# Anisotropic two-dimensional Heisenberg model studied by the Schwinger-boson Gutzwiller-projection method

T. Miyazaki, D. Yoshioka, and M. Ogata Institute of Physics, College of Arts and Sciences, University of Tokyo, Komaba, Meguro-ku Tokyo 153, Japan (Received 1 August 1994)

A two-dimensional Heisenberg model with anisotropic couplings in the x and y directions ( $J_x \neq J_y$ )  $J_y$ ) is considered. The model is first solved in the Schwinger-boson mean-field approximation. Then the solution is Gutzwiller projected to satisfy the local constraint that there is only one boson at each site. The energy and spin-spin correlation of the obtained wave function are calculated for systems with up to  $20 \times 20$  sites by means of the variational Monte Carlo simulation. It is shown that the antiferromagnetic long-range order remains down to the one-dimensional limit.

#### I. INTRODUCTION

Stimulated by the discovery of cuprate superconductors, the ground state of the two-dimensional S =1/2 quantum antiferromagnetic Heisenberg model has been extensively investigated by various kinds of approaches. Although the model has never been solved exactly, the properties of its ground state have been carefully investigated by numerical and analytical calculations. It has been found that the ground-state energy per site is  $(-0.6696 \pm 0.0004)J$  by series expansions,<sup>1</sup> and [-0.66934(3)]J by the Green's-function Monte Carlo method.<sup>2,3</sup> As for the existence of long-range order, it is believed that it has an antiferromagnetic long-range order. The staggered magnetization per site is estimated to be  $0.308 \pm 0.008$  by series expansions and  $0.3075 \pm 0.008$ 0.0025 by the Green's-function Monte Carlo method.<sup>4</sup>

On the other hand, a one-dimensional S=1/2 quantum antiferromagnetic Heisenberg model is solved exactly by means of the Bethe ansatz. The exact groundstate energy per site is  $(\ln 2 - 0.25)J = -0.4431J$ and the excitation is gapless.<sup>5</sup> Since the system is onedimensional, it does not have a long-range order.

From these results, we expect an order-disorder phase transition in an anisotropic Heisenberg model, which interpolates the one- and two-dimensional systems:

$$\mathcal{H} = J_x \sum_{i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}} + J_y \sum_{i} \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{y}} \quad , \tag{1}$$

where  $i+\hat{x}$   $(i+\hat{y})$  means the site next to the ith site in the x(y) direction, and  $J_x = J$  and  $J_y = \alpha J$  are the coupling constants in the x and y direction, respectively. Since the ground state of this Hamiltonian has no long-range order at  $\alpha = 0$  (one-dimensional case) and it has the antiferromagnetic long-range order at  $\alpha = 1$  (two-dimensional isotropic case), we can expect a quantum phase transition as  $\alpha$  is changed between 0 and 1. It had been believed that this phase boundary is at  $\alpha = 0$ . When  $\alpha$  is infinitesimally small, the system can be regarded as a collection of weakly coupled one-dimensional chains. Several mean-field theories indicated that infinitesimally small  $\alpha$  makes the system ordered. However, very recently Parola, Sorella and Zhong<sup>9,10</sup> asserted that they found evidence for an order-disorder transition at a finite value of  $\alpha$ . They investigated the magnetization using the spin-wave theory and the Lanczos method. The spin-wave theory predicted a breakdown of the antiferromagnetic long-range order at about  $\alpha_c \sim 0.03(0.07)$  at first order (second order) in 1/S expansions. Below this critical anisotropy, the staggered state disappeared and the disordered state was realized. They also found that the spin-wave theory generalized to finite systems agreed with the results of the Lanczos method for  $\alpha > 0.1$ . However, this agreement did not persist for  $\alpha < 0.1$ . The result of the Lanczos method showed finite magnetization at  $\alpha = 0$ . Although they concluded the order-disorder phase transition at finite  $\alpha$  from their results, it is far from conclusive.

