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Stability of the ferromagnetic state with respect to a single spin flip: Variational calculations for the $U=\infty$ Hubbard model on the square lattice

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We generalize a variational wave function for the $U=\infty$ Hubbard model recently proposed by Shastry *et al.* [Phys. Rev. B **41**, 2375 (1990)] to study the stability of the ferromagnetic state with respect to a single spin flip, and for the square lattice find an instability above a hole density $\delta=0.41$. The form of our wave function is consistent with the picture suggested by Roth [J. Phys. Chem. Solids **28**, 1549 (1967); Phys. Rev. **184**, 451 (1969); **186**, 428 (1969)] that the flipped spin binds an electron of opposite spin. We also obtain good upper bounds on the energy of spin-wave excitations for $\delta<0.41$. Our values for the effective spin-wave stiffness are smaller but generally in agreement with those of Shastry *et al.*

The $U=\infty$ Hubbard model was originally introduced as a theory of itinerant ferromagnetism[1] and has recently enjoyed renewed interest as a limiting case of related Hubbard models of relevance to the theory of high-T_c superconductivity.[2] However, progress on this difficult model has been slow and only a small number of analytical results,[3-9] and exact numerical calculations[10-12] are available. The earliest rigorous result by Nagaoka,[6] and independently Thouless,[7] showed that the ground state of one hole in the $U=\infty$ Hubbard model on a bipartite lattice is the ferromagnetic state (also called Nagaoka state). This theorem breaks down with even two holes and certainly says nothing about a finite density of holes in the thermodynamic limit. More recently Shastry, Krishnamurthy, and Anderson[3] set a rigorous upper bound to the ground-state energy of a finite density of holes with one spin flipped. Their results show that for sufficiently large hole density the Nagaoka state is unstable with respect to a single spin flip. Moreover, at low hole density the positive excitation energy of their flipped spin state is closely reproduced by Barbieri, Riera, and Young[12] who obtained the exact ground state for up to four holes and one flipped spin on an 8×8 lattice. An essential step in the latter calculation was an *average* over boundary conditions that minimizes the effects of shell closure in the hole distribution on a finite lattice.

The purpose of this Rapid Communication is to introduce a generalization of the Shastry *et al.* trial wave function in a simplified language which admits a systematic sequence of improvements. With this generalization we decrease the critical hole density above which the Nagaoka state is unstable on the square lattice from the Shastry *et al.* value $\delta=0.49$ to 0.41. We propose a second trial wave function for the calculation of the spin-wave excitations and again improve on the results of Shastry *et al.* In both of our wave functions correlations are introduced in the real-space neighborhood of the flipped spin. We conclude by suggesting further refinements of our wave functions.

In the usual language of the dynamics of the electrons, the $U=\infty$ Hubbard Hamiltonian is given by

$$H=-\sum_{\langle ij\rangle,\sigma}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma}+\text{H.c.}), \tag{1}$$

where $\tilde{c}_{i\sigma}=c_{i\sigma}(1-c^{\dagger}_{i,-\sigma}c_{i,-\sigma})$, $c_{i\sigma}$ annihilates an electron of spin σ at site i, $\langle ij\rangle$ are nearest-neighbor pairs, and H.c. stands for Hermitian conjugate. We measure all energies in units where the hopping matrix element is unity. Clearly H in (1) commutes with the z component of the total spin s_z and the total crystal momentum $\mathbf{p}$, and so can be transformed into blocks where both s_z and $\mathbf{p}$ have definite values. Concentrating on that spin sector with only one flipped spin, one realizes that H can be equivalently written in a language of the dynamics of holes (spinless fermions) in the presence of a flipped spin (which is always translated to the origin). Namely,

$$H=H_0+H_I, \tag{2}$$

where

$$H_0=-\sum_{\langle ij\rangle}(a^{\dagger}_{\mathbf{r}_i}a_{\mathbf{r}_j}+\text{H.c.}), \tag{3a}$$

$$H_0=\sum_{\mathbf{k}}\varepsilon(\mathbf{k})a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}, \tag{3b}$$

and

$$H_I=\sum_{\mathbf{s}}(a^{\dagger}_{\mathbf{s}}a_0+\text{H.c.})-\sum_{\mathbf{s}}\exp(i\mathbf{s}\cdot\mathbf{p})a^{\dagger}_{-\mathbf{s}}T_{\mathbf{s}}a_{\mathbf{s}}, \tag{4a}$$

$$H_I=-\frac{1}{N_s}\sum_{\mathbf{k}_1,\mathbf{k}_2}a^{\dagger}_{\mathbf{k}_1}[\varepsilon(\mathbf{k}_1)+\varepsilon(\mathbf{k}_2)-\varepsilon(\mathbf{p}+\mathbf{k}_1+\mathbf{k}_2+\Sigma_{\mathbf{k}}\mathbf{k}a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}})]a_{\mathbf{k}_2}. \tag{4b}$$

