Static-hole energies in the t-J model and a t-J-ϵ model of the high-temperature superconductors

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We present Monte Carlo results for the energies of static holes in the t-J model. We consider the cases of zero, one, two, and four holes on square lattices of side $L=4$, 6, and 8 and extrapolate these results to give estimates for the bulk limit. We find that the hole energies and finite-size effects are in good agreement with spin-wave theory. Our results are consistent with phase separation in the static limit of the t-J model, but indicate that the incorporation of long-range Coulomb repulsion between holes prevents phase separation. We find that hole pairs alone are bound for a certain range of dielectric constant ϵ, which is $52<\epsilon<104$ in the static limit of a t-J-ϵ model with $1/r$ Coulomb repulsion, given the currently accepted value of J. The large observed value of the in-plane dielectric constant of La_2CuO_4, $\epsilon=30\pm3$, is not far from the lower limit of this theoretical pairing range, so the t-J-ϵ model may provide a useful approximate description of the mechanism of hole pairing in the high-temperature superconductors. Hole Cooper pairs that act as mediators of high-temperature superconductivity may thus arise from a competition between the large antiferromagnetic coupling J, which encourages hole clustering, and the ϵ-suppressed hole Coulomb repulsion, which restricts hole binding to pairs.

I. INTRODUCTION: THE t-J MODEL, SPIN-WAVE THEORY, AND PHASE SEPARATION

The search for the mechanism of high-temperature superconductivity[1] has motivated many recent investigations of the behavior of holes in quantum antiferromagnets, due to experimental indications of an association between the onset of superconductivity and the disruption of long-range antiferromagnetic order as hole doping is increased.[2] If this association is not accidental, a model Hamiltonian that incorporates both hole hopping and long-range spin antialignment on a two-dimensional lattice may implicitly describe the mechanism of high-T_c superconductivity. Several models of these effects have been proposed,[3] including the two-dimensional Hubbard model and the closely related t-J model.[4] The t-J model, which is the subject of this study, is described by the Hamiltonian

$$H=-t\sum_{\langle ij\rangle,\sigma}(c_{i\sigma}^{\dagger}c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\ . \tag{1}$$

Numerical studies of this Hamiltonian on small lattices using exact diagonalization techniques have appeared in the literature (for a review see Dagotto[5]), but it is unfortunately very difficult to simulate these dynamical fermion models using Monte Carlo methods due to the "minus-sign problem." Although the t-J model has not been studied numerically on large lattices, various approximate methods have been applied to this system. Bulut, Hone, Scalapino, and Loh[6] used spin-wave theory in the static hole ($t=0$) limit to estimate hole energies and hole-pair binding energies on finite lattices and in the bulk limit. They actually quote results for static holes in the Heisenberg model

$$H=J\sum_{\langle ij\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \tag{2}$$

which is equivalent to the static limit of the t-J model once the energy of each hole sector is decreased by $J\sum_{\langle ij\rangle}n_in_j/4$. The eigenstates of (1) and (2) are trivially identical in the static limit. This spin-wave calculation finds large finite-size effects, which is not encouraging for small-lattice studies. However they also indicate that the asymptotic finite-size energy dependences are simple powers of the lattice size, with relatively small nonleading corrections on a 4×4 lattice, so that extrapolation to the bulk limit may be straightforward. It is clearly of interest to test these predictions of finite-size effects, since accurate numerical studies of high-T_c models are currently restricted to small lattices.

There is another more fundamental problem encountered in studies of the t-J model; although it is widely discussed as a model of high-T_c superconductors, it is also believed to predict phase separation in the hole-doped system.[7,8] This prediction can be motivated by simple energy arguments in the static-hole limit. An isolated hole in a Heisenberg spin background breaks four antiferromagnetically ordered spin-pair bonds, with a corresponding increase in the energy of the system. To minimize the increase in energy for a given number of holes we must minimize the number of broken bonds, which is accomplished by arranging the holes in a compact cluster. This phenomenon of hole phase separation is not observed in the high-T_c superconductors and is thus an unphysical feature of the t-J model. (To avoid possible confusion we emphasize that the hole phase separation considered here is distinct from the separation of an oxygenrich phase of $La_2CuO_{4+\delta}$ reported by Jorgensen *et al.*[9])

