

## Criterion for a good variational wave function

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The variance of the Hamiltonian in a given variational wave function measures how good an eigenstate this wave function is. In some instances, as for the two-dimensional antiferromagnetic Heisenberg Hamiltonian (2D AFH), the energy expectation value is not enough to distinguish between different trial *Ansätze*. Here we propose the variance as a simple criterion, which allows for further differentiation between degenerate trial wave functions. We show that this criterion establishes the projected wave functions as candidates for the ground state of the 2D AFH. A strong interference effect is discovered in computer experiment.

### INTRODUCTION

Variational wave functions are powerful tools in condensed matter physics. The *variational principle* guarantees that they provide an exact upper bound for the estimate of the ground-state energy of a given physical system. Their usefulness lies in the presumption that the lower the variational estimate of the ground-state energy, the better the wave function. This, the usual criterion of wave-function quality, has been used successfully in many circumstances.

Lately, in the context of strongly correlated electron systems, a breakdown has been observed of this simple measure of quality, i.e., how close to the ground state a given variational wave function is. More specifically, a variety of different trial wave functions<sup>1,2</sup> have been proposed for the ground state of the two-dimensional (2D) antiferromagnetic Heisenberg Hamiltonian (AFH), which may be viewed as the limiting model of the  $t$ - $J$  Hamiltonian at zero doping. These wave functions have physically very distinct properties. Some of them show antiferromagnetic long-range order, others do not. Some are formulated in terms of spin operators, others in terms of anticommuting fermion operators. Nevertheless, many of them yield about the same variational estimate for the ground-state energy, which is very close to that obtained by other numerical methods, especially by the Green's-function Monte Carlo method.<sup>3</sup> On the basis of energy expectation values alone, one cannot choose a best trial wave function for the 2D antiferromagnetic Heisenberg Hamiltonian from among those proposed so far.

Recently, some successful calculations have been performed in order to attest the quality of a given wave function by other means than the energy expectation value alone. One of the prominent studies is that of the Laughlin wave function for the fractional quantum Hall effect,<sup>4</sup> where the overlap matrix element with the exact ground state for systems with 3 to 5 particles could be evaluated. Similar studies of variational wave functions have been performed for the case of the  $t$ - $J$  model<sup>5</sup> and that of fractional-statistics particles.<sup>6</sup>

In a different context, the question of the ground state of atoms and small molecules continues to attract attention. One of the problems of interest in this field is the

functional form for the wave functions which recovers most of the correlation energy. Umrigar, Wilson, and Wilkins<sup>7</sup> have shown that in this context it might be more efficient not to minimize the energy, but the variance of the Hamiltonian (see Ref. 7 also for reference to earlier ideas on this subject).

In this paper we consider a criterion for what constitutes a good trial wave function which may be evaluated for relatively large systems (with 50–150 degrees of freedom) by a Monte Carlo method. We will define the variance of the Hamiltonian as a measure that indicates how good an eigenstate a variational wave function is. We have calculated this measure for a projected wave function which supports a superposition of both an antiferromagnetic and a  $d$ -wave order parameter. The measure shows an extraordinary interference effect which proves it a valuable criterion for the goodness of a given trial wave function. Since the measure is very easy to compute (in many evaluations of trial wave functions it could be obtained as a by-product), the knowledge of its behavior is of general interest. Furthermore, we will discuss some of the physical consequences for the case of projected wave functions.

### HAMILTONIAN

Let us first define the Hamiltonian to which we will apply the method to be developed in this paper. The antiferromagnetic Heisenberg Hamiltonian with a coupling anisotropy is given by

$$H_{J_z, J_\perp}(N \times N) = \sum_{\langle i, j \rangle} [J_z S_i^z S_j^z + J_\perp / 2 \times (S_i^+ S_j^- + S_i^- S_j^+)] , \quad (1)$$

where  $J_z \geq J_\perp > 0$  are the strengths of the Ising and transverse couplings, and  $\langle i, j \rangle$  are pairs of a nearest neighbor of an  $N \times N$  square lattice with periodic boundary conditions. The spin operators are given in terms of the underlying fermion operators as  $S_i^z = \frac{1}{2} (c_{i,1}^\dagger c_{i,1} - c_{i,1}^\dagger c_{i,1})$  and  $S_i^+ = c_{i,1}^\dagger c_{i,1}$ . When considering a variational approach to this Hamiltonian, a key feature to keep in mind is that the thermodynamic and the isotropic limits

do not commute:

$$H_1 \equiv \lim_{N \rightarrow \infty} \lim_{J_{\perp} \rightarrow J_z} H_{J_z, J_{\perp}}(N \times N) \neq \lim_{J_{\perp} \rightarrow J_z} \lim_{N \rightarrow \infty} H_{J_z, J_{\perp}}(N \times N) \equiv H_2. \quad (2)$$

