Effect of Anderson disorder on the correlation functions and binding energy of excess carriers in a Cu_4O_8 cluster

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The effect of Anderson disorder on the binding energy Δ of the excess carriers, and on the correlation functions of the ground state of a Cu_4O_8 cluster has been studied numerically. Calculations were carried out for the cases of p-type and n-type doping, through an exact diagonalization of the Emery Hamiltonian. The results show that $|\Delta|$ decreases with increasing value of the disorder parameter W, vanishing at a certain critical value W_c. The ratio $W_c/|\Delta(W=0)|$ remains constant (at ≈ 9 and ≈ 7 for holes and electrons, respectively) over a broad range of values of $\Delta(W=0)$, corresponding to various choices of the parameters of the Hamiltonian. An increase in W weakens the antiferromagnetic correlations in the undoped insulating state, while it leads to a partial restoration of these correlations if the system contains excess carriers. The results found here can be explained by the hypothesized magnetic mechanism for effective attraction of carriers.

1. INTRODUCTION

The high-T_c superconductors are sensitive to nonmagnetic impurities and to defects of the crystal structure which result from a deviation from stoichiometry,[1] from a change in composition,[2] or from irradiation.[3] An increase in disorder is known to cause a transition to an insulating state[4] and vanishing of the superconducting transition temperature.[3,5–7] The changes which occur in the critical properties of superconductors associated with atomic disordering depend on the superconducting pairing mechanism. A study of the effect of defects on the properties of the high-T_c superconductors is thus of fundamental as well as practical interest, since it may prove helpful in reaching an understanding of high-T_c superconductivity.

Various versions of a nonphonon magnetic mechanism for the superconductivity of these superconductors have been studied actively in recent years.[8–12] This mechanism is based on strong Coulomb correlations, which lead to antiferromagnetic ordering of spins at copper sites in the initial undoped compounds.[13] Efforts to carry out an analytic study of the interrelationships between disorder and superconductivity on the basis of the magnetic mechanism[14] run into serious computational difficulties. In the thermodynamic limit, such studies can be carried out only by perturbation theory.

Even if there is no disorder, the problem of the electronic structure and (especially) the superconductivity of strongly correlated systems is a very difficult one, which has yet to be finally resolved. The results which have been found by various analytic methods are ambiguous and lean heavily on various approximations. Numerical methods become particularly important in such a situation. One numerical method is the exact-diagonalization method, which makes it possible to find the energy of the ground state and the corresponding eigenvector (and thus the various correlation functions) in finite clusters with any prescribed accuracy (Refs. 15–19, for example). An exact solution for small clusters leads to a qualitative understanding of the properties of the system of interest. It may also serve as a test of analytic methods using approximations which cannot be tested.

Exact calculations of the hole binding energy Δ_h (Refs. 15–19) and of the electron binding energy Δ_e (Ref. 19) in Cu–O clusters have been carried out previously on the basis of the $2D$ Emery model.[20] Those results showed that, in the absence of disorder, there is a certain region of the values of the parameters of the model in which both excess holes ($\Delta_h < 0$) and excess electrons[1)] ($\Delta_e < 0$) are effectively attracted. The changes which occur in the antiferromagnetic correlations in the copper sublattice[15,16,19] are such that the addition of the first excess carrier (a hole or an electron) to the insulating state of the cluster produces a far greater disruption of the antiferromagnetic correlations than is caused by the subsequent addition of a second excess carrier of the corresponding sign. It has accordingly been suggested[15,16,19] that the effective attraction of carriers stems from an energy advantage due to a decrease in the dimensions of the region with the disrupted antiferromagnetic correlations upon the formation of a bound pair. We wish to stress that these results are exact, although they were derived for systems of finite dimensions (see Refs. 19, 23, and 24, for example, regarding the effect of the size of the clusters on the binding energy). To some extent, these results may be taken as support for the hypothesis of a magnetic mechanism for the superconductivity of the high T_c materials.

This hypothesis might be confirmed (or refuted) directly by exact calculation of the carrier binding energy Δ in several Cu–O clusters with various numbers of atoms, N_a. Such calculations would make it possible to find the dependence $\Delta(N_a)$ at a fixed density n of the excess carriers and to attempt to determine $\Delta(N_a \to \infty)$ by interpolation. Moreover, such calculations might make it possible to find the dependence $\Delta(n)$ and to study the nature of the changes in the antiferromagnetic correlations at values of n corresponding to the disappearance of the effective attraction. However, the values of N_a which can be handled are severely restricted by the limited memory and speed of existing computers. As we know, the smallest Cu–O cluster which has the symmetry of the CuO_2 plane (so that periodic boundary conditions can be employed) and which is consistent with

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the use of the exact-diagonalization method to study the unreduced Emery model is the 12-site Cu_4O_8 cluster (Fig. 1).