Here $a^{\dagger}_{\mathbf{r}_i}$ creates a hole at site i in an otherwise all spin-up background and obeys fermionic anticommutation relations, $\mathbf{s}$ is one of the four nearest neighbors to the origin $\mathbf{r}=0$, N_s is the number of lattice sites which we take to infinity, and $T_{\mathbf{s}}$ is the operator which translates all the holes by $-\mathbf{s}$,

$$T_{\mathbf{s}}=\prod_{\mathbf{k}}\exp(i\mathbf{s}\cdot\mathbf{k}a^{\dagger}_{\mathbf{k}}a_{\mathbf{k}}). \tag{5}$$

On the square lattice $\varepsilon(\mathbf{k}) = -2(\cos k_x + \cos k_y)$. The presence of the flipped spin has been entirely incorporated in H_I: terms in H_0 which hop a hole onto the origin are replaced by effective hops of length two that result when the flipped spin is restored to the origin (requiring a translation of the whole system).

In our language, the Shastry *et al.* wave function (unnormalized) takes on the following form:

$$|\psi_S\rangle = a_0 |F+1\rangle . \tag{6}$$

Here $|F+1\rangle$ is the ground state of H_0 with one extra hole at the Fermi surface, i.e.,

$$|F\rangle = \prod_{\mathbf{k}<\mathbf{k}_F} a_{\mathbf{k}}^\dagger |0\rangle , \quad |F+1\rangle = a_{\mathbf{k}_F}^\dagger |F\rangle , \tag{7}$$

where $\mathbf{k} < \mathbf{k}_F$ indicates that $\mathbf{k}$ is below a hole Fermi surface and $|0\rangle$ is the *vacuum state,* i.e., all sites occupied by spin-up electrons. This wave function gives the upper bound,[3]

$$\Delta_S = \left(\varepsilon_F - \frac{\varepsilon_0}{\delta}\right) - \varepsilon(\mathbf{p})\left(\delta - \frac{\varepsilon_0^2}{16\delta}\right) , \tag{8}$$

where $\varepsilon_F = \varepsilon(\mathbf{k}_F)$, and

$$\varepsilon_0 = \frac{E_F}{N_s} = \frac{1}{N_s}\sum_{\mathbf{k}<\mathbf{k}_F} \varepsilon(\mathbf{k}) , \tag{9}$$

is the ground-state energy per site of H_0. The quantity E_F in (9) also represents the energy of the fully spin-aligned (ferromagnetic) state. The minimum of Δ_S occurs at $\mathbf{p} = (\pi,\pi)$ for all δ.

Our generalization of (6) is

$$|\psi_T\rangle = a_0 a_0^\dagger \sum_{\mathbf{r}} f_{\mathbf{r}} a_{\mathbf{r}} |F+1\rangle , \tag{10}$$

where $f_{\mathbf{r}}$ are variational parameters and $a_0 a_0^\dagger$ ensures that no hole is at the origin. Since $|\psi_T\rangle$ is unnormalized, we are required to minimize

$$\Delta_T = \frac{\langle\psi_T|(H-E_F)|\psi_T\rangle}{\langle\psi_T|\psi_T\rangle} . \tag{11}$$