In this paper we investigate this order-disorder transition using a different method. Here, we consider a resonating valence bond (RVB) state<sup>11,12</sup> and adopt the Schwinger-boson description of the spin operators. 13-16 For the isotropic two-dimensional case ( $\alpha = 1$ ), wave functions based on the RVB singlet have been studied by many authors. Liang, Douçot, and Anderson<sup>17</sup> made a variational RVB wave function with long-range bonds and found that the optimal energy per site is -0.6688Jand that the ground state has an antiferromagnetic longrange order. The staggered magnetization is 0.225 per site. The variational energy is very close to the best estimated value. 1 Furthermore, recently Chen and Xiu<sup>18</sup> made a trial wave function by the Gutzwiller projection of the state obtained in the Schwinger-boson mean-field theory. Though the wave function has no variational parameter, they found that it can describe the isotropic ground state quite accurately. The energy per site is -0.6688J, which is 99.9% of the best estimation and the staggered magnetization is also very close to the best estimated value. In this paper, we extend the wave function of Chen and Xiu into the anisotropic Hamiltonian for  $0 \le \alpha \le 1$  to investigate the order-disorder transition.

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To this end, we first solve the model in the mean-field approximation. Next, using the mean-field solution, we make variational wave functions without doubly occupied sites and calculate the energy and staggered magnetization to investigate the phase transition.

In Sec. II, we solve the Hamiltonian in the Schwingerboson mean-field theory. Using this mean-field solution, we make RVB wave functions without doubly occupied sites in Sec. III. In Sec. IV, numerical results for energies and spin-spin correlations as a function of anisotropy are studied by means of Monte Carlo simulations. In Sec. V, we discuss the accuracy of our wave function and the boundary of the order-disorder transition.

#### II. MEAN-FIELD SOLUTION

In this section we solve the Hamiltonian in the Schwinger-boson mean-field approximation. <sup>15,16,14</sup> First we introduce two kinds of Bose operators,  $s_{i,\uparrow}$  and  $s_{i,\downarrow}$ , to express the spin operators,

$$S_i^+ = s^{\dagger}_{i,\uparrow} s_{i,\downarrow} \text{ and } S_i^z = \frac{1}{2} (s_{i,\uparrow}^{\dagger} s_{i,\uparrow} - s_{i,\downarrow}^{\dagger} s_{i,\downarrow}).$$
 (2)

The commutation relations of the spin operators  $S_i$  are satisfied in this replacement. We impose a constraint,

$$s_{i,\uparrow}^{\dagger} s_{i,\uparrow} + s_{i,\downarrow}^{\dagger} s_{i,\downarrow} = 1,$$
 (3)

in order to guarantee S = 1/2. Then the Hamiltonian is rewritten as follows:

$$\mathcal{H} = \sum_{i} \sum_{z} J_{z} (\mathbf{S}_{i} \cdot \mathbf{S}_{i+\hat{z}} - \frac{1}{4} n_{i} n_{i+\hat{z}}) + \mu \sum_{i} n_{i}$$

$$= \frac{1}{2} \sum_{i} \sum_{z} \sum_{\sigma} J_{z} (s^{\dagger}_{i,\sigma} s^{\dagger}_{i+\hat{z},-\sigma} s_{i+\hat{z},\sigma} s_{i,-\sigma}$$

$$-s^{\dagger}_{i,\sigma} s^{\dagger}_{i+\hat{z},-\sigma} s_{i+\hat{z},-\sigma} s_{i,\sigma})$$

$$+\mu \sum_{i} \sum_{\sigma} s^{\dagger}_{i,\sigma} s_{i,\sigma} . \tag{4}$$

Here z=x or  $y,\ i+\hat{z}$  represents a site next to the site i in the z direction,  $n_i=s_{i,\uparrow}^{\dagger}s_{i,\uparrow}+s_{i,\downarrow}^{\dagger}s_{i,\downarrow}$ , and  $\mu$  is a chemical potential to be adjusted to satisfy Eq. (3) on the average.