In this paper we use the exact-diagonalization method to study the effect of an atomic disorder on the antiferromagnetic correlations and the value of Δ in a Cu_4O_8 cluster (these are apparently the first such calculations). We consider the Emery model with a diagonal Anderson disorder (the increments in the site potentials are distributed at random over an energy interval of width W). A distinctive feature of the present study is a comparative analysis of the cases of p-type and n-type doping. We will see that $|\Delta_h|$ and $|\Delta_e|$ fall off monotonically as the degree of disorder W increases, and they vanish at a certain critical value W_c. The ratios $W_c/|\Delta_h(W=0)|$ and $W_c/|\Delta_e(W=0)|$ remain constant (at ≈ 9 and ≈ 7, respectively) over broad ranges of the values of $|\Delta_h(W=0)|$ and $|\Delta_e(W=0)|$, corresponding to various choices of the values for the parameters of the Emery model. An increase in W weakens the antiferromagnetic correlations in the undoped insulating state, while in a state with excess carriers, of one sign or the other, the antiferromagnetic correlations remain constant at $W \sim W_c$ or even undergo a partial restoration. According to the magnetic mechanism, changes of this sort in the antiferromagnetic correlations are consistent with the disappearance of the effective carrier attraction.

1. STATEMENT OF THE PROBLEM

The Emery Hamiltonian describing the system of correlated charge carriers in the CuO_2 plane (which is a common structural element of the high T_c superconductors) is

$$H_1 = -t\sum_{\langle ik\rangle,\sigma}(d_{i\sigma}^{+}p_{k\sigma}+\text{H.a.}) + t'\sum_{\langle kk'\rangle,\sigma} p_{k\sigma}^{+}p_{k'\sigma} + \varepsilon\sum_{k,\sigma} n_{k\sigma} + U_d\sum_i n_{i\uparrow}n_{i\downarrow} + U_p\sum_k n_{k\uparrow}n_{k\downarrow} + V\sum_{\langle ik\rangle,\sigma,\sigma'} n_{i\sigma}n_{k\sigma'}, \quad (1)$$

where the operators $d_{i\sigma}^{+}$ and $p_{k\sigma}^{+}$ create a hole in the states $d_{x^2-y^2}$ and p_x, p_y, respectively; $\langle ik\rangle$ means a summation over nearest neighbors; the index i refers to copper sites; the index k refers to oxygen sites; $n_{i\sigma} = d_{i\sigma}^{+}d_{i\sigma}$; $n_{k\sigma} = p_{k\sigma}^{+}p_{k\sigma}$; t and t' are the matrix elements for copper-oxygen and oxygen-oxygen hops, respectively; $\varepsilon = \varepsilon_p - \varepsilon_d$ is the difference between the energies of a hole at an oxygen site and at a copper site; and U_d, U_p, and V are the energies of the Coulomb repulsion of holes at copper sites, at oxygen sites, and between them, respectively. The vacuum for the Hamiltonian (1) is the electronic configuration $Cu3d^{10}O2p^6$ (with a $Cu^{2+}O^{2-}$ valence state).

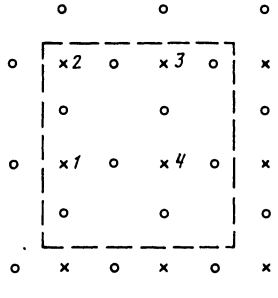

FIG. 1. A Cu_4O_8 cluster. ×—Copper atoms; O—oxygen atoms.