In this paper we use a Monte Carlo method to determine the ground-state energies of static holes in the *t-J* model, which allows a direct comparison with the spin-wave theory of Bulut *et al.* and also allows us to estimate the energies associated with phase separation. In Sec. II we briefly describe the Monte Carlo algorithm and give more complete references to related applications. Section III gives our results for hole energies and compares them to previous numerical and spin-wave results, and shows that they lead to a simple approximate result for hole energies which supports phase separation in the *t-J* model. As an indicator of phase separation we measure a two-pair condensation energy in addition to the usual hole-pair binding energy. In Sec. IV we discuss the effect of introducing the Coulomb interaction between holes in a "t-J-ϵ" model. We argue that phase separation is prevented by the incorporation of any amount of $1/r$ Coulomb repulsion between holes, and that Coulomb repulsion with a dielectric constant near the value observed in La_2CuO_4 may lead to hole pairing as is suggested experimentally. Finally, Sec. V gives a summary and conclusions.

II. METHOD: THE DGRW ALGORITHM

Our results were obtained using the discrete guided random walk (DGRW) Monte Carlo algorithm,[10] which simulates the evolution of a given initial state in Euclidean time τ by running random walks in the configuration space of the system. The ground-state energy and matrix elements can be extracted from the averages of certain weight factors, which depend on the path followed by each walk in configuration space and on a trial ground-state wave function $\psi_0^{\rm trial}$ used to guide the walks. For this study we used

$$\psi_0^{\rm trial} \propto \exp(-\xi V_{\rm Ising}/J) ,$$

where $V_{\rm Ising}$ equals the $\hat{z}$ terms of (2) and the optimum guiding parameter $\xi \approx 0.25$ was estimated by minimizing the variance of the weight factors. In the DGRW algorithm the choice of $\psi_0^{\rm trial}$ affects the rate of convergence to ground-state matrix elements and energies but does not bias their limiting values. The initial configuration was chosen to be a "dimer state"[11] with appropriate vacancies for the first walk in each simulation, and successive walks were "bootstrapped" by using the final configuration of the nth walk as the starting point for the $(n+1)$th walk. This procedure was chosen because it gave the best convergence in tests on 4×4 lattices; we confirmed that other initialization procedures gave consistent energies. The random-walk program was implemented on a 128-node iPSC/860 Intel hypercube sited at Oak Ridge National Laboratory. Each node was used to generate weight factors for a large number of random walks and the combined results were averaged in eight subsets to generate statistical errors. As the program has very modest memory requirements no internode communication was required, so programming was straightforward. We determined a τ-dependent effective energy for a range of τ values from measurements of the mean weight factor at two Euclidean times, τ_1 and $\tau_2=\tau_1+1$. We typically chose $\tau_1=1-6$ in steps of 1, which was a sufficiently large range to confirm that the energies had converged to within our statistical errors. (For a more detailed description of the algorithm in this type of application see Barnes *et al.*[11]). In this study each energy measurement at each Euclidean time τ_1 represents an average over 2^{23} random walks. We also tested for bias due to the use of a finite Euclidean time step size, which was usually taken to be $h_\tau=0.1/L^2$; a correction of $-0.000\,08(3)$ in the ground-state energy per spin was found in the 4×4 simulations and is incorporated in our result for E_0/L^2, but no significant h_τ bias was observed on the larger lattices.

III. RESULTS AND DISCUSSION

We used the Monte Carlo algorithm described above to measure static-hole energies in the *t-J* model for comparison with the spin-wave calculations of Bulut *et al.* and to determine the energies involved in phase separation. The quantities measured were the ground-state energy per site E_0/L^2, the ground-state energy of a single hole relative to the no-hole state ($e_h=E_h-E_0$), and similarly for two nearest-neighbor holes ($e_{2h}=E_{2h}-E_0$) and four adjacent holes in a square ($e_{4h}=E_{4h}-E_0$). These energies were measured on square lattices of side $L=4$, 6, and 8. Our choice for the initial spin configuration restricted the algorithm to subspaces with $S^z_{\rm tot}=0$ for an even number of holes and $S^z_{\rm tot}=\frac{1}{2}$ for a single hole, but as this does not constrain $S_{\rm tot}$ we expect the algorithm to find the energy of the true ground state independent of its $S_{\rm tot}$.