By straightforward algebra, the numerator in (11) is given by

$$\sum_{\mathbf{r}_1,\mathbf{r}_2} f_{\mathbf{r}_1}^* f_{\mathbf{r}_2} M_{\mathbf{r}_1\mathbf{r}_2} ,$$

where

$$M_{\mathbf{r}_1\mathbf{r}_2} = [\varepsilon_F - \varepsilon(\mathbf{p})]V(\mathbf{r}_1)V(\mathbf{r}_2) + [(1-\delta)\varepsilon_F - \varepsilon_0]V(\mathbf{r}_2-\mathbf{r}_1) + \sum_{\mathbf{s}} V(\mathbf{r}_2-\mathbf{r}_1-\mathbf{s})[(1-\delta) - \exp(i\mathbf{s}\cdot\mathbf{p})V(\mathbf{s})] , \tag{12}$$

and

$$V(\mathbf{r}) = \int_{\mathbf{k}<\mathbf{k}_F} \frac{d^2k}{(2\pi)^2} \cos(\mathbf{k}\cdot\mathbf{r}) . \tag{13}$$

In deriving (12), we have used the identity

$$\varepsilon(\mathbf{k}) = -\sum_{\mathbf{s}} \exp(i\mathbf{s}\cdot\mathbf{k}) . \tag{14}$$

Similarly, the denominator in (11) is given by

$$\sum_{\mathbf{r}_1,\mathbf{r}_2} f_{\mathbf{r}_1}^* f_{\mathbf{r}_2} N_{\mathbf{r}_1\mathbf{r}_2} ,$$

where

$$N_{\mathbf{r}_1\mathbf{r}_2} = (1-\delta)V(\mathbf{r}_2-\mathbf{r}_1) + V(\mathbf{r}_1)V(\mathbf{r}_2) . \tag{15}$$

Minimizing (11) is equivalent to finding the ground state of an effective Hamiltonian operating on the real-space components $f_{\mathbf{r}}$:

$$H_{\text{eff}} = N^{-1/2} M N^{-1/2} . \tag{16}$$

As a technical point, we note that the two-dimensional (2D) integral (13) can be done by integrating over k_x first and doing the remaining 1D integral by Gaussian Tchevyshev integration with at least 20 points. We restrict our cluster size to the 61 lattice sites closest to and including the origin, so that M and N are 61×61 matrices. The energy expectation Δ_T is well converged with this cluster size.

Figure 1 compares Δ_T with the old bound Δ_S. Again, we find that Δ_T is minimized for $\mathbf{p} = (\pi,\pi)$. The new instability point, above which $\Delta_T < 0$, occurs at $\delta = 0.41$. (The ferromagnetic state is actually slightly unstable at exactly $\delta = 0.41$.) An examination of the amplitudes $f_{\mathbf{r}}$ shows that the region of hole depletion near the flipped spin is strongly localized. The ground-state $f_{\mathbf{r}}$ values for $\delta = 0.41$ are given in Table I. We note that these amplitudes decay rapidly away from the origin and have an interesting angular variation. Since a localized deficit of one hole is equivalent to an excess of one spin-aligned electron near the flipped spin, our results bear out the Green's-function calculation of Roth.[4,5]

Next we address the question of spin-wave excitations (Goldstone modes) for densities where the Nagaoka state is stable. For this we consider the following wave function which explicitly contains particle-hole excitations:

$$|\psi_{\text{SW}}\rangle = a_0 a_0^\dagger \left(g_0 + \sum_{\mathbf{r}_1,\mathbf{r}_2} g_{\mathbf{r}_1\mathbf{r}_2} a_{\mathbf{r}_1}^\dagger a_{\mathbf{r}_2}\right) |F\rangle . \tag{17}$$

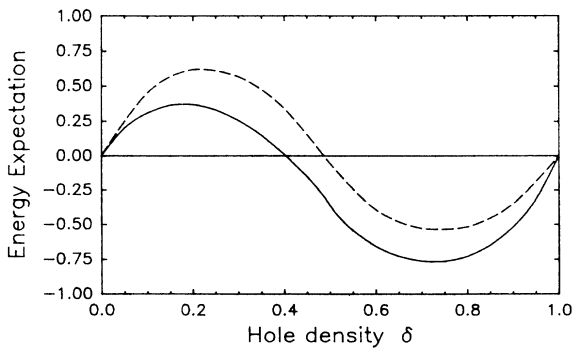

FIG. 1. The energy expectations of $|\psi_S\rangle$ (dashed line) and $|\psi_T\rangle$ (solid line), as a function of hole density.

TABLE I. The ground-state f_r values for $\delta=0.41$. The positions of the values in the table correspond to lattice sites with the underlined position as the origin. The probability of a hole being annihilated in this 25-site region of the 61-site cluster is 94%.