Since there is one hole per copper atom in the CuO_2 plane in the insulators La_2CuO_4, Nd_2CuO_4, $YBa_2Cu_3O_6$, etc. (the valence state is $Cu^{2+}O^{2-}$), the undoped insulating state of the Cu_4O_8 cluster corresponds to $N=4$ holes. Values $N>4$ correspond to a p-type doping of the CuO_2 plane ($La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$, etc.), while values $N<4$ correspond to n-type doping ($Nd_{2-x}Ce_xCuO_4$, etc.). For $\varepsilon>0$, the excess holes occupy $O2p$ orbitals predominantly according to experimental data,[25-27] while the excess electrons occupy $Cu3d$ orbitals predominantly.[2)]

To describe the effect of atomic disorder on the electronic structure of the CuO_2 plane, we use the diagonal Anderson disorder model. The total Hamiltonian is

$$H = H_1 + H_2 = H_1 + \sum_{j=i,k} w_j(n_{j\uparrow}+n_{j\downarrow}), \quad (2)$$

where H_1 is the Emery Hamiltonian in (1), H_2 is an "impurity" Hamiltonian, and w_j are the increments in the site potentials of the copper and oxygen atoms. The quantities w_j take on random values in an energy interval of width W, with a distribution function

$$P(w_j) = \begin{cases} 1/W, & |w_j| \leqslant W/2, \\ 0, & |w_j| > W/2. \end{cases}$$

The parameter W characterizes the degree of disorder (at $W=0$, there is no disorder).

The binding energy of the excess carriers is given by[15-19]

$$\Delta = E(0) + E(2) - 2E(1), \quad (3)$$

where $E(m)$ is the energy of the ground state of the system, with m excess carriers.

For the numerical calculations of the ground-state energies $E(N)$ and the eigenvectors of the Hamiltonian (2) for various numbers N of holes in the Cu_4O_8 cluster, we used the iterative Lanczos algorithm.[19,34] The relative error of these calculations was less than 10^{-8}. The hole binding energy Δ_h and the electron binding energy Δ_e were found from (3), with the understanding that the number of excess carriers is $m = N-4$ in the case of p-type doping, while it is $m = 4-N$ in the case of n-type doping.

Our calculations dealt in most detail with the following region of values of the parameters of Hamiltonian (1): $\varepsilon = 0-3$, $U_d \leqslant 10$, and $U_p = V = t' = 0$ (here and below, all quantities with the dimension of energy are expressed in units of t; i.e., we are setting $t=1$). Our choice agrees with estimates in the literature ($t = 1$–1.5 eV, $t' = 0.3$–0.6 eV, $\varepsilon = 1.5$–4 eV, $U_d = 6$–10 eV, $U_p = 1$–6 eV, $V = 0$–4 eV; Refs. 35–40). We selected these values because it is in this region of parameter values that there is an effective attraction of both excess holes and excess electrons: $\Delta_h < 0$ and $\Delta_e < 0$ ($|\Delta_h| \lesssim 0.10$; $|\Delta_e| \lesssim 0.03$) (Ref. 19). In the case of the p-type doping, we also considered the case with $U_p \neq 0$ and $V \neq 0$.

At a fixed value of W, the characteristics of the ground state of the clusters depend on the specific realization of the site disorder, i.e., on the specific set $\{w_j\}$. If this circum-

stance is ignored, erroneous results may be found. For example, the exact-diagonalization method was used in Ref. 41 to study the influence of Anderson disorder on the correlation functions of a ten-site Hubbard chain. A totally nonphysical oscillatory dependence of the correlation function $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ on W was found as a result. The reason, we believe, is that, for each value of W, the calculations of $\langle n_{i\uparrow} n_{i\downarrow} \rangle$ in Ref. 41 were carried out for a common set $\{w_j\}$, which was changed each time W was changed.

A correct description of the influence of defects on the electronic structure of small clusters requires taking a suitable average over the various configurations of the disorder and determining both mean values and mean square deviations. We carried out calculations in the following manner: For each of L different random sets $\{w_i^l\}$ $(l = 1, L)$, at fixed values of all the other parameters of Hamiltonian (2), we calculated $\Delta_h^l(W)$ and $\Delta_e^l(W)$. Mean values of the binding energies $\Delta_h(W)$ and $\Delta_e(W)$ were then found as the arithmetic means over L configurations. Using the same approach, we calculated the spin-spin correlation functions $S_{ij} = \langle (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}) \rangle$, the density-density correlation functions $D_{ij} = \langle (n_{i\uparrow} + n_{i\downarrow})(n_{j\uparrow} + n_{j\downarrow}) \rangle$, and the occupation numbers of the copper and oxygen orbitals ($\langle n_{\mathrm{Cu}} \rangle$ and $\langle n_{\mathrm{O}} \rangle$, respectively).