Our results for E_0/L^2, e_h, e_{2h}, and e_{4h} are presented in Table I in units of J. (A factor of J is implicit in the energies in the following discussion as well.) The *t-J* values of E_0/L^2 have been increased by $\frac{1}{2}$ for comparison with more familiar Heisenberg numbers. The 4×4 Monte Carlo result for E_0/L^2 reproduces the Lanczos number quite accurately, within 1σ of the total estimated error of 3×10^{-5}. The 6×6 and 8×8 values are consistent with the most accurate previous results for these lattices, which are due to Trivedi and Ceperley,[12] and at least equal their statistical accuracy. To estimate the bulk limit energy we extrapolate using the spin-wave form[13] $E_0/L^2=c_0+c_1/L^3$, which Carlson[14] found to be very accurate on lattices of size 4×4 to 32×32. Fitting this form to our data gives $c_1=2.083(8)$ and

$$\lim_{L\to\infty}\frac{E_0}{L^2}=-0.669\,23(13) , \tag{3}$$

which may be compared to the $-0.669\,18(10)$ of Carlson and the $-0.6692(2)$ of Trivedi and Ceperley.[12,15] Since Carlson fits a larger range of L values, his estimate $E_0/L^2\approx-0.669\,18+2.086/L^3$ may have a smaller systematic error than our result and in any case is consistent with our numbers; for this reason we used his fit to determine hole energies relative to E_0.

The single-hole energy e_h for $L=4$, 6, and 8 is also given in Table I; we did not extend these measurements

TABLE I. Ground-state energies for zero, one, two, and four static holes on square lattices with $L=4$, 6, and 8 and their extrapolated bulk limit values.

L	$(E_0/L^2)^a$	e_h	$(e_h^{SWT})^b$	e_{2h}	$(e_{2h}^{SWT})^b$	e_{4h}
4	−0.701 780 201[c]	2.348 5631[d]		3.882 7352[d]		6.698 3460[d]
	−0.701 78(3)	2.3486(6)	2.3270	3.8825(4)	3.8872	6.6973(6)
6	−0.6789(1)	2.263(5)	2.2332	3.838(5)	3.8332	6.645(7)
8	−0.6732(2)	2.226(13)	2.2000	3.814(19)	3.8172	6.626(26)
∞	−0.669 23(13)	2.193(7)	2.1552	3.801(8)	3.7936	6.602(12)

[a]The t-J E_0/L^2 has been increased by 0.5 in this table to correspond to Heisenberg conventions.
[b]Spin-wave result of Bulut *et al.* (Ref. 6).
[c]Lanczos result of Gross *et al.* (Ref. 20).
[d]Lanczos result, this reference.

to larger lattices because the statistical errors were found to grow rapidly with L, and the smaller lattices sufficed to determine bulk limit values to our required accuracy. For comparison we have also tabulated the spin-wave results of Bulut *et al.* with conventions changed to correspond to the t-J Hamiltonian. The t-J hole energy is J larger than the Heisenberg results quoted by Bulut *et al.* due to the $-J\sum_{\langle ij\rangle} n_i n_j/4$ term in (1). Similarly the static t-J e_{2h} and e_{4h} are larger than Heisenberg energies by $7J/4$ and $3J$, respectively. To compare our Monte Carlo results with spin-wave theory (SWT) we also fitted both sets of numbers to the asymptotic form c_0+c_1/L^2 which Bulut *et al.* found empirically in their spin-wave calculation. For the spin-wave energies we estimated these coefficients from the 8×8 and bulk limit results. This fit to the spin-wave energy of a static hole in the t-J model gives

$$e_h^{SWT} \approx 2.155+\frac{2.87}{L^2}\ , \tag{4}$$

and the fit to our Monte Carlo (MC) data gives

$$e_h^{MC}=2.193(7)+\frac{2.49(13)}{L^2}\ . \tag{5}$$

In Fig. 1 we display the Monte Carlo and spin-wave results for this hole energy versus $1/L^2$. Evidently there is quite good agreement, the most important discrepancy being an underestimate of the hole energy in the spin-wave calculation by ≈ 0.03.

