Spin-Peierls ground states of the quantum dimer model: A finite-size study

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Exact diagonalization results on the quantum dimer Hamiltonian of Rokhsar and Kivelson on lattice sizes up to 6×6 are presented. Correlation functions of a new order parameter characterizing the crystalline states of the model are calculated. All of the results are consistent with the existence of a direct transition between a columnar crystalline state and a staggered crystalline state with no intermediate spin-fluid state. However, the existence of a spin-fluid state over a small, but finite, range of parameters has not been definitively ruled out.

INTRODUCTION

The quantum dimer model was introduced recently by Rokhsar and Kivelson[1] (RK) as a phenomenological description of a non-Néel phase of the spin-$\frac{1}{2}$ Heisenberg quantum antiferromagnet on a square lattice. Interest in the latter model is motivated partly by the suggestion of Anderson[2] that properties of the non-Néel phase are important in understanding the occurrence of high temperature superconductivity in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-x}$.[3] In a phase with exponentially decaying *two-spin* correlation functions, RK argued that it was a reasonable approximation to truncate the Hilbert space to states that can be expressed as a tensor product of nearest-neighbor singlet pairs of spins. There is clearly a one-to-one mapping between such states and the set of all close-packed dimer coverings of the square lattice. RK also argued that the effects of the nonorthogonality of these states could be absorbed into a redefinition of the parameters in the following phenomenological Hamiltonian H acting upon an orthogonal basis set of states represented by all the different close-packed dimer coverings of the square lattice:

$$H=-J\sum_{\square}|\,\|\,\rangle\langle\,=\,|+\text{H.c.}+V\sum_{\square}|\,\|\,\rangle\langle\,\|\,|+V\sum_{\square}|\,=\,\rangle\langle\,=\,|\,. \tag{1}$$

The dark lines denote dimers on the links of the square lattice and all the sums extend over all the elementary plaquettes of the square lattice. The first term is a dimer kinetic energy and the last two terms are the diagonal potential energies. Read and Sachdev[4] have recently shown that H may be obtained in a formal $1/N$ expansion of a particular nearest-neighbor SU(N) antiferromagnet with the states at each site transforming with an appropriately chosen representation of SU(N), and exchange constant J_s; at order $1/N$ the parameters obtained in this expansion are $J=2J_s/N$ and $V=0$. We also have the correspondence $n_d(\mathbf{r}+\hat{\mathbf{e}}/2)\sim-\mathbf{S}(\mathbf{r})\cdot\mathbf{S}(\mathbf{r}+\hat{\mathbf{e}})$ between the dimer number operators $n_d(\mathbf{R})$ and the spin-$\frac{1}{2}$ generators $\mathbf{S}$ of the Heisenberg model ($\hat{\mathbf{e}}$ is an elementary link of the square lattice). The symbol $\sim$ implies that correlation functions of n_d in the ground state of the dimer Hamiltonian H should have the same asymptotic form as the corresponding correlation functions of $\mathbf{S}(\mathbf{r})\cdot\mathbf{S}(\mathbf{r}+\hat{\mathbf{e}})$ in the non-Néel phase of the Heisenberg antiferromagnet.

In a separate development, Read and Sachdev[4,5] have shown, using several different semiclassical and $1/N$ expansions of SU(N) antiferromagnets, that the non-Néel phase exhibits spin-Peierls or valence-bond solid order. For the quantum-dimer model, these phases correspond to a *crystallization* of the dimer bosons into a "column" state with the *symmetry* of Fig. 1(a); note that this state is fourfold degenerate and completely breaks the Z_4 lattice rotational symmetry.

We briefly review known results and open questions on the properties of H:

(i) The dimer states are characterized by conserved winding numbers (N_x,N_y) (Ref. 1) (specified below) with $-L/2<N_x,N_y<L/2$ on a $L\times L$ lattice.

(ii) For $V>J$ the exact ground state is the fourfold degenerate "staggered" crystalline state[1] shown in Fig. 1(b). These states have winding numbers $(\pm L/2,0)$ and $(0,\pm L/2)$.

(iii) At exactly $V=J$, the lowest energy states in *all* the

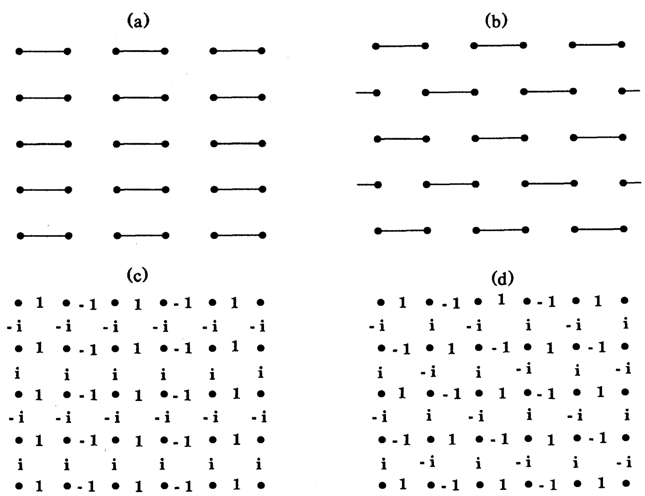

FIG. 1. (a) The *perfectly* ordered column state and (b) the staggered state; this state is the ground state of H for $V>J$. (c) The phase factors θ and (d) ζ on the links of the lattice.