In most cases we restricted the calculations to $L = 8$–15 disorder configurations. This decision made it possible to avoid an excessive demand on computing time, while leading to fairly accurate results (increasing L to 30–40 or using a different set of $L \sim 10$ configuration realizations resulted in changes of 10%–20% in Δ and in the mean square deviations). For systems of large dimensions, there is no need to take an average over a large number of configurations. For example, in a study of the $1D$ Hubbard-Anderson model by the Monte Carlo method, the number of disorder realizations required for chains of $N_a = 8$–24 sites was $L = 40$–60 (Ref. 42), while at $N_a = 120$ a single realization ($L = 1$) proved sufficient.[43]

2. RESULTS OF THE CALCULATIONS

Figure 2 shows some typical results on the behavior of the binding energies Δ_h and Δ_e as a function of the Anderson-disorder parameter W. We recall that we are dealing with a region of values of the Emery-model parameters for which the excess carriers experience an effective attraction in the absence of disorder: $\Delta_h(W=0) < 0$ and $\Delta_e(W=0) < 0$. The primary features of the $\Delta_h(W)$ and $\Delta_e(W)$ curves are:

1) The absolute values of $|\Delta_h(W)|$ and $|\Delta_e(W)|$ always decrease with increasing W, and they vanish at a critical value W_c of the degree of atomic disorder.

2) The functions $\Delta_h(W)$ and $\Delta_e(W)$ are linear over a very broad range of W, including values $W \gg W_c$.

3) The mean square deviations of the binding energies Δ_h and Δ_e also increase linearly with W (we will not take up this point again; we will cite only values of the binding energies averaged over the various realizations of the disorder).

In the absence of disorder, the binding energies $\Delta_h(W=0)$ and $\Delta_e(W=0)$ depend on the values of the parameters of Hamiltonian (1). With $\varepsilon = 1$, for example, the quantity $|\Delta_h(W=0)|$ increases monotonically with increasing U_d (Fig. 3a), and at $U_d = 6$ it has a maximum at

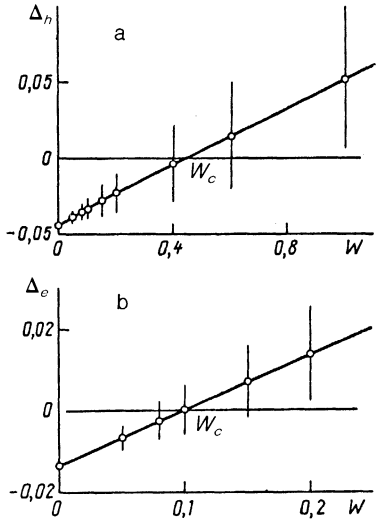

FIG. 2. Plots of (a) Δ_h, (b) Δ_e, and (vertical lines) the corresponding mean square deviations versus W for $\varepsilon = 1$, $U_d = 8$, and $U_p = V = 0$.

$\varepsilon \approx 1.5$ (Fig. 4a). The maximum of $|\Delta_e(W=0)|$ is reached at $U_d \approx 5$ and $\varepsilon \approx 1$ (Figs. 5a and 6a). Note the correlation between W_c and $|\Delta_h(W=0)|$, $|\Delta_e(W=0)|$. As can be seen from Figs. 3b–6b, W_c increases with increasing binding energy at $W = 0$. This is true over a very broad range of the values of $|\Delta_h(W=0)|$ and $|\Delta_e(W=0)|$, corresponding to various sets of parameter values in Hamiltonian (1). Figure 7 combines the results calculated on W_c for $\varepsilon \leqslant 3$, $U_d \leqslant 10$, and $U_p = V = 0$. We see that W_c is directly proportional to $|\Delta(W=0)|$, for both p-type and n-type doping: $W_c/|\Delta_h(W=0)| \approx 9$, and $W_c/|\Delta_e(W=0)| \approx 7$. It follows that at fixed values of ε and U_d the value of W_c for holes is larger than that for electrons by a factor of 3 to 6, since we have $|\Delta_h(W=0)|/|\Delta_e(W=0)| = 2$–$5$ (Ref. 19).