Fitting the two-hole energies in Table I to the spin-wave form gives

$$e_{2h}^{MC}=3.801(8)+\frac{1.31(14)}{L^2}\ , \tag{6}$$

which is in good agreement with the approximate spin-wave formula

$$e_{2h}^{SWT} \approx 3.794+\frac{1.51}{L^2} \tag{7}$$

and with the numerical spin-wave results, which are also given in Table I. The four-hole energy was not calculated by Bulut *et al.* nor has it been determined elsewhere using Lanczos techniques. As a check we determined this and the other hole energies using a Lanczos method, and these are given in Table I as well. The Monte Carlo and Lanczos results for e_{4h} agree to within 2σ. A fit of our data to c_0+c_1/L^2 gives

$$e_{4h}^{MC}=6.602(12)+\frac{1.54(19)}{L^2}\ . \tag{8}$$

Note that the finite-size corrections to the $2h$ and $4h$ energies are smaller than for the single hole; this is presumably due to the unpaired spin in the single-hole state.

Our bulk limit results show that the hole energies are approximately linear in the total number of broken spin-pair bonds N_B. If this were exact, the ratio of energies would equal the ratio of broken bonds, and for illustration the actual ratios in the $2h$ and $4h$ cases are

$$\frac{N_B(4h)}{N_B(2h)}=\frac{12}{7}=1.714\ldots \tag{9}$$

and

$$\frac{e_{4h}}{e_{2h}}=1.736(7)\ , \tag{10}$$

which is good agreement for such a simple estimate. This

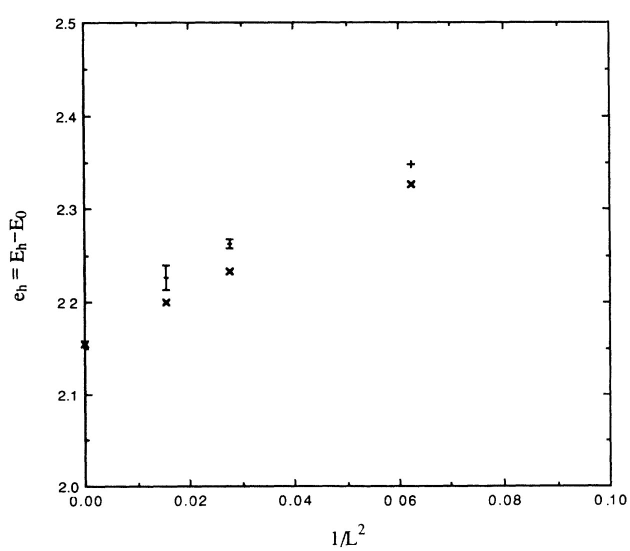

FIG. 1. Spin-wave theory and Monte Carlo results for the static-hole energy in the t-J model. + indicates Lanczos and Monte Carlo data; I, Monte Carlo data; ×, spin-wave theory.

suggests that the bulk limit ground-state energy of a state of N_h closely associated static holes is approximately $0.55N_B$. This number compares well with the ground-state energy of the t-J model in the no-hole sector, which is $-0.5846N_B$.

As we wish to test for hole pairing and phase separation, we introduce a two-hole binding energy relative to the energy of two separate holes,

$$\Delta_{2,1^2}=e_{2h}-2e_h\ , \tag{11}$$

and a condensation energy for a four-hole square cluster relative to two separate hole pairs,

$$\Delta_{4,2^2}=e_{4h}-2e_{2h}\ . \tag{12}$$

If $\Delta_{2,1^2}<0$ but $\Delta_{4,2^2}>0$, hole pairs would form but further condensation to four-hole clusters would not occur; this is the situation we expect to find in a realistic model of hole-doped high-T_c superconductors such as $La_{2-x}Sr_xCuO_4$. If both energy differences are positive, the hole clusters are not bound; if both are negative, four-hole clusters are energetically favorable, and holes will presumably condense into larger clusters and phase separation will result unless additional effects arise.

