RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 37, NUMBER 7 1 MARCH 1988

Large-n limit of the Heisenberg-Hubbard model: Implications for high-T_c superconductors

Ian Affleck
Physics Department, University of British Columbia, Vancouver, British Columbia V6T 2A6, Canada

J. Brad Marston
Joseph Henry Laboratories, Princeton University, Princeton, New Jersey 08544
(Received 13 October 1987)

The Heisenberg-Hubbard model is solved in the large-n limit to gain insight into its relevance to the copper-oxide materials. A gapless disordered ground state is found for the Heisenberg model. Electronically induced orthorhombic-tetragonal symmetry breaking is observed as a function of doping, with the greatest tendency towards superconductivity occurring in the orthorhombic phase.

Anderson[1] has proposed that the correct model to describe the CuO_2 planes in the high-T_c superconductors is the two-dimensional Hubbard model *without phonons:* only the electrons in the outer d orbitals of the Cu^{2+} ions are retained, and the O^{2-} ions are ignored entirely. The electron density is believed to be 1 for pure La_2CuO_4 and decreases with Sr or Ba doping. Adjusting the O-deficiency in $YBa_2Cu_3O_{7-x}$ should adjust the filling factor in this material as well, although in a less obvious way (due to the presence of the CuO chains). It is well known that in the limit $U/|t| \gg 1$ for a half-filled band the model reduces to the Heisenberg antiferromagnet, with no charge transport. Estimates suggest that $U \approx 5$ eV, $t \approx 1$ eV, and indeed undoped La_2CuO_4 seems to be an insulator well described by the Heisenberg model. The doped compound $La_{2-\delta}Sr_\delta CuO_4$, with electron density $1-\delta$, is superconducting for $\delta \approx 0.15$.[2] Meanwhile, an orthorhombic to tetragonal structural transition occurs at approximately the same value of δ, with the orthorhombic phase being stable at lower δ.[2]

It is clearly very important to understand whether the Hubbard model can produce this behavior. Anderson and collaborators[3,4] have developed a language and a mean-field theory for understanding these phenomena based on the notion of "resonating valence bonds." Almost nothing is known rigorously about either the $s=\frac{1}{2}$ Heisenberg model or the Hubbard model on a square lattice.

Diagonalization of small systems[5] suggests that the Heisenberg model Néel orders at $T=0$. Indeed Néel order has been observed in some La_2CuO_4 samples.[6] Recent experimental studies[7] of the two-dimensional magnetic correlations have also been performed. It is possible that the Néel order is purely a three-dimensional effect and the two-dimensional system might *not* order, even at $T=0$.

A related issue is the nature of the gap for spin excitations. Experimental indications of a linear low-temperature specific heat have been reported[8] suggesting a gapless Fermi surface as was predicted by RVB theory.[3,4] A theorem due to Lieb, Schultz, and Mattis[9] seems to imply[10] that either gapless excitations or broken translational symmetry occurs.

In this paper we attempt to shed light on these issues by applying a systematic approximation to the Heisenberg and Hubbard models based on the large-n limit.[11] We replace the two spin components of the electron by n "flavor" components, and let n become large. In lowest order in $1/n$ we essentially perform a Hartree-type factorization. However, unlike other mean-field theories, in this approach systematic calculations of corrections (in higher powers of $1/n$) are possible. We do not make any *a priori* assumptions about symmetry breaking. Furthermore, the lowest-order calculation is the exact solution of a physically sensible model (albeit not the right one). If $n=2$ is sufficiently large we should expect our conclusions to be at least qualitatively correct. Alternatively, certain phase transitions may occur as a function of n.