It had been shown previously[16,17,19] that large values of V, combined with a strong repulsion at the copper sites, U_d, strengthen the tendency for the holes to attract ($|\Delta_h|$ increases), although an instability may result[3)] (similar re-

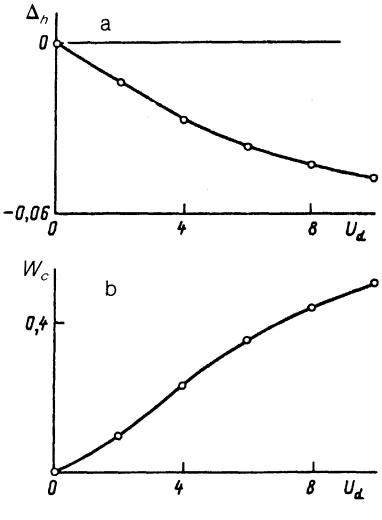

FIG. 3. Plots of (a) $\Delta_h(W=0)$ and (b) W_c versus U_d for $\varepsilon = 1$ and $U_p = V = 0$.

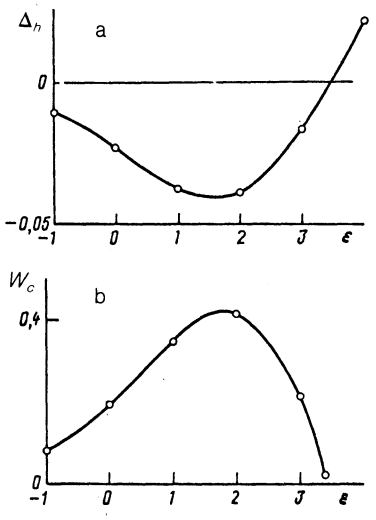

FIG. 4. Plots of (a) $\Delta_h(W=0)$ and (b) W_c versus ε for $U_d=6$ and $U_p=V=0$.

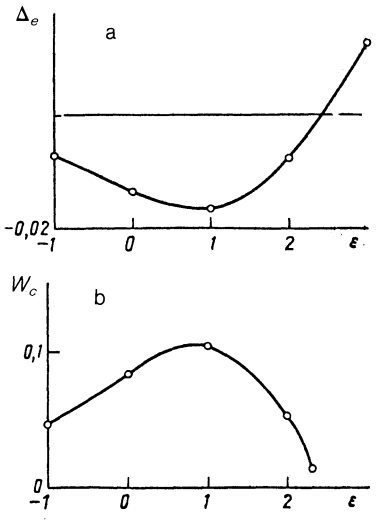

FIG. 6. Plots of (a) $\Delta_e(W=0)$ and (b) W_c versus ε for $U_d=6$ and $U_p=V=0$.

sults were found in Ref. 12 in a study of a reduced Emery model). Our calculations of W_c for the case of p-type doping (in the case of n-type doping, an increase in V erases the effective attraction[19]) with $\varepsilon=1$–2, $U_d=6$–8, $V=1$–3, and $U_p=0$–2 show that the ratio $W_c/|\Delta_h(W=0)|\approx 9$ remains constant over a range of binding energies ($|\Delta_h(W=0)|\lesssim 0.5$), substantially wider than in Fig. 7.

Another question of considerable interest is the possibility that an increase in the degree of atomic disorder will stimulate an effective attraction of excess carriers in strongly correlated systems.[41,44] In Ref. 41, for example, a numerical study of the correlation functions $\langle n_{i\uparrow} n_{i\downarrow}\rangle$ in the $1D$ Hubbard model revealed indications of the appearance of local attraction of holes at a site with increasing W. We carried out calculations of $\Delta_h(W)$ and $\Delta_e(W)$ for several values of the parameters of Hamiltonian (1) corresponding to initial repulsion: $\Delta_h(W=0)$, $\Delta_e(W=0)>0$. In all cases considered, $\Delta_h(W)$ and $\Delta_e(W)$ increased monotonically, remaining positive.

Figure 8 shows results calculated on the spin correlation functions S_{ij} between the nearest and next-nearest copper sites (S_{12} and S_{13}, respectively; Fig. 1), for the typical parameter values $\varepsilon=1$, $U_d=8$, and $U_p=V=0$ [$\Delta_h(W=0)=-0.044$, $\Delta_e(W=0)=-0.013$, and $W_c=0.43$ and 0.10, for holes and electrons, respectively]. The mean square deviations for the correlation functions are $<10\%$ of the mean values, so we are showing only these mean values of S_{ij} in Fig. 8.