winding-number sectors are degenerate; these states are equal superpositions of all dimer coverings with a fixed winding number.[1] Correlation functions in the equal-superposition state on a square lattice with free boundary conditions [this restricts the state to be in the (0,0) winding-number sector] can be exactly calculated using the results of Fisher and Stephenson;[6] we shall refer to this particular eigenstate as the Fisher-Stephenson (FS) state. The FS state has no broken lattice symmetry: correlations of the column state order parameter, introduced below, fall off as $1/r^2$.[7]

(iv) For $V<\kappa J$, where $\kappa \leq 1$ is an unknown constant, the ground state of H breaks lattice rotational symmetry and crystallizes into a state with the symmetry of the column state shown in Fig. 1(a). Thus, there is a possible range of values $\kappa J \leq V \leq J$ over which H displays a spin-fluid ground state. In fact, RK suggested that $\kappa<1$ and that the spin fluid was thus stable over a finite range of V.

The primary purpose of this paper is to obtain more information on the value of κ by exact diagonalization of H on a $L\times L$ lattice with periodic boundary conditions with sizes up to $L=6$. Our results allow us to conclude with reasonable certainty that $\kappa>0.5$, although all of our results are consistent with a value $\kappa=1$. Thus for the parameters obtained in the $1/N$ expansion ($V=0$), we find a crystalline ground state.

It is useful at this juncture to introduce the complex order parameters $\Psi_{\rm col}^p(\mathbf{r})$ to measure the breaking of rotational symmetry in the column phase

$$\Psi_{\rm col}^p(\mathbf{r})=\sum_{\hat{\mathbf{e}}}[\theta(\mathbf{r}+\hat{\mathbf{e}}/2)]^p n_d(\mathbf{r}+\hat{\mathbf{e}}/2)\,, \tag{2}$$

where, as before, the sum over $\hat{\mathbf{e}}$ extends over $\hat{\mathbf{x}}$, $-\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $-\hat{\mathbf{y}}$; the $\theta(\mathbf{R})$ take the fixed values 1, i, -1, and $-i$ on the links of the square lattice, as shown in Fig. 1(c), and are chosen such that under a rotation by $n\pi/2$ about any point on the A sublattice $\Psi_{\rm col}^p \rightarrow e^{in\pi p/2}\Psi_{\rm col}^p$, while on the B sublattice $\Psi_{\rm col}^p \rightarrow e^{-in\pi p/2}\Psi_{\rm col}^p$. These properties imply that $\langle \Psi_{\rm col}^p\rangle=0$ for $p\neq(\mathrm{mod}4)$ in any spin-fluid state with unbroken lattice rotational symmetry while $|\langle\Psi_{\rm col}^p\rangle|\neq 0$ for $p\neq(\mathrm{mod}4)$ in the column phase.

The order parameter associated with the staggered state is

$$\Psi_{\rm st}^p(\mathbf{r})=\sum_{\hat{\mathbf{e}}}[\zeta(\mathbf{r}+\hat{\mathbf{e}}/2)]^p n_d(\mathbf{r}+\hat{\mathbf{e}}/2)\,, \tag{3}$$

where $\zeta(\mathbf{R})$ takes the values shown in Fig. 1(d). Note that $\Psi_{\rm col}^2=\Psi_{\rm st}^2$. It can also be shown that $\sum_{\mathbf{r}\in A}\Psi_{\rm st}^1(\mathbf{r})=L(N_y+iN_x)$, where the summation over $\mathbf{r}$ extends over the A sublattice, and N_x and N_y are the *conserved winding numbers.*[1] The connection of $\Psi_{\rm st}$ with the conserved winding numbers will restrict its utility in the finite-size calculations presented below.

NUMERICAL RESULTS

With momentum and winding-number conservation the calculation required diagonalization of matrices of dimensions up to 1256: the diagonalization was carried out by a modified Lanczos method.[8] We note that an analogous procedure on a 8×8 lattice would require diagonalization of matrices of order 10^6, which is clearly prohibitive. For all $V<J$ the ground state of H was found in the winding number $(N_x,N_y)=(0,0)$ sector. All of the correlation functions presented below are obtained with the Hilbert space *restricted to the (0,0) winding-number sector for all values of V.* For $V<J$, this implies that, for large enough system sizes, the low-energy states will consist of domains of the staggered states in different orientations; the domains are chosen in a manner that restricts the global winding number to (0,0). The order parameter correlation functions are trivially calculable in the exact staggered ground state [Fig. 1(b)] for $V>J$ and do not yield any useful information.