We begin by discussing the Heisenberg model in the large-n limit. In the ordinary ($n=2$) case, we may write the Heisenberg interaction in terms of electron operators as $\mathbf{S}_i \cdot \mathbf{S}_j = (\frac{1}{2}) c_{i\alpha}^\dagger c_{i\beta} c_{j\beta}^\dagger c_{j\alpha} +$ constant. (Repeated flavor indices such as α and β are summed over the two spin components.) To obtain the Hilbert space of the spin model, rather than an itinerant electron model, we must project out states with one electron on each site. We generalize this to arbitrary n by writing the interaction the same way but letting the spin indices α and β run from 1 to n and projecting out states with $n/2$ electrons per site, assuming that n is even. (The model with one electron on the even sublattice and $n-1$ on the odd sublattice is also interesting and will be discussed elsewhere.) For the ordinary ($n=2$) antiferromagnet, an arbitrary singlet state can be represented by a valence bond diagram in which each site is attached to precisely one other site. For general n, we must draw $n/2$ valence bonds eminating from each site. (For general n, a valence bond represents a diagonal sum over electron and hole indices on two different sites.) Thus, there will be, in general, a large number of valence bonds on each link. In the ordinary ($n=2$) case, when the Hamiltonian acts on a link not containing a valence bond it annihilates the two bonds terminating at the ends of the link and creates a bond on that link and another (non-nearest-neighbor) bond between the two disconnected spins. The same is true for arbitrary n. Although there are $n/2$ bonds terminating at each site, acting with the Hamiltonian annihilates only *two* bonds and creates two new ones, with a linear superposition of all the

possible ways of doing this. Thus fluctuations in the relative number of valence bonds on each link are suppressed at large n. This bond number becomes a classical quantity in our large-n approximation. One attractive feature of these models is that the Lieb-Schultz-Mattis theorem[9] generalizes to arbitrary n.[12]

We solve the model at large n by a path-integral method. This allows us to introduce the valence bond operator $\chi_{ij} = (J/n) c_{i\alpha}^{\dagger} c_{j\alpha}$ by a Hubbard-Stratonovich transformation. At large n we may ignore its fluctuations. The Hamiltonian can be written as

$$H = \sum_{(i,j)} [(n/J) |\chi_{ij}|^2 + (c_{j\alpha}^{\dagger} c_{i\alpha} \chi_{ij} + \text{H.c.})] .$$

An additional Lagrange multiplier field must be introduced to enforce the constraint on the number of electrons on each site. However, it plays no role to leading order at large n and will be dropped in this simplified discussion. We now simply minimize the ground-state energy (or free energy) with respect to the classical numbers χ_{ij}. A subtlety arises because of gauge invariance. The exact conservation of the particle number at *each site* implies invariance under phase rotations of the c_j's with arbitrary space and time dependence[13] $c_j \rightarrow c_j \exp(i\theta_j)$. χ transforms as $\chi_{jk} \rightarrow \chi_{jk} \exp[i(\theta_j - \theta_k)]$. Thus, the phases of $\chi_{jk} = |\chi_{jk}| \exp(i\theta_{jk})$ act as components of the gauge field. The sum of the θ_{jk}'s around an elementary plaquette is gauge invariant; it corresponds to the magnetic flux through the plaquette. Compact gauge symmetries are not broken in lattice gauge theories. Gauge-equivalent saddle points must be averaged over so that only gauge-invariant quantities have nonzero expectation values. In particular,

$$\chi_{jk}^{\dagger} \chi_{jk} = (J/n)^2 (c_{k\alpha}^{\dagger} c_{j\alpha})(c_{j\beta}^{\dagger} c_{k\beta}) \propto \mathbf{S}_j \cdot \mathbf{S}_k + \text{const}$$

may be nonzero. $(n/J^2)\chi_{jk}^{\dagger}\chi_{jk}$ is the number of valence bonds on the link jk, a classical number for large n. [For $n=2$ the number of valence bonds on any link is at most one, but we may interpret $(n/J^2)\chi_{jk}^{\dagger}\chi_{jk}$ as the probability of a valence bond lying on the link.]