In the absence of disorder ($W=0$), the undoped insulating state of the Cu_4O_8 cluster ($N=4$) is characterized by strong antiferromagnetic correlations in the copper sublattice: $S_{12}<0$, $S_{13}>0$, $S_{13}\approx 0.5|S_{12}|$. Doping disrupts the antiferromagnetic correlations for both p-type doping ($N>4$) and n-type doping ($N<4$). An important result is that the addition of the very first excess carrier to a cluster ($N=3$ or 5) leads to a far greater disruption of the antiferromagnetic correlations then is caused by the subsequent addition of a second excess carrier ($N=2$ or 6): $S_{12}(N=4)/S_{12}(N=3$

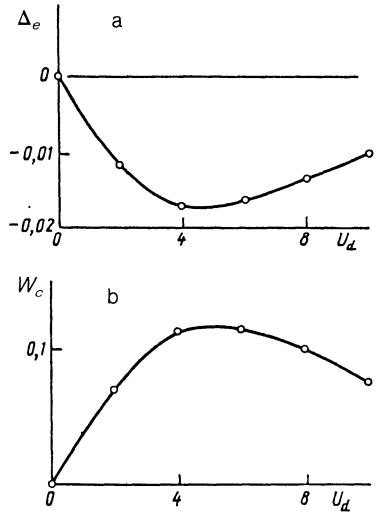

FIG. 5. Plots of (a) $\Delta_e(W=0)$ and (b) W_c versus U_d for $\varepsilon=1$ and $U_p=V=0$.

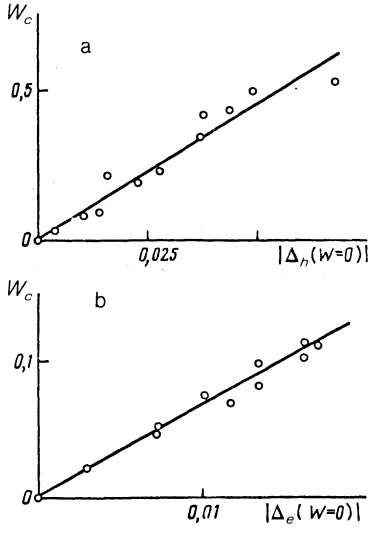

FIG. 7. Plots of W_c versus (a) $|\Delta_h(W=0)|$ and (b) $|\Delta_e(W=0)|$ for $0\leqslant\varepsilon\leqslant 3$, $0\leqslant U_d\leqslant 10$, and $U_p=V=0$.

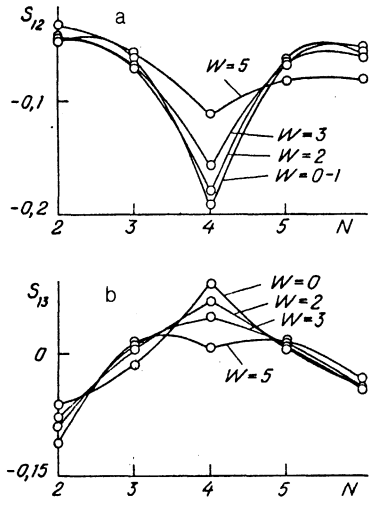

FIG. 8. The spin correlation functions (a) S_{12} and (b) S_{13} in the copper sublattice for various numbers of holes ($N=2$–6) in the Cu_4O_8 cluster (the numbering of the sites is explained in Fig. 1). Here $\varepsilon=1$, $U_d=8$, and $U_p=V=0$.

or 5) ≈ 3, $S_{12}(N=4)/S_{12}(N=2$ or 6) ≈ 4, $S_{13}(N=3$ or 5) ≈ 0, $S_{13}(N=4)/S_{12}(N=2$ or 6) ≈ -2. It was suggested in Refs. 15, 16, and 19 on this basis that the reason for the effective attraction of carriers is an energetic advantage when the two excess holes or two excess electrons are close together, so they reduce the size of the region with the disrupted antiferromagnetic correlations. Note that we have $S_{ij}(N=3)\approx S_{ij}(N=5)$ and $S_{ij}(N=2)\approx S_{ij}(N=6)$; i.e., there is a sort of (incomplete) symmetry in the disruption of the antiferromagnetic correlations by the p-type doping and the n-type doping.[19]