We begin by measuring the correlation function

$$\chi^1=\frac{1}{L^2}\left\langle\left|\sum_{\mathbf{r}\in A}\Psi_{\rm col}^1(\mathbf{r})\right|^2\right\rangle. \tag{4}$$

In a phase with long-range column-phase order we expect $\chi^1 \sim L^2$ for large L, while $\chi^1\sim O(1)$ in a spin-fluid or staggered phase. In the FS ground state at $V=J$ we find $\chi_{\rm FS}^1\sim(\log L)^2$. The results of the numerical calculations of χ^1 for $L=4$ and $L=6$ are shown in Fig. 2. We note that (i) for $V<J$, the strong size dependence of χ^1 and its almost linear dependence upon V/J are consistent with presence of long-range column phase order, and (ii) for $V>J$, the large value of χ^1 for the 4×4 lattice is due to the impossibility of inserting two domains of the staggered phase in this lattice size; the (0,0) winding-number sector is thus strongly frustrated.

A further probe of the nature of the ground state is offered by the quantity g:

$$g=\frac{\left\langle\left|\sum_{\mathbf{r}\in A}\Psi_{\rm col}^1(\mathbf{r})\right|^4\right\rangle}{\left\langle\left|\sum_{\mathbf{r}\in A}\Psi_{\rm col}^1(\mathbf{r})\right|^2\right\rangle^2}\,, \tag{5}$$

the ratio of the fourth moment of the order parameter to the square of its second moment. In a phase with long-range column-phase order we expect $g\rightarrow 1$ as $L\rightarrow\infty$. However, in a spin-fluid or staggered phase, the fluctuations in $\Psi_{\rm col}^1$ can be expected to be Gaussian, in which case

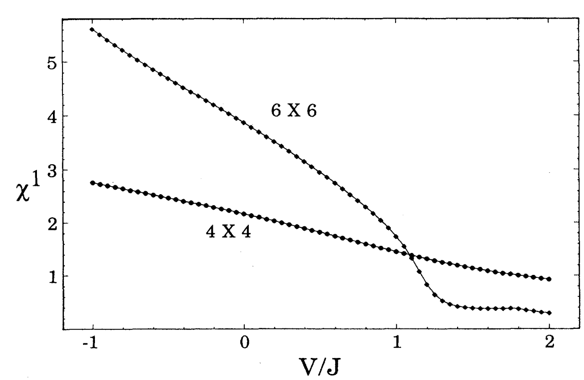

FIG. 2. The correlation function χ^1 [Eq. (4)] as a function of V/J.

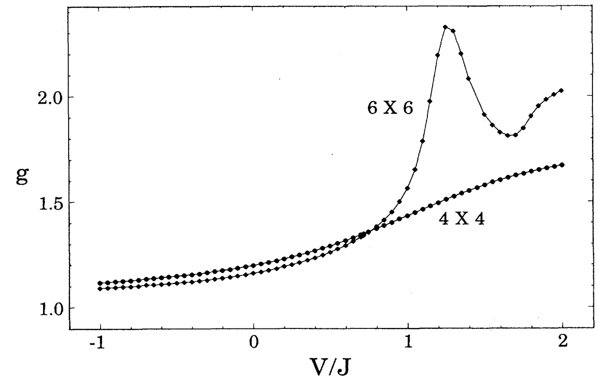

FIG. 3. The quantity g [Eq. (5)] as a function of V/J.

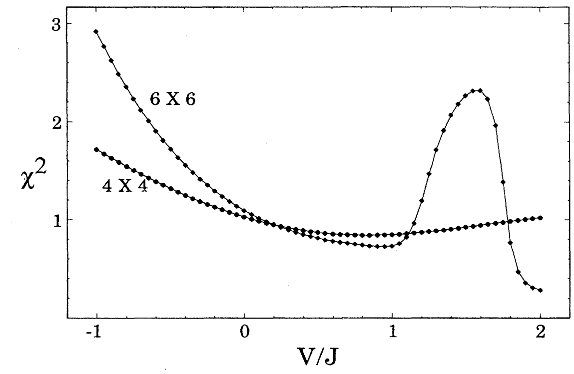

FIG. 5. The correlation function χ^2 [Eq. (7)] as a function of V/J.

$g \to 2$ and $L \to \infty$. The values of g are shown in Fig. 3. We note (i) the rapid increase in the value of g for $L=6$ near $V/J \approx 1$ as indicating a crossover from a column phase to the staggered phase; (ii) the oscillations in the value of g for $L=6$ and $V>J$ can be traced to (a) changes in the structure of the domain walls as a function of V/J, and (b) the small value of χ^1 whose square appears in the denominator for the expression for g; (iii) the value of g for the FS state can be calculated to be $g_{\mathrm{FS}}=2$.