To solve this Hamiltonian in a mean-field approximation, we introduce the following mean-field parameters, which give the amplitude of the nearest-neighbor singlet pairs and an averaged occupation number,

$$\Delta_z = \frac{1}{2} \langle s_{i,\downarrow} s_{i+\hat{z},\uparrow} - s_{i,\uparrow} s_{i+\hat{z},\downarrow} \rangle, \tag{5}$$

$$n_{\sigma} = \langle s_{i,\sigma}^{\dagger} s_{i,\sigma} \rangle = \frac{1}{2}.$$
 (6)

After decoupling the Hamiltonian, we rewrite the operator using its Fourier transform:

$$s_{i,\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} s_{\mathbf{k},\sigma},$$
 (7)

where N is the total number of lattice sites, and  ${\bf k}$  are two-dimensional wave vectors. The mean-field Hamiltonian is then written as

$$\mathcal{H}_{\mathrm{MF}} = \sum_{\mathbf{k}} \left[ \lambda (s_{\mathbf{k},\uparrow}^{\dagger} s_{\mathbf{k},\uparrow} + s_{-\mathbf{k},\downarrow}^{\dagger} s_{-\mathbf{k},\downarrow}) + \gamma_{\mathbf{k}} s_{\mathbf{k},\uparrow}^{\dagger} s_{-\mathbf{k},\downarrow}^{\dagger} + \gamma_{\mathbf{k}}^{*} s_{-\mathbf{k},\downarrow} s_{\mathbf{k},\uparrow} \right] + 2N \left[ J |\Delta_{x}|^{2} + J\alpha |\Delta_{y}|^{2} \right] + \frac{1}{4} N (1 + \alpha) J,$$
 (8)

where

$$\lambda = \mu - \frac{1}{2}(1+\alpha)J,\tag{9}$$

$$\gamma_{\mathbf{k}} = 2i(J\Delta_x \sin k_x + J\alpha\Delta_y \sin k_y). \tag{10}$$

This Hamiltonian is diagonalized using the Bogoliubov transformation:

$$s_{\mathbf{k},\uparrow} = u_{\mathbf{k}} \alpha_{\mathbf{k}} - v_{\mathbf{k}} \beta_{\mathbf{k}}^{\dagger}, \tag{11}$$

$$s_{-\mathbf{k},\perp} = -v_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} + u_{\mathbf{k}} \beta_{\mathbf{k}}, \tag{12}$$

where

$$u_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \frac{\lambda}{E_{\mathbf{k}}} + 1 \right)^{\frac{1}{2}} \exp\left( \frac{i}{2} \theta_{\mathbf{k}} \right), \tag{13}$$

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$$v_{\mathbf{k}} = \frac{1}{\sqrt{2}} \left( \frac{\lambda}{E_{\mathbf{k}}} - 1 \right)^{\frac{1}{2}} \exp\left( \frac{i}{2} \theta_{\mathbf{k}} \right).$$
 (14)

 $\theta_{\mathbf{k}}$  is the phase of  $\gamma_{\mathbf{k}}$ ,  $\gamma_{\mathbf{k}} = |\gamma_{\mathbf{k}}| \exp(i\theta_{\mathbf{k}})$ , and

$$E_{\mathbf{k}} = \sqrt{\lambda^2 - |\gamma_{\mathbf{k}}|^2}. (15)$$

After this transformation the Hamiltonian becomes

$$\mathcal{H}_{\mathrm{MF}} = \sum_{\mathbf{k}} E_{\mathbf{k}} (\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}}) + \text{const.}$$
 (16)