How are the antiferromagnetic correlations affected by site disorder (Fig. 8)? We are concerned primarily with values $W\sim W_c=0.1$–1. At $N=4$, an increase in W results in monotonic decrease in $|S_{12}|$ and S_{13}. In other words, it leads to disruption of the antiferromagnetic correlations, but this disruption does not become important until $W>2$. At smaller values of W, the strong antiferromagnetic correlations persist in the undoped state (these correlations disappear completely for a sufficiently large value of $W\gtrsim 5$). For $N=3$ and 5 (for one excess carrier per cluster), the correlation functions S_{13} increase monotonically with increasing W (in the case of the n-type doping, the correlation function S_{13} changes from negative to positive), while for $W\lesssim 2$ the correlation function S_{12} either remains unchanged (for $N=5$) or increases in absolute value ($N=3$). This behavior of $S_{12}(W)$ and $S_{13}(W)$ can be interpreted as a partial restoration of the antiferromagnetic correlations which are disrupted when an excess carrier is added to the cluster. We find a similar picture for $N=6$ (for two excess holes): $|S_{12}|$ and S_{13} increase with increasing W. In the case $N=2$ (two excess electrons), the antiferromagnetic correlations are not restored as W is increased: We find $S_{12}\approx$const, while S_{13} decreases, remaining negative (we should not say that the antiferromagnetic correlations are weakened, since in this case there are essentially no such correlations in the cluster, even at $W=0$).

The correlation functions D_{ij} are vastly less sensitive than the correlation functions S_{ij} to a disorder. The reason is that the system has no charge correlations in the case $U_d\gg V$ and $W=0$. For $W<2$, the occupation numbers $\langle n_{Cu}\rangle$ and $\langle n_O\rangle$ remain essentially constant. A further increase in W leads to a decrease in $\langle n_{Cu}\rangle$ and $\langle n_O\rangle$.

3. DISCUSSION OF RESULTS

It follows from our calculations that the effect of a diagonal Anderson disorder on the antiferromagnetic correlations of copper spins in a Cu_4O_8 cluster depends strongly on the number of excess carriers in the cluster. In the initial insulating state, an increase in W leads first to a weakening of the antiferromagnetic correlations (for $W\lesssim 2$) and then to their complete suppression (for $W\sim 5$). In a state with a single excess carrier (a hole or an electron), the antiferromagnetic correlations are partially restored. In a state with two excess carriers, the antiferromagnetic correlations are again partially restored in the case of p-type doping, while in the case of n-type doping they are not.

A result which we found somewhat surprising was the partial restoration of the antiferromagnetic correlations when the doped state was disordered. However, a corresponding result had been found previously[43] in a numerical study of the $1D$ Hubbard–Anderson model by the Monte Carlo method (although this result was not stressed in Ref. 43): At a hole density $n=0.4$ (reckoned from a half-filled band), the Fourier component of the spin correlation function

$$S(\mathbf{q})=\frac{1}{N_a}\sum_i\sum_l S_{il}\cos[\mathbf{q}(\mathbf{R}_l-\mathbf{R}_i)]$$

increases with increasing W at $q=\pi$ (i.e., the antiferromagnetic correlations, which are weakened by the doping, are strengthened again). At $n=0$, on the other hand, we observe a decrease in $S(\pi)$ (as expected): The disorder suppresses the antiferromagnetic correlations in the insulating state of the Hubbard model.

The Fourier representation is very convenient for analyzing antiferromagnetic correlations, since a single Fourier component contains information on the spin correlation functions between different lattice sites (in the case at hand, information on S_{12} and S_{13}). Figure 9 shows results calculated on $S(\pi,\pi)$ in a Cu_4O_8 cluster for various values of W. We see from Fig. 9 that the W dependence of $S(\pi,\pi)$ is determined by the type and number ($|N-4|$) of excess carriers in the cluster. With increasing W, the quantity $S(\pi,\pi)$

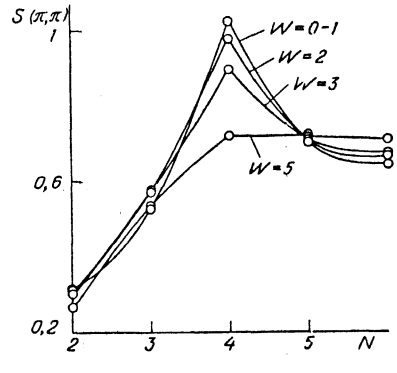

FIG. 9. The Fourier component $S(\pi,\pi)$ of the spin correlation functions in the copper sublattice for various numbers of holes ($N=2$–6) in the Cu_4O_8 cluster. Here $\varepsilon=1$, $U_d=8$, and $U_p=V=0$.

falls off monotonically for $N = 2$ and 4, increases monotonically for $N = 5$ and 6, and goes through a maximum at $W = 2$–3 for $N = 3$. These results confirm our conclusion, reached above on the basis of analysis of the correlation functions S_{12} and S_{13}, that the antiferromagnetic correlations undergo changes upon disordering.