Our results for $\Delta_{2,1^2}$ and $\Delta_{4,2^2}$ are given in Table II, and as both are negative, hole pairing and continued condensation to phase separation is indicated. Note that the pair binding energy $\Delta_{2,1^2}$ has a relatively large finite-size dependence, which is primarily driven by the finite-size dependence of e_h. We find the bulk limit of the pair binding energy to be 0.72(2) of the 4×4 result. Bulut *et al.* quote a rather larger finite-size effect in their spin-wave calculation, due to their use of the Heisenberg Hamiltonian; on incorporating the additional t-J energy shifts due to the $-J\sum_{\langle ij\rangle}n_in_j/4$ term in (1), their expected decrease in binding energy becomes

$$\Delta_{2,1^2}(L=\infty)=0.67\Delta_{2,1^2}(L=4)\ ,$$

which is close to our Monte Carlo result. Note that the four-hole condensation energy shows a much smaller dependence on lattice size,

$$\Delta_{4,2^2}(L=\infty)=0.94(2)\Delta_{4,2^2}(L=4)\ .$$

This suggests that small-lattice results may more closely resemble the bulk limit when applied to bound even-hole states, as these do not have the large finite-size effects associated with an unpaired spin.

TABLE II. The static-hole pair binding energy $\Delta_{2,1^2}$ and two-pair condensation energy $\Delta_{4,2^2}$ for $L=4$, 6, and 8 and their extrapolated bulk limit values.

L	$\Delta_{2,1^2}$	$(\Delta_{2,1^2}^{\rm SWT})^{\rm a}$	$\Delta_{4,2^2}$
4	$-0.814\,3910^{\rm b}$		$-1.067\,1244^{\rm b}$
	$-0.8147(12)$	-0.7668	$-1.0677(10)$
6	$-0.688(11)$	-0.6332	$-1.031(12)$
8	$-0.638(32)$	-0.5828	$-1.002(46)$
$\infty^{\rm c}$	$-0.584(15)$	-0.5168	$-1.000(20)$

[a]Spin-wave result of Bulut *et al.* (Ref. 6).
[b]Lanczos result, this reference.
[c]These numbers follow from the bulk limits of e_h, e_{2h}, and e_{4h} in Table I.

IV. COULOMB HOLE REPULSION, PHASE SEPARATION, AND HOLE PAIRING

In Sec. III we presented numerical results for the energies of static holes in the t-J model and noted that these results were consistent with phase separation, at least in the static-hole limit. In summary, we found that the energy of of closely associated static holes is approximately $0.55N_BJ$, where N_B is the number of broken spin-pair bonds. To minimize this energy for a given number of holes one must pack the holes as closely as possible, which corresponds to phase separation.

There are obvious objections to applying these t-J model results to high-temperature superconductors. One objection is that the static limit may overestimate binding energies in the t-J model; this is difficult to test on large lattices at present. Our results given above suggest, however, that small lattices may suffice to study the t dependence of these energies, and we shall argue that binding energies may actually increase with t in a more realistic "t-J-ϵ" model. A second objection, which has been raised in a number of theoretical studies,[5,7,8,16] is that the neglect of the hole Coulomb interaction may be an unwarranted approximation and that phase separation probably does not occur when long-range Coulomb repulsion is incorporated. The Coulomb energy is certainly not negligible relative to the spin-spin interaction; the energy scale of the nearest-neighbor spin-spin interaction is $J\approx125$ meV (from a fit to neutron scattering data[17]), whereas the Coulomb energy of two holes separated by the mean CuO_2 spacing of 3.8 Å is also ≈125 meV, assuming a dielectric constant of $\epsilon=30$ (an in-plane value of $\epsilon=30\pm3$ has been reported[18] for undoped La_2CuO_4). We shall show that $1/r$ hole Coulomb repulsion does indeed prevent phase separation in a simple model of the separated hole system, and even the formation of hole pairs appears marginal given current experimental values for J and ϵ.

