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Spin disorder in the two-dimensional Hubbard model: A mean-field theory

G. Vignale

Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, Missouri 65211

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A scheme of symmetry breaking is proposed for the two-dimensional Hubbard model at less than half filling. The self-induced mean field is a random spin-dependent potential. The energy of the spin-disordered state is shown to be lower than that of commensurate or incommensurate antiferromagnetic states. Long-wavelength charge and spin fluctuations obey the diffusion equation, leading to deviations from Fermi-liquid behavior. At wave vector $\mathbf{q}=(\pi,\pi)$ the transverse spin-excitation spectrum has a gap.

The recently discovered copper oxide–based superconductors[1] have a rich phase diagram. Transitions between antiferromagnetic (AFM) and superconducting phases are induced by relatively small compositional changes.[2] The simplest model that appears to have the potential to describe such complex behavior is the two-dimensional Hubbard model.[3] At half filling (filling fraction $x=50\%$) this model has a commensurate AFM ground state.[4] Far away from half filling its ground state is paramagnetic. An outstanding theoretical question is to determine the character of the ground state at intermediate filling fractions. Most theoretical work thus far has focused on the case of very small departures from half filling. In that regime the AFM state has been found to be unstable with respect to various types of incommensurate structures[5–8] and/or localized defects.[9,10] For larger departures from half filling—characteristic of superconducting composition—even these defective AFM states become unstable.

In this paper I study the ground state of the Hubbard model at filling fractions $x<50\%$ within the frame of Hartree-Fock mean-field theory. I show that, at least in a range of concentrations ($20\%<x<45\%$) and interaction strengths, the system admits an enormous number of spin-disordered states (SDS) whose mean-field energies are lower than those of the commensurate AFM state, or its incommensurate version.[5] These SDS's are characterized by a random spin density and by a finite Edwards-Anderson order parameter. Effectively then, the SDS is a spin-glass phase, except that spin disorder is entirely *self-induced.*

I start from the standard one-band Hubbard Hamiltonian

$$H=-t\sum_{\langle i,j\rangle s}(c_{is}^{\dagger}c_{js}+c_{js}^{\dagger}c_{is})+U\sum_{i}n_{i\uparrow}n_{i\downarrow}\,, \tag{1}$$

where c_{is} is the destruction operator of an electron at site i, with spin projection s, and $\langle i,j\rangle$ indicates summation over all nearest-neighbor pairs on a square lattice. Although in the region of interest the Coulomb repulsion U is comparable to the bandwidth $W=8t$, the Hartree-Fock (HF) approximation is still the natural starting point for a systematic treatment of many-body effects. Inclusion of many-body corrections can be achieved by standard techniques (e.g., the loop expansion) which have already enjoyed considerable success in the half-filled case.[9–11]

Obtaining an unrestricted solution of the HF equations for the Hamiltonian (1) at arbitrary filling fraction is a very complex numerical task. A good deal of insight into the character of the solution can be obtained by considering the phase diagram of Fig. 1, showing the regions of relative stability (within HF) of the paramagnetic (PM), commensurate antiferromagnetic, and ferromagnetic (FM) states. The most remarkable feature is the close proximity of the AFM and FM regions: the energies of the two phases coincide along the boundary line. This suggests that near the phase boundary, the system may be a mixture of ferro- and antiferromagnetic regions. This idea is supported by the observation[5] that doping the AFM state with few holes creates domain walls across which the phase of the AFM order parameter slips by π. The relative orientation of a pair of neighboring spins on opposite sides of a linear wall is ferromagnetic. As the density of domain walls increases so does the number of ferromagnetic pairs of spins. Like in conventional spin glasses, the most likely result of a competition between ferro- and antiferromagnetic pairings is a randomly disor-

