chains with no degeneracy at the Fermi level in the noninteracting ($U=0$) limit. However, we found significant binding ($\Delta<0$), comparable to that seen in two-dimensional Hubbard lattices, in chains which had such a degeneracy.

In the degenerate chains, for $U/t<4.5$, we found that binding initially increased dramatically with lattice size before beginning a slow decay to zero in the thermodynamic limit. For $U/t>4.5$, there was no binding on small lattices. However, as the lattice size was increased, binding eventually set in, increased in magnitude, and then began to decay, as before. We noted that a nonmonotonic behavior of $\Delta(N)$ with N of this sort could prove deceptive in attempts to extrapolate to the thermodynamic limit.

Our results suggest that, in general, great care must be exercised in inferring binding energies in the thermodynamic limit from binding energies calculated for finite systems. In particular, they suggest that the two-dimensional systems studied to data may be too small to determine whether binding persists in the thermodynamic limit.

Nonetheless, the use of different boundary conditions may provide further useful information within current size limitations. As an example, the largest two-dimensional Hubbard lattices for which binding calculations have been done,[5] and in which binding was observed, have periodic boundary conditions in both the x and y directions. This gives a $U=0$ degeneracy at the Fermi level in the half-filled case, as in the degenerate (binding) one-dimensional chains. For a square lattice, the degeneracy persists if antiperiodic boundary conditions are used in both directions. However, if "mixed" boundary conditions are used, periodic in one direction and antiperiodic in the other, there is *no* $U=0$ degeneracy at the Fermi level. Further, the one-particle energies are symmetric about the Fermi energy, as in the one-dimensional nondegenerate (nonbinding) chains (see Fig. 1). Thus, for instance, the existence of binding in two-dimensional Hubbard lattices with mixed boundary conditions would provide a clear-cut difference between the one- and two-dimensional systems, suggesting (though not yet proving) that binding might survive in the thermodynamic limit. Conversely, the disappearance of binding in the "mixed" case, by analogy, might lead one to question whether the observed binding could be a finite-size effect. Another alternative would be to look at binding slightly off half-filling.

These same considerations apply equally to the t-J model, due to its close relationship with the Hubbard model.[15] Further, variable boundary conditions may also prove helpful in studying Hubbard, CuO_2, and other related clusters,[16] though the prescription there is less clear.

Lastly, it is possible that the appearance of binding in finite systems may be associated with other indications of superconductivity, such as enhanced pairing correlations or susceptibilities. If this is so, our results suggest similar caution in interpreting such indications. As for the binding energy, mixed or other variable boundary conditions might prove generally useful in obtaining better control over finite-size effects.

ACKNOWLEDGMENTS

One of us (R.M.F.) is indebted to D. J. Scalapino, R. L. Sugar, A. Moreo, and P. Littlewood for helpful discussions. R.M.F. is grateful to IBM for partial financial support. M.J.M. would like to acknowledge support by Conselho Nacional de Desenvolvimento Científico e Tecnológico and by NSF Grant No. PHY86-14185. This research was supported in part by the National Science Foundation under Grant No. DMR86-15454.

*On leave from Departamento de Física, Universidade Federal de São Carlos, São Carlos, 13560, Brazil.

[1]For example, see V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990), and references therein.

[2]J. E. Hirsch, S. Tang, E. Loh, Jr., and D. J. Scalapino, Phys. Rev. Lett. **60**, 1668 (1988); J. E. Hirsch, E. Loh, Jr., D. J. Scalapino, and S. Tang, Phys. Rev. B **39**, 243 (1989).

[3]C. A. Balseiro, A. G. Rojo, E. R. Gagliano, and B. Alascio, Phys. Rev. B **38**, 9315 (1988).

[4]J. A. Riera and A. P. Young, Phys. Rev. B **39**, 9697 (1989).

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

[6]J. Callaway, D. P. Chen, D. G. Canhere, and Qiming Li, Phys. Rev. B **42**, 465 (1990).

[7]E. Kaxiras and E. Manousakis, Phys. Rev. B **38**, 866 (1988).

[8]J. Bonca, P. Prelovsek, and I. Sega, Phys. Rev. B **39**, 7074 (1989).

[9]Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989).

[10]E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[11]M. J. Martins and R. M. Fye (unpublished).

[12]B. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).

[13]This value, $\Delta = -0.090$, is close to the maximum binding seen for *any* U or N, and is comparable to the 4×4 Hubbard lattice value $\Delta = -0.10 \pm 0.02$ when $t=1$ and $U=4$ observed in Ref. 5.

[14]The $N=16$ and 64 curves will, however, cross for some U sufficiently large.

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

[16]Y. Hatsugai, M. Imada, and N. Nagaosa, J. Phy. Soc. Jpn. **58**, 1347 (1989).