Both  $H_1$  and  $H_2$  might be viewed as representations of the antiferromagnetic Heisenberg model on an infinite lattice. They are expected to support a linearly dispersing Goldstone mode, as a consequence of the continuous spin-rotation symmetry. The first one,  $\lim_{J_{\perp} \rightarrow J_z} H_{J_z, J_{\perp}}(N \times N)$ , which is normally studied in numerical approaches on finite lattices, has a singlet ground state and shows antiferromagnetic long-range order<sup>3</sup> in the thermodynamic limit without breaking spin-rotation symmetry explicitly. Consequently, in the ground state

$$\langle S_i^z S_j^z \rangle = \frac{1}{2} (\frac{1}{2} \langle S_i^+ S_j^- + S_i^- S_j^+ \rangle),$$

for all  $N$  and all dimensions. [The factor  $\frac{1}{2}$  inside the parentheses originates from the  $J_{\perp}/2$  in Eq. (1).] On the other side, the ground state of  $H_2$  does break spin-rotational symmetry explicitly and shows a staggered moment in the  $z$  direction. (This might also be called a spontaneously broken symmetry.) It is this Hamiltonian which most variational approaches attempt to describe. A less-well-known property of the ground state of  $H_2$  is that  $\langle S_i^z S_j^z \rangle \approx 1.00 (\frac{1}{2} \langle S_i^+ S_j^- + S_i^- S_j^+ \rangle)$ , to a high level of accuracy.<sup>8</sup> This factor  $\approx 1.00$  is a consequence of the two dimensionality, in higher dimensions  $\langle S_i^z S_j^z \rangle \gg \langle S_i^+ S_j^- + S_i^- S_j^+ \rangle$ . (In infinite dimensions the Néel state will become asymptotical to the exact ground state.) It is this property of  $H_2$  that we will take into account later on.

### METHOD

Now I will explain the method. Let us denote by  $|\psi\rangle$  some favorite trial wave function. In order to calculate the properties of  $|\psi\rangle$ , we must know the amplitudes  $\langle \alpha | \psi \rangle$  and corresponding matrix elements for at least one complete set of states  $\sum_{\alpha} |\alpha\rangle \langle \alpha|$ . In the case of a spin Hamiltonian, as considered above, the  $|\alpha\rangle$  are normally the set of all spin configurations. The expectation value of any operator  $\theta$  in  $|\psi\rangle$  is then given by

$$\langle \theta \rangle = \frac{\langle \psi | \theta | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_{\alpha} \frac{\langle \psi | \theta | \alpha \rangle \langle \alpha | \psi \rangle}{\langle \psi | \psi \rangle} = \sum_{\alpha} f_{\theta}(\alpha) \rho(\alpha), \quad (3)$$

where we have defined  $f_{\theta}(\alpha) = \langle \psi | \theta | \alpha \rangle / \langle \psi | \alpha \rangle$  and  $\rho(\alpha) = |\langle \alpha | \psi \rangle|^2 / \langle \psi | \psi \rangle$ . In a variational Monte Carlo<sup>1</sup> (MC) approach, Eq. (3) is directly used. Since  $\rho(\alpha) \geq 0$  and  $\sum_{\alpha} \rho(\alpha) = 1$ , one can evaluate Eq. (3) by a random walk in configuration space, measuring the local quantity  $f_{\theta}(\alpha)$  and sampling the configurations with large weight  $\rho(\alpha)$ . The result is an evaluation of Eq. (3) with a certain statistical accuracy, which is inversely proportional to the square of the number of Monte Carlo measurements. The size of the systems which can be evaluated is substantially larger than what would be possible by an exact summation over configuration space.