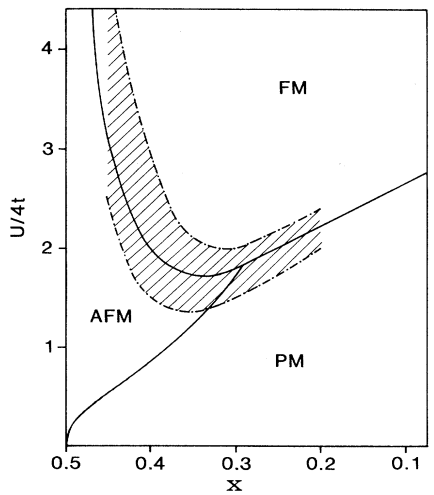

FIG. 1. Hartree-Fock phase diagram for the two-dimensional Hubbard model. AFM, FM, and PM denote antiferromagnetic, ferromagnetic, and antiferromagnetic ground states, respectively. The shaded region indicates the approximate stability region of the model spin disorder state introduced in the text. x is the filling fraction.

dered spin state.[12]

To make the above ideas more quantitative, I propose as a variational wave function for (1) the ground-state wave function of the following one-electron Hamiltonian:

$$H_{\text{eff}} = -t \sum_{\langle i,j\rangle s} (c_{is}^{\dagger} c_{js} + c_{js}^{\dagger} c_{is}) + \sum_{i,ss'} (\mathbf{V}_i \cdot \boldsymbol{\sigma})_{ss'} c_{is}^{\dagger} c_{is'} . \quad (2)$$

The symmetry-breaking field $\mathbf{V}_i$ is regarded as a set of variational parameters. The expectation value of H in the ground state of H_{eff} must be minimized with respect to $\mathbf{V}_i$'s. Usually $\mathbf{V}_i$ is taken to be a highly symmetric function in real space; but in this case I regard $\mathbf{V}_i$ as a random function of position. To simplify the subsequent calculations I assume that the spin densities point in the z direction, i.e.,

$$\mathbf{V}_i = (0,0,V_i) , \quad (3)$$

where V_i is a random variable that can take the values $+\Delta$ and $-\Delta$ with equal probability. The V_i's on different sites are assumed to be uncorrelated. This schematic model[13] is already sufficient to give lower variational energy than commensurate or incommensurate AFM states.

I have calculated the average energy of the model SDS by two different methods. (i) Exact diagonalization of H_{eff} on a 10×10 lattice with periodic boundary conditions. In this case the energy to be minimized with respect to Δ is given by

$$E_1(\Delta) = \sum_{as} \varepsilon_{as} f_{as} + U \sum_i \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle - \sum_i V_i (\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle) , \quad (4a)$$

where ε_{as} are the exact eigenvalues of H_{eff}, and f_{as} is the Fermi distribution at zero temperature. (ii) Coherent-potential approximation[14] (CPA) for an infinite lattice. The energy functional to be minimized in this case is

$$E_2(\Delta) = -2\pi^{-1} \sum_{\mathbf{k}} \int_{-\infty}^{E_f} \varepsilon_{\mathbf{k}} \operatorname{Im} \bar{G}(\mathbf{k}, \omega + i\eta) d\omega + U \sum_i \langle\langle n_{i\uparrow}\rangle\rangle_{+\Delta} \langle\langle n_{i\downarrow}\rangle\rangle_{+\Delta} , \quad (4b)$$

where $\epsilon_k = -2t(\cos k_x + \cos k_y)$ is the usual tight-binding dispersion, $\bar{G}(k,\omega)$ is the average CPA Green's function, E_F is the Fermi energy, and $\langle\langle n_{is}\rangle\rangle_{\pm\Delta}$ are disorder averages of $\langle n_{is}\rangle$ subject to the condition that the potential on site i be $\pm\Delta$. Notice that because the energy is self-averaging, it only depends on the parameters characterizing the statistical distribution of the V_i's. (To within fluctuations of order 1 per size of the system.)