The ground state  $|G\rangle$  is defined as the vacuum of the Bose operators  $\alpha_{\mathbf{k}}$  and  $\beta_{\mathbf{k}}$ :  $\alpha_{\mathbf{k}}|G\rangle = \beta_{\mathbf{k}}|G\rangle = 0$ . For a finite-size system,  $\lambda, \Delta_x$ , and  $\Delta_y$  are determined from the self-consistent equations

$$\langle G|s_{i,\uparrow}^{\dagger}s_{i,\uparrow} + s_{i,\downarrow}^{\dagger}|G\rangle = 1$$
 (17)

and

$$\langle G|s_{i,\downarrow}s_{i+\hat{z},\uparrow} - s_{i,\uparrow}s_{i+\hat{z},\downarrow}|G\rangle = 2\Delta_z,$$
 (18)

which read

$$2 = \frac{1}{N} \sum_{\mathbf{k}} \frac{\lambda}{E_{\mathbf{k}}} \tag{19}$$

and

$$\Delta_z = \frac{1}{N} \sum_{\mathbf{k}} \sin k_z \frac{J_x \Delta_x \sin k_x + J_y \Delta_y \sin k_y}{E_{\mathbf{k}}}.$$
 (20)

The solution depends on the size of the system N; so does  $u_k$  and  $v_k$ . We will use the solutions for finite-size systems in the following sections.

When N is finite,  $E_{\mathbf{k}}$  never becomes zero. However,

in the limit of  $N \to \infty$  it is possible that  $E_{\mathbf{k}}$  vanishes at  $\mathbf{k} = \mathbf{K}_{\pm} = \pm (\pi/2, \pi/2)$ . In such a case it is known that we need to introduce the Bose condensate  $n_B$ , <sup>15,16</sup> and Eqs. (19) and (20) are rewritten as

$$2 = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \frac{\lambda}{E_{\mathbf{k}}} + 2n_B, \tag{21}$$

$$\Delta_z = \frac{1}{(2\pi)^2} \int_{-\pi}^{\pi} dk_x \int_{-\pi}^{\pi} dk_y \sin k_z \frac{J_x \Delta_x \sin k_x + J_y \Delta_y \sin k_y}{E_{\mathbf{k}}} + n_B.$$
 (22)

Here  $n_B$  becomes finite only when the spectrum is gapless, i.e., when  $\lambda = 2(J_x\Delta_x + J_y\Delta_y)$ . The finite value of  $n_B$  means the existence of the antiferromagnetic longrange order. The staggered magnetization is  $\sqrt{3/2}$   $n_B$ .

Before discussing the mean-field solution for an arbitrary anisotropy, it is worthwhile to see what happens in the one-dimensional limit, where  $\alpha=0$ . It is easy to see that the spectrum  $E_{\mathbf{k}}$  cannot be gapless, and thus  $n_B=0$ . In this case the self-consistent equations are expressed by elliptic integrals. By introducing  $\epsilon=2J\Delta_x/\lambda$ , we can express Eqs. (21) and (22) as

$$2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \frac{\lambda}{E_{\mathbf{k}}} = \frac{2}{\pi} K(\epsilon)$$
 (23)

and

$$\frac{\lambda}{J} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \frac{\sin^2 k_x}{\sqrt{1 - \epsilon^2 \sin^2 k_x}}$$

$$= \frac{2}{\epsilon^2} - \frac{2}{\pi \epsilon^2} E(\epsilon). \tag{24}$$

Here  $K(\epsilon)$  and  $E(\epsilon)$  are the complete elliptic integrals. By solving these equations we obtain  $\lambda=1.379\,962J$ , and  $\Delta_x=0.679\,239\,7$ . The excitation energy  $E_k$  has a gap:  $E_k\geq 0.242\,547J$ .

For an intermediate value of  $\alpha$ , we must solve the self-consistent equations numerically. The results are shown in Fig. 1, where the RVB order parameters  $\Delta_x$  and  $\Delta_y$ , the Bose condensate  $n_B$ , and the energy gap  $E_{\rm g}$  are plotted. When  $\alpha$  is decreased from unity, both  $\Delta_y$  and  $n_B$  decrease. The Bose condensate vanishes first at  $\alpha=0.1356$ . This is the point where the antiferromagnetic long-range order vanishes. Below this value of  $\alpha$ , the energy gap in the spin excitation develops quite rapidly, and  $\Delta_y$  is suppressed.  $\Delta_y$  finally vanishes at  $\alpha=0.1286$ . Below  $\alpha=0.1286$  the system reduces to a collection of independent chains running parallel to the x direction. In this region the order parameter  $\Delta_x$  and the gap  $E_{\rm g}$  become constant.