It is tempting to assume that χ_{ij} has a uniform real value on all links. In this case, the reduced Hamiltonian is simply the standard tight-binding model with hopping parameter χ. However, as discussed below, this is *not* the minimum energy configuration. Due to the Fermi surface instability (which results from perfect nesting in the tight-binding model), the energy can be reduced by allowing χ_{ij} to have an alternating part. The reduced Hamiltonian is then a tight-binding model with a nonuniform hopping parameter. We will assume the simplest form of χ consistent with a locally stable minimum. This configuration has a unit cell of length $\sqrt{2}$, corresponding to symmetry of translation across diagonals of the original square lattice. This symmetry permits four independent χ's as shown in Fig. 1. We must calculate the dispersion relation for the tight-binding model with these nonuniform hopping parameters. Because there are two inequivalent sublattices, this dispersion relation has two branches,

$$E_{\pm}(K_x,K_y) = \pm |\chi_1 \exp(ik_x) + \chi_2^* \exp(ik_y) + \chi_3 \exp(-ik_x) + \chi_4^* \exp(-ik_y)| .$$

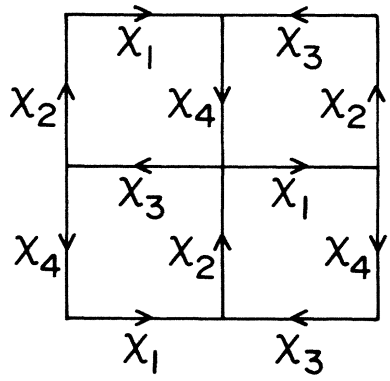

FIG. 1. Definition of the four χ's consistent with invariance under translation across a diagonal.

To calculate the ground-state energy as a function of the χ's we must sum the energies of the lower branch (since the band is half filled) and then add the term quadratic in χ. We have done a computer search and find two locally stable minima. The first one, which we refer to as the Peierls phase, has only one of the four χ's nonzero. Each spin forms a dimer with one of its nearest neighbors; hence the electronic spectrum is completely localized, with a gap $E_{\pm}(\mathbf{k}) = \pm |\chi|$.

The second phase, which we call the flux phase, has all four χ's equal in *magnitude* and the sum of the four phases, the flux, is π. There is only one gauge-inequivalent state of this kind. Choosing the gauge in which all the $\chi_i = |\chi| e^{i\pi/4}$, the electronic spectrum becomes

$$E(\mathbf{k}) = \pm |2\chi| [\cos^2 k_x + \cos^2 k_y]^{1/2} .$$

Note that the gap only vanishes at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$. It vanishes linearly here, and the low-energy theory is the $(2+1)$ dimensional relativistic free fermion quantum-field theory. Consequently, the spin-correlation function drops off as $1/(\text{distance})^4$. Note that the translational symmetry appears to be broken because of the nonzero phase, since χ_1 and χ_3, for example, are oriented in opposite directions (see Fig. 1). This phenomena is a gauge artifact however, since we can always find a gauge transformation that makes χ_1 and χ_3 real. The constraint on the number of particles implies that only particle-hole excitations are permitted with gapless modes at $(0,0)$, $(\pi,0)$, $(0,\pi)$, (π,π).

These results are consistent with the Lieb-Schultz-Mattis theorem.[9,10] In the Peierls phase the symmetry of translation by one site is spontaneously broken, and in the flux phase there are gapless excitations of wave vector $(\pi,0)$.

We have, in fact, checked that these solutions are local minima with respect to arbitrary *space-dependent* variations of χ. We find that the Peierl's phase is slightly lower in energy, the energies per site being $-nJ/8$ and $-0.115nJ$.