The curve for $E_1(\Delta)$ is plotted in Fig. 2, for the representative case $U=8t$, filling fraction $x=40\%$. The curve for $E_2(\Delta)$ would be barely distinguishable from the one for $E_1(\Delta)$ on the scale of this graph. The minimum is found at $\Delta = 0.35U$. The close agreement between the CPA and the finite lattice calculation convincingly demonstrates that localization and finite-size effects do not significantly affect the energy functional.

In Fig. 2 I have also plotted the energy of the AFM state and of the incommensurate AFM (IAFM) state, with parameters as proposed by Schulz.[5] Both curves lie above the SDS one, although the IAFM is considerably closer. The CPA density of states at the optimum Δ is

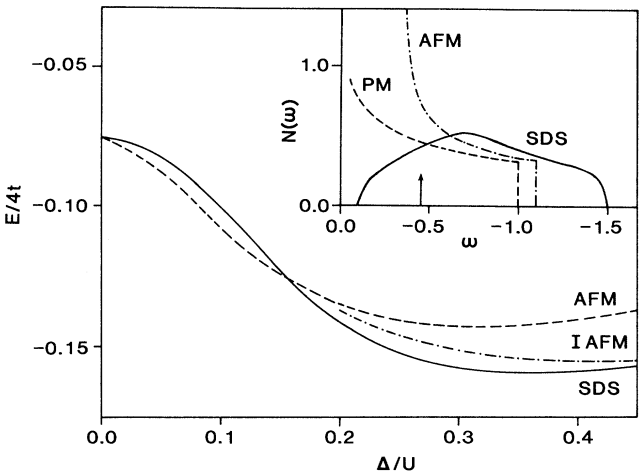

FIG. 2. Energy vs "order parameter" Δ for AFM, IAFM, and SDS ground states at $U=8t$, $x=40\%$. IAFM has wave vector $\mathbf{q}=(2.712,\pi)$ as suggested in Ref. 5. Inset: density of states for PM ($\Delta=0$), AFM ($\Delta=0.32U$), and model SDS ($\Delta=0.35U$). The arrow indicates the position of the Fermi energy in the SDS.

shown in the inset of Fig. 2. The mechanism of energy reduction in the SDS appears to be mainly associated with the "softening" of the gap compared to the AFM state.

The region of stability of the present model at $T=0$ is sketched in Fig. 1. I believe that this region can be extended by allowing for more variational flexibility, for instance, by including some degree of short-range order. At finite temperature, thermal fluctuations will greatly favor the SDS relative to an ordered state. This agrees with the fact that neither ferro- nor antiferromagnetism was observed in computer simulations of the two-dimensional Hubbard model in the non-half-filled case.[4]

It is important to appreciate the profound difference between the present theory and previous "alloy analogy" treatments of the Hubbard model.[15,16] In the latter, a random potential was introduced to model the effect of correlations (i.e., the many-body self-energy) in the paramagnetic state. This led to violations of Fermi-liquid theory in the weak-coupling limit. In the present work no correlation effects have been considered. The SDS is a mean-field solution characterized by true static spin disorder, which can be experimentally measured.

Of course, one cannot rule out the possibility that strong fluctuations, not included in the present calculation, might completely destroy any static arrangement of spins. In that case, the correct physical picture would be that of a paramagnetic spin liquid—a sort of time-dependent SDS in which the spin-orientations fluctuate in space and time. The present solution should then be regarded as a static approximation to the true dynamical state.