## III. RVB WAVE FUNCTIONS

The ground-state wave function obtained in the meanfield theory is expressed as

$$|G\rangle = \prod_{\mathbf{k}} \exp\left(-\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^*} s_{\mathbf{k},\uparrow}^{\dagger} s_{-\mathbf{k},\downarrow}^{\dagger}\right) |0\rangle \quad ,$$
 (25)

where  $|0\rangle$  is the vacuum of the Schwinger bosons. By the Fourier transformation for  $s^{\dagger}_{\mathbf{k},\uparrow}, s^{\dagger}_{-\mathbf{k},\downarrow}$ , we get a real-space representation for this ground state:

$$|G
angle = \exp\left(\sum_{i,j} a_{i,j} s_{i,\uparrow}^{\dagger} s_{j,\downarrow}^{\dagger}\right) |0
angle \quad ,$$
 (26)

$$a_{i,j} = -\frac{1}{N} \sum_{\mathbf{k}} \left( \frac{v_{\mathbf{k}}}{u_{\mathbf{k}}^*} \right) \exp(-i\mathbf{k} \cdot \mathbf{r}_{i,j}) \quad ,$$
 (27)

where  $\mathbf{r}_{i,j} = \mathbf{r}_i - \mathbf{r}_j$ . It is evident that the local constraint, Eq. (3), is not satisfied in this wave function. This is why the energy of the mean-field ground state is too low.<sup>19</sup> We remove this difficulty by projecting the wave function to a space where every site is singly occupied. Namely, we perform the Gutzwiller projection,

$$|G
angle = P\Biggl(\sum_{i 
eq j} a_{i,j} s_{i\uparrow}^\dagger s_{j\downarrow}^\dagger\Biggr)^{rac{N}{2}} |0
angle \quad .$$

The operator P on the right-hand side is the Gutzwiller-projection operator. From now on, we consider this wave function. Since  $a_{i,j} = -a_{j,i}$ , the ground state of Eq. (28) is nothing but an RVB state, which includes long-range bonds with weights  $a_{i,j}$ .

Although it would be possible to regard every  $a_{i,j}$  as

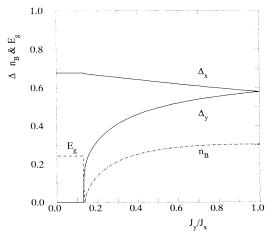


FIG. 1. Mean-field values of order parameters  $\Delta_x, \Delta_y$ , Bose condensate  $n_B$  and energy gap  $E_g$  as a function of  $\alpha$ .

a variational parameter, we here restrict  $a_{i,j}$  to be those given in Eq. (27). In the isotropic case  $(J_x = J_y)$ , this restriction is justified by the result itself: Chen and Xiu<sup>18</sup> have shown that this choice of  $a_{i,j}$  gives excellent results for the ground-state energy and the staggered magnetization. To see if Eq. (27) gives similarly good results for anisotropic case or not is one of our aims in the present paper. It should be noticed that for the anisotropic system we still have one variational parameter, namely,  $u_k$  and  $v_k$  depend on the anisotropy parameter  $\alpha = J_y/J_x$ . It is not evident that, for a given value of  $\alpha$  in the Hamiltonian, the same value of  $\alpha$  in the variational wave function gives the best result. Thus we consider  $\alpha$  in the mean-field equations as a variational parameter, which we denote  $\alpha_p$ .

#### IV. NUMERICAL RESULTS

In this section, we show numerical results of the variational energy, spin-spin correlation, and staggered magnetization for the anisotropic Heisenberg Hamiltonian. We perform Monte Carlo simulations for lattices with various number of sites up to  $20 \times 20$  for the energy and the spin-spin correlation. All the numerical calculations are performed with periodic boundary conditions. For each system size we solve the self-consistent equations (19) and (20) and calculate  $a_{i,j}$  to be used to construct the wave function at that system size. Instead, we could have used  $a_{i,j}$  for an infinite-size system. However, we did not take this approach, since the energy is higher and size-scaling does not coincide with the prediction of the spin-wave theory in this case.