We may always rewrite the expression for the expecta-

tion value of  $\theta$  in  $|\psi\rangle$  in operator form

$$\theta | \psi \rangle = \frac{\langle \psi | \theta | \psi \rangle}{\langle \psi | \psi \rangle} | \psi \rangle + | \phi_{\theta} \rangle, \quad (4)$$

where  $\langle \psi | \phi_{\theta} \rangle = 0$ . Most importantly, if  $|\psi\rangle$  is an *exact* eigenstate of  $\theta$ , then the correction  $|\phi_{\theta}\rangle \equiv 0$ .<sup>9</sup> For example, if we consider the case of the Hamiltonian, then  $\langle \phi_H | \phi_H \rangle$  measures how good an eigenstate the trial wave function is. In the following we will show that this quantity is very easy to calculate.

Let us assume here for simplicity that  $\theta$  is Hermitian. Using Eq. (4) we define the relative measure

$$\sigma_{\theta}^2 \equiv \frac{\langle \phi_{\theta} | \phi_{\theta} \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi | (\theta - \langle \theta \rangle)^2 | \psi \rangle}{\langle \psi | \psi \rangle}. \quad (5)$$

A simple calculation using Eq. (3) shows that

$$\sigma_{\theta} = \left[ \sum_{\alpha} [f_{\theta}^*(\alpha) - \langle \theta \rangle][f_{\theta}(\alpha) - \langle \theta \rangle] \rho(\alpha) \right]^{1/2}. \quad (6)$$

This equation shows that no new matrix elements have to be evaluated in order to calculate  $\sigma_{\theta}$ , since the quantities  $f_{\theta}(\alpha)$  were already needed for Eq. (3). We can interpretate  $\sigma_{\theta}$  in three different ways. (i) Equation (4) tells us that  $\sigma_{\theta}$  measures how good an eigenstate  $|\psi\rangle$  is of  $\theta$ . (ii) Equation (5) tells us that  $\sigma_{\theta}$  measures the quadratic fluctuations of  $\theta$  in  $|\psi\rangle$ . (iii) Equation (6) tells us that  $\sigma_{\theta}$  can be viewed as the standard deviation (variance) of the local quantity  $f_{\theta}(\alpha)$  in  $|\psi\rangle$ .

### WAVE FUNCTION

The concept formulated above is completely general. It applies to any operator or Hamiltonian and any wave function. Now we will apply it to a concrete case of current interest. Intensive studies have shown that projected wave functions are interesting variational wave functions for the 1D and 2D antiferromagnetic Heisenberg model. We define a class of projected wave functions<sup>10</sup> as

$$|\psi\rangle = P_0 \prod_{\mathbf{k} \in \text{RBZ}} (u_{\mathbf{k}} + v_{\mathbf{k}} d_{\mathbf{k}\uparrow}^{\dagger} d_{-\mathbf{k}\downarrow}^{\dagger}) \times \prod_{\mathbf{k} \in \text{RBZ}} (u_{\mathbf{k}+\mathbf{Q}} + v_{\mathbf{k}+\mathbf{Q}} e_{\mathbf{k}\uparrow}^{\dagger} e_{-\mathbf{k}\downarrow}^{\dagger}) |0\rangle. \quad (7)$$