I now discuss some of the physical consequences of the SDS. The response of the system to an external probe is determined by the average two-particle correlation functions

$$\chi^{c(zz)}(\mathbf{q},\Omega) = \chi_0^{l}(\mathbf{q},\Omega)[1-(+)\chi_0^{l}(\mathbf{q},\Omega)]^{-1} \quad (5a)$$

for charge $(-)$ and longitudinal spin $(+)$ correlations, and

$$\chi^{+-}(\mathbf{q},\Omega)=\chi_0^t(\mathbf{q},\Omega)[1+U\chi_0^t(\mathbf{q},\Omega)]^{-1} \quad (5b)$$

for transverse spin correlations. χ_0^l and χ_0^t are the longitudinal and transverse response functions of $H_{\rm eff}$, evaluated at a locally stable configuration of the effective field.[17] In the CPA, χ_0^l and χ_0^t are given by

$$\chi_0^{l(t)}(\mathbf{q},\Omega)=\sum_{\mathbf{k}}\int\frac{d\omega}{2\pi i}\bar{G}(\mathbf{k}+\mathbf{q},\omega+\Omega)\bar{G}(\mathbf{k},\omega)\times\Gamma^{l(t)}(\mathbf{q},\omega+\Omega,\omega), \quad (6)$$

where Γ is the well-known CPA vertex correction.[18]

The calculation of χ_s is a cumbersome numerical task. However, some elegant analytic results can be derived for the special cases $\mathbf{q}\cong 0$ and $\mathbf{q}=\mathbf{Q}=(\pi,\pi)$.

(i) $\mathbf{q}\cong\mathbf{0}$. The CPA vertex correction $\Gamma(\mathbf{q},\omega+\Omega+i\eta,\omega-i\eta)$ has a pole when q and Ω tend to zero and $\omega=E_F$. Hence, the longitudinal response function takes the familiar diffusion form

$$\chi_0^l(\mathbf{q},\Omega)=N(E_F)\frac{Dq^2}{-i\Omega+Dq^2}. \quad (7)$$

Here $N(E_F)$ is the density of states per spin at the Fermi energy, and $D>0$ is the bare diffusion constant, which can be calculated in the CPA. Equation (7) is just a statement that density fluctuations of either spin obey a diffusion equation at long wavelength and low frequency. The presence of diffusion, combined with the electron-electron interaction in two dimensions leads to several interesting deviations from standard Fermi-liquid theory.[19] For instance, the inverse lifetime $1/\tau$ of an exact eigenstate of $H_{\rm eff}$ scales at $T=0$ as $E-E_F$,[20] rather than $(E-E_F)^2$. A linear behavior of the quasiparticle width as a function of $E-E_F$ has been indeed observed in photoemission experiments on high-T_c superconductors.[21] I note, incidentally, that the observation of a Fermi surface in angle-resolved photoemission experiments is *not* incompatible with the existence of spin disorder. A Fermi surface can still be seen because the spectral function of quasiparticles remains peaked in momentum space.[22] However, since the quasiparticle width is comparable to its energy, the system is at best a "marginal" Fermi liquid.

(ii) $\mathbf{q}=(\pi,\pi)$. At this value of q the spectrum of *noninteracting* transverse spin excitations can be calculated exactly. The result is

$$-\pi^{-1}\mathrm{Im}\chi_0^t(\mathbf{q},\Omega+i\delta)=\tfrac{1}{2}N(\Omega/2)\theta(|\Omega|-2|E_F|). \quad (8)$$

Note that the spectrum vanishes for $|\Omega|<2|E_F|$, irrespective of the form of the random potential. Thus, the noninteracting transverse spin spectrum has a gap of magnitude $2|E_F|$. This result is a consequence of the following theorem: *For V_i in the form of Eq. (3), if $\psi_{as}(\mathbf{l})$ is an eigenfunction of $H_{\rm eff}$, with energy E and spin s, then $\psi_{-a-s}(\mathbf{l})\equiv e^{i\mathbf{Q}\cdot\mathbf{l}}\psi_{as}(\mathbf{l})$ is also an eigenfunction of $H_{\rm eff}$ with energy $-E$ and spin $-s$.* (The proof is by direct substitution.) The application of a transverse probe with momentum transfer $\mathbf{Q}$ will therefore excite a spin s electron with energy $E<E_F(<0)$ to a $-s$ state with energy $E>-E_F$. The minimum excitation energy in the process is $2|E_F|$. Since there is a finite density of states at E_F, the excitation spectrum will have a finite discontinuity at $2|E_F|$.