The absence of phase separation may be illustrated by considering the ground state of a large number N_h of static holes in a "t-J-ϵ" model with $1/r$ Coulomb repulsion,

$$H=-t\sum_{\langle ij\rangle,\sigma}(c_{i\sigma}^\dagger c_{j\sigma}+\text{H.c.})+J\sum_{\langle ij\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)+\frac{e^2}{\epsilon}\sum_{\langle ij\rangle}(1-n_i)\frac{1}{r_{ij}}(1-n_j)\ . \tag{13}$$

This Hamiltonian models the hole Coulomb repulsion using the pure dielectric form $E^2/\epsilon r$, which is most appropriate for light doping and small t in the insulating phase. A $-e^2/\epsilon r$ Coulomb energy was previously used by Chen *et al.*[18] to model the acceptor-hole bound state in La_2CuO_{4+y}. As the Coulomb interaction in the CuO_2 planes becomes better understood it may prove appropriate to generalize the $e^2/\epsilon r$ term in (13) accordingly. First assume that the Coulomb repulsion is totally screened ($\epsilon=\infty$), so that we recover the t-J model. From our earlier results the static-hole energy relative to the no-hole state is approximately c_BN_BJ, where $c_B\approx0.55$ and N_B is the number of broken spin-pair bonds. To minimize the energy of the N_h-hole state, we arrange the holes in a compact cluster; approximating this cluster by a disc of radius $R=a\sqrt{N_h/\pi}$, we have $N_s=2\pi R/a$ "surface" holes that break approximately three bonds each and N_h-N_s "volume" holes that break two bonds each. (We emphasize that this is only a simple estimate, and that the determination of the actual lowest-energy state as a function of J and ϵ is a complicated problem.) The magnetic energy of this disc of holes is the sum of a volume term ($\propto N_h$) and a surface term ($\propto N_h^{1/2}$),

$$E_J \approx c_B N_B J \approx (N_h+\sqrt{\pi}N_h^{1/2})2c_B J \ . \tag{14}$$

Now suppose we introduce the Coulomb repulsion; approximating the charged-hole disc as a smooth charge distribution gives a Coulomb energy of

$$E_C \approx N_h^{3/2}\frac{2\sqrt{\pi}}{3}\frac{e^2}{\epsilon a} \tag{15}$$

and the total energy is the sum of these contributions. Since the Coulomb contribution grows as $N_h^{3/2}$, for a sufficiently large number of holes it will dominate the magnetic $N_h^{1/2}$ surface term, and it will be energetically favorable to divide the N_h-hole disc into smaller clusters. We can estimate this critical number by determining the $N_h^{\rm crit}$ for which two discs of $N_h/2$ holes have the same total energy as a single N_h-hole disc, which is

$$N_h^{\rm crit} \approx 3\sqrt{2}\frac{c_B J}{e^2/\epsilon a} \ . \tag{16}$$

Thus, any arbitrarily large but finite ϵ will stop phase separation in an infinite system with a finite hole density (for which $N_h=\infty > N_h^{\rm crit}$), and we will instead find a ground state consisting of finite hole clusters of approximately $N_h^{\rm crit}$ holes.

As the electrostatic repulsion $e^2/\epsilon a$ is comparable to $c_B J$ in La_2CuO_4, the estimate (16) leads one to expect that only small hole clusters may be bound in the high-T_c materials; indeed, the observed parameters lead to an estimate of $N_h^{\rm crit}=2.3$ for La_2CuO_4. In the specific cases of hole pairs and four-hole clusters considered in this paper, the Coulomb term changes the binding energies to

$$\Delta_{2,1^2}=\Delta_{2,1^2}(0)+\frac{e^2}{\epsilon a} \tag{17}$$

and

$$\Delta_{4,2^2}=\Delta_{4,2^2}(0)+(2+\sqrt{2})\frac{e^2}{\epsilon a} \ . \tag{18}$$

These binding energies are shown in Fig. 2 in units of J as a function of $1/\epsilon$ for $a=3.8$ Å. For completely screened charges and $J=125$ meV, a static-hole pair is bound by about 73 meV and a four-hole cluster is favored over two pairs by 125 meV. As we decrease the dielectric constant and thereby unscreen the Coulomb repulsion, the four-hole cluster becomes less deeply bound, and for $\epsilon<104$ the hole pair alone is bound. The hole pair remains bound until $\epsilon=52$, below which it is unstable with respect to dissociation. Since the observed in-plane dielectric constant of La_2CuO_4 is $\epsilon=30\pm3$, the static limit of this simple t-J-ϵ model does not support hole-pair formation given currently accepted values of J and ϵ.