+0.0015	−0.1209	−0.0826	−0.1209	+0.0015
−0.1209	−0.0446	−0.2433	−0.0446	−0.1209
−0.0826	+0.2433	+0.7417	+0.2433	−0.0826
−0.1209	−0.0446	+0.2433	−0.0446	−0.1209
+0.0015	−0.1209	−0.0826	−0.1209	+0.0015

Here, g_0 and $g_{r_1r_2}$ are variational parameters. The wave function proposed by Shastry *et al.* for calculating the spin-wave excitations corresponds to setting $g_0=0$, $g_{r_1r_2}=0$ whenever $r_2\neq 0$, and not insisting that r_1 is localized near the origin.

We proceed to evaluate Δ_{SW} using (11) with $|\psi_{SW}\rangle$ replacing $|\psi_T\rangle$ and obtain expressions similar to (12) and (15). To reduce computational time, the low-energy eigenvalues of the effective Hamiltonian can be obtained (using a Lanczos algorithm) by calculating $H_{\text{eff}}=N^{-1}M$ rather than (16). Both give the same energy spectrum, although their eigenvectors differ. We are then able to consider cluster sizes up to 21 sites about the origin.

We find, consistent with previous work,[3–5] that the spectrum has a spin-wave branch $\varepsilon_{SW}(\mathbf{p})$ separated from a continuum of states by a gap. Figure 2 depicts our results for $\varepsilon_{SW}(\mathbf{p})$ and the top of the gap for crystal momenta along the (1,1) direction with $\delta=0.34$ and 0.41. For $\delta=0.34$ a comparison with the calculation of Shastry *et al.* is possible and we find lower energies for $\varepsilon_{SW}(\mathbf{p})$, although we are qualitatively in agreement. However, our calculation of the top of the gap does not show the same qualitative agreement; in particular, we find that the gap persists to the zone boundary, whereas the Shastry *et al.* calculation shows that it vanishes at an intermediate value of $\mathbf{p}$. Our form of $|\psi_{SW}\rangle$ only contains local correlations in the vicinity of the flipped spin, but the continuum states are not expected to be localized. Therefore, we do not expect our calculation of the gap to be conclusive and in fact find slow convergence with cluster size implying that our maximum cluster size of 21 sites is too restrictive. This question may be better addressed by relaxing the constraint that r_1 be localized in (17) although keeping (as Shastry *et al.* do) r_2 localized.

Of particular interest is the behavior of $\varepsilon_{SW}(\mathbf{p})$ for small $\mathbf{p}$, as a function of δ, especially near the critical density $\delta=0.41$. The spin-wave stiffness D is defined by

$$\varepsilon_{SW}(\mathbf{p})=Dp^2+O(p^4), \tag{18}$$

in units where the lattice constant is unity. We obtain D

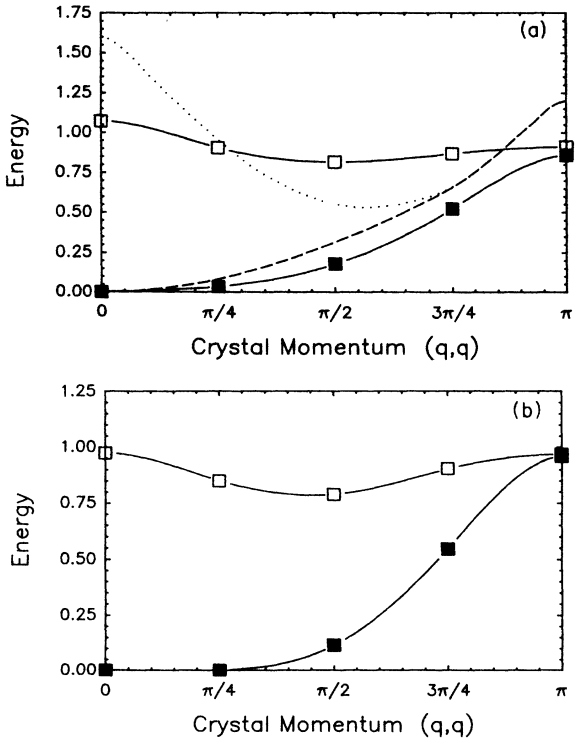

FIG. 2. Spin-wave dispersion, $\varepsilon_{SW}(\mathbf{p})$ (solid squares) and the top of the gap (open squares) along the (1,1) direction for (a) $\delta=0.34$ and (b) $\delta=0.41$. In (a) we compare with the Shastry *et al.* calculation of $\varepsilon_{SW}(\mathbf{p})$ (dashed line) and the top of the gap (dotted line). The solid lines connecting our points are only guides for the eye.