The spatial structure of the state can be investigated by the correlation function

$$G(\mathbf{r})=\langle \Psi_{\mathrm{col}}^{1*}(\mathbf{r}_1)\Psi_{\mathrm{col}}^{1}(\mathbf{r}_1+\mathbf{r})\rangle . \tag{6}$$

For $\mathbf{r},\mathbf{r}_1 \in A$, the function $G(\mathbf{r})$ can be shown to be real. The results for $G(\mathbf{r})$ are shown in Fig. 4 for $L=6$ and a range of values of V/J. Also shown are the values of $G_{\mathrm{FS}}(\mathbf{r})$, the correlation functions in the FS state. The differences in the values of $G_{\mathrm{FS}}(\mathbf{r})$ and $G(\mathbf{r})$ for $V=J$ in (0,0) winding-number sector (shown in Fig. 5 by the inverted triangles) are due to finite-size corrections. Thus the nonmonoticity of $G(\mathbf{r})$ at the two largest values of $|\mathbf{r}|$ is a finite-size correction. For $V=0$ and $V=0.5J$, the function $G(\mathbf{r})$ clearly appears to asymptote at a nonzero value as $|\mathbf{r}| \to \infty$, implying long-range column-phase order. The order parameter $\langle \Psi_{\mathrm{col}}^{1} \rangle$ satisfies $\lim_{\mathbf{r}\to\infty} G(\mathbf{r}) = |\langle \Psi_{\mathrm{col}}^{1} \rangle^2$: we thus obtain estimates of $|\langle \Psi_{\mathrm{col}}^{1} \rangle|$ of 0.53 and 0.40 for $V=0$ and $V=0.5J$, respectively. (Ψ_{col}^{1} has been chosen such that a completely ordered rigid column state would have an order-parameter expectation value of 1.)

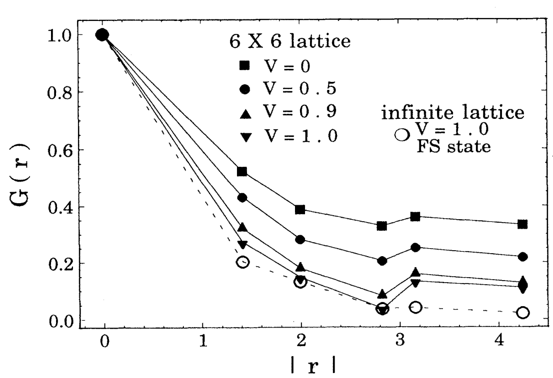

FIG. 4. The correlation function $G(\mathbf{r})$ [Eq. (6)] as a function of the Euclidean distance $|\mathbf{r}|$ for various values of V/J on a 6×6 lattice. Also shown are the correlation functions in the infinite lattice FS state.

Finally, we measure x-y symmetry breaking by examining the order parameter Ψ^2 (as $\Psi_{\mathrm{col}}^2=\Psi_{\mathrm{st}}^2$, we will drop the subscript). We numerically evaluated the correlation function

$$\chi^2=\frac{1}{L^2}\left\langle \left| \sum_{\mathbf{r}\in A} \Psi^2(\mathbf{r}) \right|^2 \right\rangle . \tag{7}$$

We now expect $\chi^2 \sim L^2$ in *both* the column and the staggered phases. An intermediate spin-fluid phase would have $\chi^2 \sim O(1)$. The values of χ^2 for $L=4$ and $L=6$ are shown in Fig. 5. The sharp minimum in χ^2 for $L=6$ at $V=J$ is consistent with the restoration of Z_2 symmetry at precisely $V=J$ and nowhere else. The sharp dropoff in the value of χ^2 at $V=1.6J$ for $L=6$ is due to changes in the structure of the domain walls between the different staggered-phase domains; we obtain staggered phases rotated by 90° with respect to each other, which drastically reduces the value of $\sum_{\mathbf{r}\in A}\Psi^2$.

CONCLUSIONS

We have found convincing evidence for the crystallization of the dimers into a state with the symmetry of Fig. 1(a) for $V<0.5J$. However, the simplest scenario consistent with all of the data is the persistence of the column phase right up to $V=J$. For $V>J$, the model is known to be in the staggered ground state; the point $V=J$ will then be a special singular point displaying power-law dimer correlations. It is notable that none of the data show any *explicit* signal of the existence of spin-fluid order over a finite range of V. We cannot, however, definitively rule out the existence of the spin-fluid phase over a small, but finite, range of V. Monte Carlo simulations on an 8×8 lattice will therefore be of considerable interest.

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