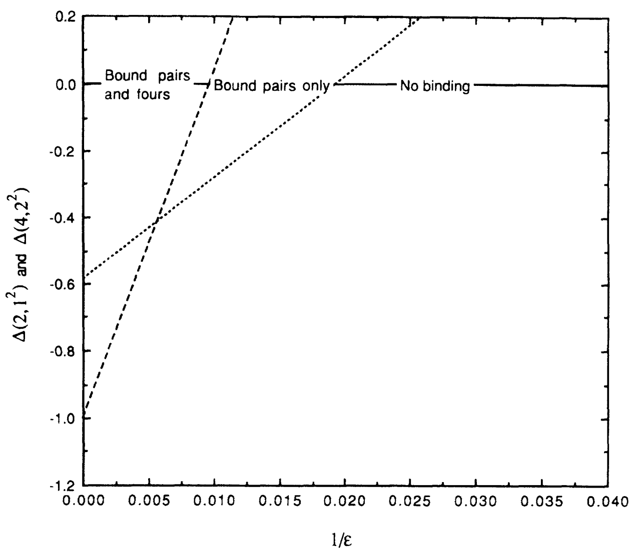

FIG. 2. Static-hole pairing and condensation energies divided by J vs dielectric constant. The solid line indicates the binding threshold; dotted line, the hole-pair binding energy $\Delta(2,1^2)$; dashed line, the four-hole condensation energy $\Delta(4,2^2)$.

However, in view of the unusually large dielectric constant of La_2CuO_4, we suggest that this hole-pairing mechanism may actually be correct and that the discrepancy between the theoretical pairing limit of $\epsilon=52$ and the observed value of 30 ± 3 is due to the simplifications of the t-J-ϵ model. We note in passing that it may also be possible to describe electron pairing in the electronlike high-temperature superconductors such as $Nd_{2-x}Ce_xCuO_4$ using a similar mechanism in the t-J-ϵ model; if excess electrons in the CuO_2 lattice pair with the Cu^{2+} spins, they would cancel the local spin-spin interaction just as a vacancy does, and additional electrons would experience Coulomb forces comparable to those between holes.

We suggest that the t-J-ϵ model should be explored in more detail as an approximate description of the interplay between magnetic effects and hole Coulomb repulsion in the high-temperature superconductors. One can study the t-J-ϵ ground state in the hole-pair binding regime using Lanczos techniques, for example, on 4×4 lattices, and the results in this paper indicate that these small lattices can give binding energies which are quite close to the bulk limit for an even number of holes, at least for small values of the hopping parameter. One question of immediate interest is the behavior of binding energies and the hole-pair wave function as the hopping parameter t is increased. As the coherence length ξ_0 in the high-temperature superconductors is typically estimated to be $\approx 10-20$ Å, localized hopping, for example, to next-nearest-neighbor sites, may be an important effect; it is certainly required to disrupt long-range antiferromagnetic order in the presence of light hole doping. The inclusion of the hopping term may significantly modify our results because t is believed to be rather large compared to J ($t/J\approx3$) and one would naively expect the binding energy to decrease as the hopping parameter is increased. Note, however, that a single hop in a nearest-neighbor hole pair will greatly decrease the

Coulomb repulsion, so that a nonzero hopping parameter may actually increase the hole-pair binding energy and hence decrease the dielectric constant required to bind pairs. This question can easily be studied numerically for small t.

Interesting experimental questions related to this model involve the determination of the sites actually occupied by paired holes and measurements of the dielectric constants of La_2CuO_4 and the "precursor insulators" of the other high-temperature superconductors such as $YBa_2Cu_3O_{7-\delta}$. The hole sites are of interest because a hole-pair bound state with a larger expected separation than 3.8-Å could bind given a smaller ϵ than we estimated using the t-J-ϵ model. Since it is known that holes preferentially occupy oxygen sites, the dielectric constant required for hole-pair formation may be somewhat lower in a more realistic model, for example, in one that incorporates distinct Cu and O sites as well as the screened Coulomb repulsion. The dielectric constant itself is of interest because this parameter specifies the amount of screening of the hole Coulomb repulsion, and hence determines whether or not hole pairing is energetically favored. Note also that there has been some disagreement in the literature regarding the value of the dielectric constant of La_2CuO_4.[18,19]