$P_0$  projects onto the subspace of no doubly occupied sites. The  $d_{\mathbf{k},\sigma}^{\dagger}$  and  $e_{\mathbf{k},\sigma}^{\dagger}$  are the creation operators of bonding and antibonding bands, respectively, for a Hartree-Fock spin-density wave, defined only for  $\mathbf{k}$  in the reduced (antiferromagnetic) Brillouin zone (RBZ):  $d_{\mathbf{k},\sigma}^{\dagger} = \tilde{u}_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} + \sigma \tilde{v}_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q},\sigma}^{\dagger}$  and  $e_{\mathbf{k},\sigma}^{\dagger} = -\sigma \tilde{v}_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} + \tilde{u}_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q},\sigma}^{\dagger}$ . Here,  $\mathbf{Q} = (\pi, \pi)$  is the antiferromagnetic nesting vector, and  $\sigma = \pm 1$ . In principle, the  $u_{\mathbf{k}}, v_{\mathbf{k}}$  and  $\tilde{u}_{\mathbf{k}}, \tilde{v}_{\mathbf{k}}$  are free variational parameters. But in order to make a numerical evaluation feasible, we will use a parametrization, which can be justified by a renormalized mean-field approach. To this end, we will retain only two variational parameters, namely  $\Delta_{\text{AF}}$  and  $\Delta_{\text{SC}}$ , which control the amount of antiferromagnetic and  $d$ -wave correlations, respectively:  $u_{\mathbf{k}}/v_{\mathbf{k}} = \Delta_{\text{AF}} / [\epsilon_{\mathbf{k}} + (\epsilon_{\mathbf{k}}^2 + \Delta_{\text{AF}}^2)^{1/2}]$  and  $\tilde{v}_{\mathbf{k}}^2, \tilde{u}_{\mathbf{k}}^2 = \frac{1}{2} \{1 \pm \epsilon_{\mathbf{k}} / [\epsilon_{\mathbf{k}} + (\epsilon_{\mathbf{k}}^2 + \Delta_{\text{AF}}^2)^{1/2}]\}$ . Here we denoted  $\epsilon_{\mathbf{k}} = -2[\cos(k_x) + \cos(k_y)]$  and  $\Delta_{\mathbf{k}} = \Delta_{\text{SC}}[\cos(k_x) - \cos(k_y)]$ .

## RESULTS

Although  $\sigma_\theta$ , as defined by Eq. (6), is strictly positive, it is not bounded above. The value of  $\sigma_\theta$  for a given  $\theta$  has, therefore, no meaning per se. Nevertheless, we can obtain useful information by comparing the values of the fluctuations for different operators  $\theta$ . To test the quality of a certain trial wave function, we separate the Hamiltonian into distinct contributions. For the case of the antiferromagnetic Heisenberg Hamiltonian, a natural separation is into the Ising and the transverse part, so we will consider  $\theta = \sum_{(i,j)} S_i^z S_j^z$ ,  $\sum_{(i,j)} \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+)$ , and  $\sum_{(i,j)} S_i \cdot S_j$ , leading to  $\sigma_z$ ,  $\sigma_{xy}$ , and  $\sigma_{xyz}$ , respectively.

In Fig. 1 the results for  $\sigma_z$ ,  $\sigma_{xy}$ , and  $\sigma_{xyz}$  are shown for the projected wave function  $|\psi\rangle$ , as defined by Eq. (7). The  $d$ -wave order parameter  $\Delta_{SC}$  is held constant at  $\Delta_{SC}=0.5$ , while varying  $\Delta_{AF}$ , the order parameter which controls the amount of long-range antiferromagnetism. The calculations were done by a Monte Carlo evaluation of  $|\psi\rangle$  on a finite lattice with 50 sites; every data point is the average of 2400 MC measurements. [For details on the technique see Ref. 1(b)].

The behavior of  $\sigma_z$  is illustrative. In the limit  $\Delta_{AF} \rightarrow \infty$ , the wave function reduces to the classical Néel state. For this state, the Ising component of the interaction is diagonal and  $\sigma_z$  must vanish. We observe this behavior in Fig. 1.

While the transverse fluctuations  $\sigma_{xy}$  do not show any particular features, a strong interference effect occurs for the fluctuations in the total energy  $\sigma_{xyz}$ . They show a deep minimum at  $\Delta_{AF} \sim 0.3$ . (The exact location of the minimum is slightly size dependent.<sup>11</sup> For larger systems it is at  $\Delta_{AF} \sim 0.2$ .) While  $|\psi\rangle$  is not a particularly good