We have also solved the general Hubbard-Heisenberg

model in the large-n limit. The Hamiltonian is

$$H=\sum_{(i,j)}[t(c_{i\alpha}^{\dagger}c_{j\alpha}+c_{j\alpha}^{\dagger}c_{i\alpha})+(J/n)c_{i\alpha}^{\dagger}c_{i\beta}c_{j\beta}^{\dagger}c_{j\alpha}]$$
$$+(U/n)\sum_{i}(c_{i\alpha}^{\dagger}c_{i\alpha}-n/2)^2.$$

We again make the χ_{ij} Hubbard-Stratonovich transformation to eliminate the Heisenberg interaction. A second Hubbard-Stratonovich transformation must also be made to eliminate the Hubbard interaction. This second variable (the analog of the Lagrange multiplier needed for the pure Heisenberg model) again plays no role to leading order in $1/n$ and is dropped from the following discussion. We thus end up with the same reduced Hamiltonian as before except that the effective hopping parameter is now $\chi_{ij}+t$:

$$H=\sum_{(i,j)}\{(n/J)|\chi_{ij}|^2+[c_{j\alpha}^{\dagger}c_{i\alpha}(\chi_{ij}+t)+\text{H.c.}]\}.$$

We have again performed a computer search for the minimum with the same symmetry assumption as before (leading to the four independent χ's). The phase diagram depends on t/J and on the doping δ, defined by the number density $\frac{1}{2}n(1-\delta)$. At $\delta=0$ (half filling) we find a Fermi surface instability for arbitrarily small J/t which makes χ have an imaginary or nonuniform part. At large J/t a partially dimerized, or Peierls state, has lowest energy (one of the χ's is larger in magnitude than the rest). Thus, the number of valence bonds $(n/J^2)|\chi|^2$ is larger on one type of link on than the others. This state may be called a bond-centered charge-density wave, since we should probably regard the electron wave functions as being concentrated on the link when they form a valence bond.

For smaller J/t the ground state has all χ's equal with a nonzero phase. This breaks the translational symmetry since neighboring parallel bonds, e.g., χ_1 and χ_3 have opposite orientation. This state is not dimerized, however, because the number of valence bonds $(n/J^2)|\chi|^2$ is the same on all links. Rather, the symmetry is broken by a diamagnetic current flowing around the plaquettes in an alternating sense. [Note that the current on the link kl is $i(c_{k\alpha}^{\dagger}c_{l\alpha}-c_{l\alpha}^{\dagger}c_{k\alpha})=i(n/J)(\chi_{kl}-\chi_{kl}^{*})$.] Only at $t=0$, the pure Heisenberg case, does this current become an unobservable gauge artifact.

At sufficiently large doping (which becomes exponentially small for small J/t), this instability disappears, and the ground state has a real, uniform χ. This corresponds to a simple Fermi-liquid state, as proposed by Anderson and co-workers.[1,3,4] The only effect of the Heisenberg interaction is the renormalization of the effective hopping term.

We also found a fourth phase at intermediate doping. (See Fig. 2.) The χ's are real and $\chi_1=\chi_2\neq\chi_3=\chi_4$ (or $\chi_1=\chi_4\neq\chi_2=\chi_3$). Thus the links with a higher valence bond (or electron) density (for example, χ_1 and χ_2) form zig-zag lines through the lattice. These "strong bonds" should have an excess electron density, and hence an excess negative charge. The weak bonds (e.g., χ_3 and χ_4) should have a net positive charge. If we regard this charge excess as residing in the vicinity of the O atom in the middle of the Cu bond, then neighboring O's on strong bonds repel each other. This could lead to shifting of the O's off the Cu planes in an alternating fashion, as observed in the orthorhombic phase of $La_{2-x}Sr_xCuO_4$. However, this phase may imply a distortion of the Cu lattice of a type which is *not* observed. The strong bonds should get shorter, and the weak ones get longer, due to the attraction or repulsion of the Cu ions by the charge excess on the links. This would distort the square Cu plaquette into a "kite"—a four-sided figure with pairs of adjacent sides equal in length—which differs from the observed distortion of the square into a rhombus.