V. SUMMARY AND CONCLUSIONS

We have used a Monte Carlo method to determine the binding and phase separation energies of holes and hole clusters in the static limit of the t-J model. These energies are found to be in good agreement with spin-wave theory. We also discussed the effect of hole Coulomb repulsion in the static limit of the t-J-ϵ model and noted that phase separation of holes is prevented by any amount of Coulomb repulsion. We found that the range of ϵ which allows the formation of hole pairs only in the static limit of this model is $52 < \epsilon < 104$ given the currently accepted value of J. As the lower limit is not far from the large observed dielectric constant of La_2CuO_4 ($\epsilon \approx 30$), we suggest that the same mechanism of hole pairing may also operate in the high-temperature superconductors. Specifically, hole pairing may be the result of a competition between antiferromagnetism, which favors hole phase separation, and hole Coulomb repulsion, which dissociates large hole clusters preferentially.

Note added in proof. After completion of this work we learned of spin-wave calculations of the properties of an additional spin in a Heisenberg background[21] that are closely related to the calculations of Ref. 6.

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[1]J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
[2]A. Aharony, R. J. Birgeneau, A. Coniglio, M. A. Kastner, and H. E. Stanley, Phys. Rev. Lett. **60**, 1330 (1989).
[3]P. W. Anderson, Science **235**, 1196 (1987); J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. Lett. **60**, 944 (1988).
[4]C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987); J. Bonča, P. Prelovšek, and I. Sega, *ibid.* **39**, 7074 (1989); E. Dagotto, A. Moreo, and T. Barnes, *ibid.* **40**, 6721 (1989).
[5]E. Dagotto, Int. J. Mod. Phys. B (to be published).
[6]N. Bulut, D. Hone, D. J. Scalapino, and E. Y. Loh, Phys. Rev. Lett. **62**, 2192 (1989).
[7]M. Marder, N. Papanicolaou, and G. C. Psaltakis, Phys. Rev. B **41**, 6920 (1990).
[8]V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).
[9]J. D. Jorgensen, B. Dabrowski, S. Pei, D. G. Hinks, L. Sonderholm, B. Morosin, J. E. Schirber, E. L. Venturini, and D. S. Ginley, Phys. Rev. B **38**, 11 337 (1988).
[10]T. Barnes and G. J. Daniell, Phys. Rev. B **37**, 3637 (1988); T. Barnes, in *Computational Atomic and Nuclear Physics at One Gigaflop*, Vol. 16 of *Nuclear Science Research Conference Series*, edited by C. Bottcher, M. R. Strayer, and J. McGrory (Harwood, Academic, Chur, Switzerland, 1989), pp. 83–106.
[11]T. Barnes, K. J. Cappon, E. Dagotto, D. Kotchan, and E. S. Swanson, Phys. Rev. B **40**, 8945 (1989).
[12]N. Trivedi and D. M. Ceperley, University of Illinois at Urbana-Champaign Report No. P/89/8/115, 1989 (unpublished).
[13]D. A. Huse, Phys. Rev. B **37**, 2380 (1988); H. Neuberger and T. Ziman, *ibid.* **39**, 2608 (1989).
[14]J. Carlson, Phys. Rev. B **40**, 846 (1989).
[15]N. Trivedi and D. M. Ceperley, Phys. Rev. B **40**, 2737 (1989).
[16]J. E. Hirsch, E. Loh, Jr., D. J. Scalapino, and S. Tang, Phys. Rev. B **39**, 243 (1989).
[17]H.-Q. Ding and M. S. Makivić, Phys. Rev. Lett. **64**, 1449 (1990).
[18]C. Y. Chen, N. W. Preyer, P. J. Picone, M. A. Kastner, H. P. Jenssen, D. R. Gabbe, A. Cassanho, and R. J. Birgeneau, Phys. Rev. Lett. **63**, 2307 (1989).
[19]D. Reagor, E. Ahrens, S-W. Cheong, A. Migliori, and Z. Fisk, Phys. Rev. Lett. **62**, 2048 (1989).
[20]M. Gross, E. Sánchez-Velasco, and E. D. Siggia, Phys. Rev. B **40**, 11 328 (1989).
[21]N. Nagaosa, Y. Hatsugai, and M. Imada, J. Phys. Soc. Jpn. **58**, 978 (1989).