Under the assumption of a magnetic mechanism for the effective carrier attraction, a decrease in the binding energy with an increase in disorder agrees qualitatively with the nature of the changes in the antiferromagnetic correlations. Specifically, a weakening of these correlations in the undoped state of the disordered cluster and the partial restoration of these correlations in the cluster with one excess carrier (Fig. 9) have the result that the disruption of these correlations resulting from the addition of one excess carrier to a disordered cluster is weaker than in the absence of a disorder. The further disruption of these correlations caused by the addition of a second excess carrier to the cluster, on the other hand, either remains nearly the same as for $W = 0$ (in the case of p-type doping) or in fact increases (in the case of n-type doping). Consequently, the energetic advantage accompanying the formation of a pair (a quantitative measure of this benefit is the binding energy) decreases with increasing W.

We are talking here about only a qualitative correspondence between the changes in the antiferromagnetic correlations and those in the binding energies associated with disordering. The changes in the antiferromagnetic correlations become significant (exceeding the "error" due to the averaging over the various disorder configurations) a for $W \gtrsim 1$. For the region of parameter values discussed above, on the other hand, we have $W_c \lesssim 0.5$. The reason why the changes in these correlations "lag behind" the changes in the binding energy with increasing W may be effects of the finite size of the cluster which we are discussing.

We briefly mention the linear W dependence of the binding energies (Fig. 2). Calculations of $\Delta_h(W)$ and $\Delta_e(W)$ for $W \gg W_c$ show that for $\varepsilon \sim 1$, and for $U_d \gg t$, V, and U_p, the linearity is disrupted at $W > \tilde{W} = \alpha U_d$, where α is a constant on the order of unity. The effect of Anderson disorder on the electronic characteristics of the Emery model appears to be determined by the parameter W/U_d.

We conclude with a discussion of the relationship between our results and experimental data on the effect of radiation on the high T_c superconductors.[3,45] The point defects which are formed during low-temperature ion bombardment of these superconductors create a random impurity potential. The effect of this potential on the carriers in the CuO_2 layers is described by the Hamiltonian (2). In this case the value of W is determined by the defect concentration n_{im}, i.e., by the radiation dose Φ (in a first approximation, we can assume $W \sim n_{im} \sim \Phi$). For the "n-type" high T_c superconductor $Nd_{1.85}Ce_{0.15}CuO_4$, the critical value Φ_c, at which the superconductivity is suppressed, is lower than that for the "p-type" high T_c superconductor $YBa_2Cu_3O_7$ by a factor of 8 to 10 (Refs. 3 and 45). These results agree with our calculations of W_c: The values found in the case of n-doping are lower than those found in the case of p-type doping by a factor of 3 to 6. We might add that the superconducting transition temperature of both the p-type and the n-type high-T_c superconductors decreases linearly with increasing Φ, in agreement with the linear decrease in the binding energies with W.

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[1)] As Emery has pointed out,[21] the discovery of the high-T_c superconductor Nd–Ce–Cu–O with n-type conductivity,[22] is evidence of a certain symmetry of the insulating state of the CuO_2 plane with respect to p-type and n-type doping. This situation is in a sense a condition for choosing among the various theories of high T_c superconductivity, most of which have been derived to describe a pairing of holes.

[2)] At the moment, the results which have been found on the electronic structure of high-T_c superconductors with the general formula $R_{2-x}Ce_xCuO_4$ where R = Nd, Pr, etc., are contradictory.[28–33] However, several studies have found indications of a $3d$ symmetry of the states of the excess electrons.[28,31–33] That symmetry would correspond to our approach to the problem of n-type doping.

[3)] The condition for stability of the system with respect to the formation of an inhomogeneous state (stratification into two phases with different carrier densities) is[16,17,19] $\Delta' = E(0) + E(3) - E(1) - E(2) > 0$. We studied only that region of parameter values in which the condition $\Delta'(W = 0) > 0$ holds. As W is increased, the sign of Δ' does not change, i.e., no instability occurs.

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