Consider now the interacting transverse correlation function, given by Eq. (5b). The denominator $1+U\chi_0^t(\mathbf{Q},\Omega)$ is plotted in Fig. 3. At $\Omega=0$ its real part is found to be positive, as it must be if the SDS is stable. As $\Omega\to 2|E_F|$, it diverges logarithmically to $-\infty$, due to the discontinuity in the imaginary part. Thus, the interacting response function *must* have a pole at some frequency between 0 and $2|E_F|$. I interpret this pole as a bound exciton formed by an electron and a hole with opposite spins and energies (relative to the center of the band).

It should be clear from the above discussion that the existence of the bound exciton does not depend on the specific form of the one-electron potential and thus it does not unambiguously characterize the SDS. In particular, a paramagnetic state could also support the bound exciton. Within the frame of the Hartree-Fock theory of the Hubbard model, this does not appear to be the case: the paramagnetic state becomes unstable well before the bound exciton can emerge as a significant collective excitation of the system. However, a strongly correlated paramagnetic state, for which the HF description is invalid, *could* support the exciton.

The magnetic spectrum of the SDS is dramatically different from that of an antiferromagnet (even a "short-range" one) in that low-energy damped spin waves are absent. The SDS also has a zero-frequency Goldstone mode, corresponding to a global rotation of all spins. However, because of the random orientations of the spins, this mode does not overlap significantly with any plane-wave probe. It plays no role in neutron-scattering experiments.

The above results have interesting implications for the interpretation of inelastic neutron-scattering experiments[23] on superconducting samples of $YBa_2Cu_3O_{6+x}$. At $x=0.45$, $T_c=45$ K, it was found that the system has an antiferromagnetic correlation length extending over several lattice constants at low temperature. The low-energy excitation spectrum (3 meV) near momentum transfer $\mathbf{Q}$ was successfully interpreted in terms of

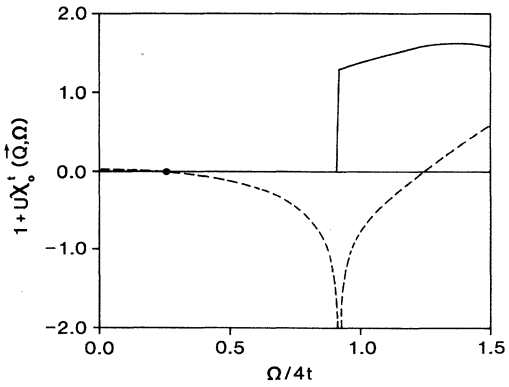

FIG. 3. Denominator of the transverse spin susceptibility, Eq. (5b), vs Ω at $q=(\pi,\pi)$. The zero of the real part determines the energy of the bound exciton.

damped spin waves.[23,24] At $x=0.5$, $T_c=50$ K, however, the antiferromagnetic correlation length appears to drop by an order of magnitude. (See Table II in Ref. 23.) The low-energy cross section also drops dramatically, but a peak in the cross section is still observed at considerably higher energy (10 meV).

I propose that the $x=0.5$ sample is a realization of the SDS. The peak at finite energy should then be interpreted as the bound exciton state.[25] This interpretation is also supported by the stability of the $x=0.5$ spectrum with increasing temperature. The $x=0.45$ sample, which is locally ordered, has a temperature-dependent spectrum, which becomes similar to that of the disordered sample as T increases.

In summary, I have proposed in this paper a scheme of symmetry breaking in which the self-induced mean field is a random spin-dependent potential. I have shown that a spin-disordered state is a definite possibility from the energy and stability point of view, and that it leads to definite predictions about the nature of the charge- and spin-excitation spectra, which can be tested by experiment.

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