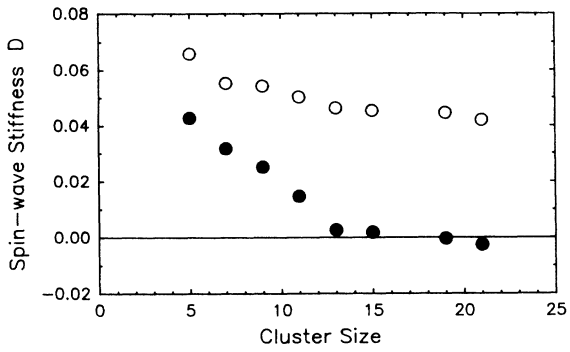

FIG. 3. The convergence of spin-wave stiffness D with cluster size for $\delta=0.2$ (open circles) and $\delta=0.41$ (solid circles). All clusters are chosen with sites closest to the origin and inversion symmetry.

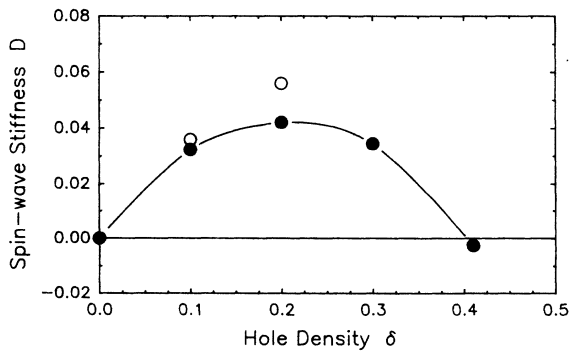

FIG. 4. The spin-wave stiffness D as a function of hole density δ calculated with a 21-site cluster (solid circles). The two open circles are stiffnesses calculated by Shastry *et al.*

by numerical differentiation using four **p** points: (q,q) with $q=0.05$, 0.10, 0.15, and 0.20. The convergence of D with cluster size is plotted in Fig. 3 for $\delta=0.2$ and 0.41. Although D is not completely converged with 21 sites it does give a good upper bound. Figure 4 shows the variation of D with δ. We see that our values of D for $\delta=0.1$ and 0.2 lie below those obtained by Shastry *et al.* Note that D becomes marginally negative at $\delta=0.41$, consistent with the fact that the Nagaoka state is unstable at exactly $\delta=0.41$. The picture that emerges from this calculation is that, for $0<\delta<0.41$, the itinerant holes give a small amount of rigidity to the aligned spins resulting in the stability of the Nagaoka state.

In conclusion, by adding real-space correlations in the vicinity of the flipped spin to the wave functions proposed by Shastry *et al.*, we have obtained a new critical density, $\delta=0.41$, above which the Nagaoka state is unstable and improved on the upper bound of the spin-wave excitation energy and stiffness for $0<\delta<0.41$. Further improvements on both of these results can be obtained by refinements of (10) and (17) in a perturbative manner, namely,

$$|\psi_T\rangle = a_0 a_0^\dagger \left(\sum_{\mathbf{r}} f_{\mathbf{r}} a_{\mathbf{r}} + \sum_{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3} f_{\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3} a_{\mathbf{r}_1}^\dagger a_{\mathbf{r}_2} a_{\mathbf{r}_3} \right) |F+1\rangle , \tag{19}$$

and

$$|\psi_{SW}\rangle = a_0 a_0^\dagger \left(g_0 + \sum_{\mathbf{r}_1,\mathbf{r}_2} g_{\mathbf{r}_1\mathbf{r}_2} a_{\mathbf{r}_1}^\dagger a_{\mathbf{r}_2} + \sum_{\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4} g_{\mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4} a_{\mathbf{r}_1}^\dagger a_{\mathbf{r}_2}^\dagger a_{\mathbf{r}_3} a_{\mathbf{r}_4} \right) |F\rangle . \tag{20}$$

Because of the substantial increase in computational effort posed by these wave functions, calculations involving them are not being contemplated.

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