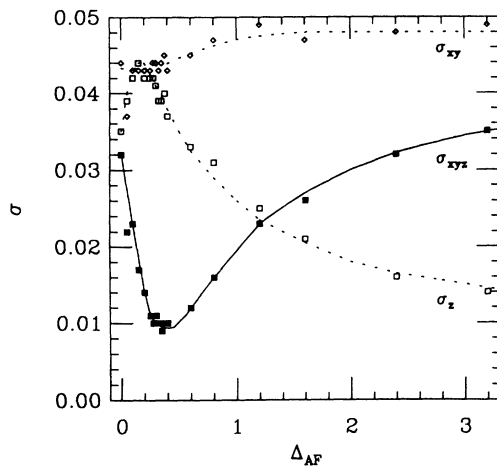


FIG. 1. The standard deviation of the nearest-neighbor transverse spin fluctuations ( $\sigma_{xy}$ , open diamonds), the Ising interaction ( $\sigma_z$ , open squares), and of the Hamiltonian ( $\sigma_{xyz}$ , solid squares), as defined by Eq. (6). The lines are guides to the eye. The data is plotted as a function of  $\Delta_{AF}$ , for a constant  $\Delta_{SC}=0.5$ . The statistical inaccuracy of the data (the corresponding error bars are omitted) shows up in the slight scattering of the data along a smooth curve. Note the strong interference effect in  $\sigma_{xyz}$ , that is the minimum at  $\Delta_{AF} \sim 0.3$ . This indicated a large overlap of  $|\psi\rangle$  with an exact eigenstate of the AFH.

eigenstate for any of the components of the Hamiltonian for this choice of parameter, when we combine both components to form the total Hamiltonian, this measure of the eigenstate quality improves by a factor of 3. This is a very strong effect. A decrease in the fluctuations of the total energy by a factor of 3 is equivalent to a decrease by a factor of 9 in the number of Monte Carlo measurements (i.e., in the time) necessary to calculate the energy expectation value with a certain accuracy. Note, however, that these results do not imply *a priori*, that the wave function has a large overlap with the exact ground state, only that it has a large overlap with some eigenstate. Only by considering additional properties of  $|\psi\rangle$ , as we will do in the following, can one establish a connection to the exact solution.

The results for  $\sigma_{xyz}$  in  $|\psi\rangle$  acquires additional significance when considered within the context of the usual criterion of variational quality, namely the expectation value of the total energy. In the upper part of Fig. 2 the ground-state energy per bond is shown for a constant  $\Delta_{SC}=0.5$ . A search in the two-dimensional space of variational parameters shows that the minimum is realized for  $\Delta_{SC} \sim 0.5$  and  $\Delta_{AF} \sim 0.3$ . At the minimum, the value of the energy per bond is  $\sim -0.3325J$ . (This value is nearly independent of system size.) This value is very close to the estimates obtained by other methods,<sup>3</sup>  $\sim -0.3346J$ .

For the case of the AFH considered here, we are able to consider a third quantity and support the notion that the interference effect shown by  $|\psi\rangle$  is of physical relevance. In the lower part of Fig. 2 we have plotted the ratio of the expectation value of the transverse part of the spin in-

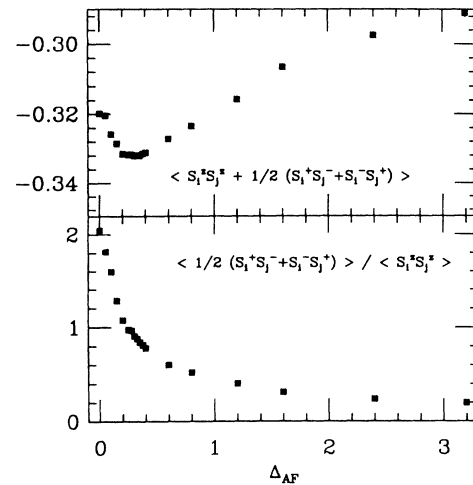


FIG. 2. Upper part: The expectation value of the Hamiltonian per bond in units of  $J$ . The data is plotted as a function of  $\Delta_{AF}$ , for a constant  $\Delta_{SC}=0.5$ . The minimum occurs at the same values of  $\Delta_{AF} \sim 0.3$  and  $\Delta_{SC} \sim 0.5$  as the interference effect described in Fig. 1. Lower part: The ratio of the expectation value of the transverse spin coupling to the Ising interaction. As discussed in the text, the data drops from a value of two for  $\Delta_{AF}=0$  to zero as  $\Delta_{AF} \rightarrow \infty$ . The important point is that the ratio crosses unity very near the point where both the energy and the standard deviation of the energy fluctuations are minimal. This ratio of *one* has been predicted for the exact ground state.

teraction to the expectation value of the Ising part. This ratio would be expected to vary between two for  $\Delta_{AF}=0$  (because  $|\psi\rangle$  is then a spin singlet) and zero for  $\Delta_{AF}\rightarrow\infty$  (because  $|\psi\rangle$  is then identical to the Néel state). This ratio is *one* at nearly the same value of parameters, at which both the energy is minimum and  $\sigma_{xyz}$  is minimum. Note that this is the value expected for the exact ground state of the  $H_2$  in 2D.<sup>8</sup> Furthermore, a search in the space of variational parameters shows that the ratio is close to *unity* only at this single point in parameter space. (The set of parameters where this occurs is slightly size dependent and is close to  $\Delta_{SC}\sim 0.5$  and  $\Delta_{AF}\sim 0.2$  in the thermodynamic limit.)