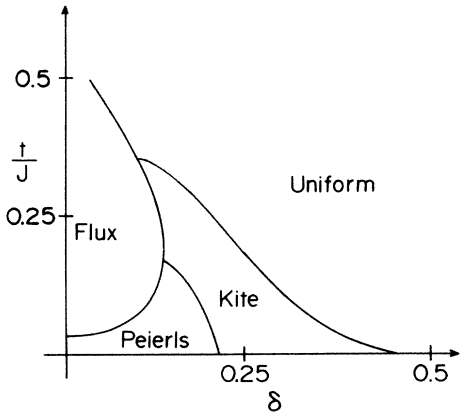

FIG. 2. Approximate phase diagram of the $n\to\infty$ Heisenberg-Hubbard model as a function of Heisenberg exchange constant and doping.

Although off-diagonal long-range order does not occur in the large-n limit, the tendency towards it, as a function of doping, can be related to the "stiffness" of the phases of the χ_{ij}'s. This stiffness determines the rigidity of the superconducting order parameter. We find the stiffness is largest in the "orthorhombic" phase and goes rapidly to zero in the tetragonal phase.

We also find that the phase diagram evolves continuously with temperature. Our results are consistent with general theorems about symmetry breaking in two-dimensional systems since we only find breaking of *discrete* lattice symmetries. A breaking of the continuous symmetries, corresponding to antiferromagnetic and superconductivity, may occur at $T=0$ for sufficiently small n. More details about the stiffness of the superconducting order parameter, the dependence on temperature, and the likely variation with n will be given elsewhere.

Our most important result is perhaps the discovery of a possible disordered gapless phase for the Heisenberg model, which is consistent with the Lieb-Schultz-Mattis theorem. We expect that a phase of this type is possible for $n=2$. It may become the true ground state for small enough n (lower in energy than the Peierls phase) if Néel order does not occur. We also found that, for large n, a Fermi-surface instability always introduces a gap for half filling, destroying the Fermi-liquid phase. Thus at small doping the specific heat should be exponential (Peierls

phase) or quadratic (flux phase). This instability can be removed by doping or by other effects such as second nearest-neighbor couplings. Once the Fermi-surface instability has been removed, the specific heat becomes linear. We also found an electronic mechanism which might drive the orthorhombic distortion. Finally, we found a dependence of the rigidity of the superconducting order parameter on doping which agrees qualitatively with the observed dependence of T_c on doping.

We thank P. W. Anderson, G. Baskaran, and E. Fradkin for useful conversations. I. A. was supported by the Canadian Institute for Advanced Research, and J. B. M. was supported by the National Science Foundation.

[1]P. W. Anderson, Science **235**, 1196 (1987).

[2]J. D. Jorgensen, H.-B. Schuttler, D. G. Hinks, D. W. Capone II, K. Zhang, M. B. Brodsky, and D. J. Scalapino, Phys. Rev. Lett. **58**, 1024 (1987).

[3]P. W. Anderson, Science **235**, 1196 (1987); G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. (to be published); P. W. Anderson, G. Baskaran, and Z. Zou (unpublished); Z. Zou and P. W. Anderson (unpublished); G. Baskaran and P. W. Anderson (unpublished).

[4]P. W. Anderson, G. Baskaran, Z. Zou, and T. Hsu, Phys. Rev. Lett. **58**, 2790 (1987).

[5]J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978).

[6]D. Vaknin, S. K. Sinha, D. E. Moncton, D. C. Johnston, J. M. Newsam, C. R. Safinya, and H. E. King, Jr., Phys. Rev. Lett. **58**, 2802 (1987).

[7]G. Shirane, Y. Endoh, R. J. Birgeneau, M. A. Kastner, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami (unpublished).

[8]N. E. Phillips, R. A. Fisher, S. E. Lacy, C. Marcenat, J. A. Olson, W. K. Ham, and A. M. Stacy (unpublished); E. Airniebl, J. Willis, J. Thompson, C. Huang, and J. Smith (unpublished).

[9]E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).

[10]I. Affleck (unpublished).

[11]I. Affleck, Phys. Rev. Lett. **54**, 966 (1987).

[12]I. Affleck and E. Lieb, Lett. Math. Phys. **12**, 57 (1986).

[13]The invariance under time-dependent gauge transformations was pointed out to us by E. Fradkin.