Here we found that the variance,  $\langle(H-\langle H\rangle)^2\rangle$ , was minimal when  $\langle H\rangle$  was so. If this relation would hold in general, the variance would merely duplicate the information contained in  $\langle H\rangle$ . Indeed this might be the case for certain classes of variational wave functions,<sup>7</sup> but not generally. It is easy to construct for nearly any given Hamiltonian a wave function with finite variance but with an energy expectation value arbitrary close to that of the exact ground state.

To be specific, let us consider the continuum version of the harmonic oscillator:  $H|\omega\rangle=\hbar\omega|\omega\rangle$  for  $\omega\in[0,\infty]$  and with  $\langle\omega'|\omega\rangle=\delta(\omega'-\omega)$ . The wave function  $|\psi\rangle=\int_0^\infty d\omega(\omega+\omega_0)^{-\gamma/2}|\omega\rangle$  has the properties  $\langle\psi|\psi\rangle=\omega_0^{-\gamma}/(\gamma-1)$  and  $\langle H\rangle=\omega_0/(\gamma-2)$  whenever  $\gamma>2$  for convergence. For fixed exponent  $\gamma$ , the ground-state energy approaches zero for  $\omega_0\rightarrow 0$ . But  $\langle(H-\langle H\rangle)^2\rangle\equiv\infty$  for  $\gamma\leq 3$  and all  $\omega_0$ . A low-energy expectation value does, therefore, *not* imply low-energy fluctuations and that the state is a relatively good eigenstate.

## CONCLUSIONS

In addition to the usual criterion of what constitutes a good variational wave function (a low expectation value of the Hamiltonian), we have examined the variance of the Hamiltonian as a measure of how good an eigenstate the trial wave function is of the Hamiltonian. This measure is easy to evaluate and might be especially useful when applied to the antiferromagnetic Heisenberg model in two dimensions. We evaluated the measure for a class of projected wave functions, as trial wave functions of the 2D AFH, and find that at a single point in the space of variational parameters, three things coincide: (i) The expectation value of the energy is minimal, (ii) the state is (relatively) the best eigenstate of the AFH (as measured by our criterion), and (iii) the spin anisotropy take a ratio which has been predicted for the exact ground state.

These results indicate, first, a close connection of the projected wave function with the exact ground state of the AFH and, second, that the evaluation of the variance as a criterion for wave-function quality might prove a valuable tool for related approaches by trial wave functions.

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<sup>8</sup>This result can be obtained by an expansion in  $J_\perp/J_z$  which converges very fast. Raji R. Singh (private communication).

<sup>9</sup>This property is well known [e.g., see E. Merzbacher, *Quantum Mechanics*, 2nd ed. (Wiley, New York, 1960), p. 313, and has been used in the context of Green's-functions Monte Carlo. For example, see D. Ceperly, *J. Stat. Phys.* **43**, 815 (1986)].

<sup>10</sup>The relevance of this class of wave functions for the phase diagram of the  $t$ - $J$  model has been discussed recently by G. J. Chen, R. J. Joynt, F. C. Zhang, and C. Gros, *Phys. Rev. B* **42**, 2662 (1990).

<sup>11</sup>The dependence of the fluctuations in total energy,  $\sigma_{xyz}$ , can be fitted nicely by  $\sigma_{xyz}=0.0018e^{2.02(2\pi/N)}$ , for constant  $\Delta_{AF}=0.25$  and  $\Delta_{SC}=0.5$ . It is amusing to note that one could interpret the factor  $2\pi/N$  in the exponent as the lowest nonzero  $k$  vector on the finite lattice ( $N$  is the linear dimension) and the constant 2.02 as the spin velocity in units of  $J$ . (In spin-wave theory, the velocity would be two.) But the interpretation of this behavior is far from certain, especially since no simple finite-size scaling behavior could be found for  $\sigma_{xy}$  or  $\sigma_z$ .