## A. Ground state

The energy per site of the anisotropic Heisenberg model is

$$E = J_x \langle \epsilon_x \rangle + J_y \langle \epsilon_y \rangle \quad , \tag{29}$$

where

$$\langle \epsilon_z \rangle = \frac{1}{N} \sum_i \langle G | \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{z}} | G \rangle.$$
 (30)

Here  $\langle \epsilon_z \rangle$ , z=x or y, is an expectation value of the nearest-neighbor spin-spin correlation in the x or y direction. These  $\langle \epsilon_x \rangle$  and  $\langle \epsilon_y \rangle$  depend on the system size N and the variational parameter  $\alpha_p$ , but independent of  $\alpha$ . Thus we first estimate the thermodynamic limit of  $\langle \epsilon_x \rangle$  and  $\langle \epsilon_y \rangle$  for several values of  $\alpha_p$ . The size dependence is studied, and we find the following size scaling:

$$\langle \epsilon_z(L) \rangle = \langle \epsilon_z(\infty) \rangle + \lambda_z L^{-3} + \cdots,$$
 (31)

where  $\lambda_z$ , is a constant and L is the linear dimension  $L^2=N$ . The size scaling coincides with the spin-wave theory for a square lattice. Then we obtain  $\alpha_p$  dependence, of the energy E at a fixed  $\alpha$  for the infinite size system. Figure 2 shows such a dependence at  $\alpha=0.6$ , for example. The error bars result both from Monte Carlo statistical errors and from a fitting error of the

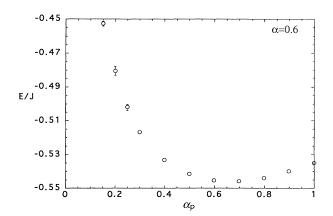


FIG. 2. Variational energy per site as a function of  $\alpha_p$  for  $\alpha=0.6$ . The optimal energy is given at  $\alpha_p=0.680$ .

size scaling. It can be seen that the optimal energy is given when  $\alpha_p = 0.680$ . In a similar way, we obtain the optimal energy for various values of  $\alpha$ , which is shown in Fig. 3. When  $\alpha$  is equal to zero, the system becomes the one-dimensional  $S=\frac{1}{2}$  antiferromagnetic Heisenberg chain. In this case, the exact energy per site is given in the Bethe-ansatz solution, which is  $(\ln 2 - 0.25)J = -0.4431J.^5$  Our variational energy per site in this case is  $(-0.4337 \pm 0.0030)J$ , which is 97.9% of the exact result. This shows that our RVB wave function can also describe fairly well the anisotropic Heisenberg Hamiltonian as well as the isotropic one.

## B. Staggered magnetization

There are several methods to estimate the staggered magnetization. In most numerical calculations, it is estimated from the spin-spin correlation. Here, we use the staggered spin-spin correlation at the longest possible distance for each direction,<sup>20</sup>

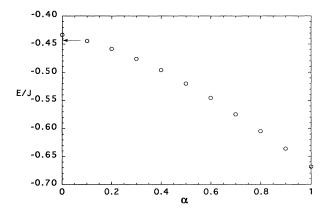


FIG. 3. Energy per site as a function of  $\alpha$ . When  $\alpha=1$ , isotropic case, the energy is  $(-0.6688 \pm 0.0008)J$ , and when  $\alpha=0$ , the one-dimensional case, it is  $(-0.4337 \pm 0.0005)J$ . The exact value at  $J_y=0$  is shown by an arrow.

$$M_z^2(L) \equiv C_z \left(\frac{L}{2}\right) \quad , \tag{32}$$

$$C_z(n) = \left(\frac{(-1)^n}{N}\right) \sum_i \langle |\mathbf{S}_i \cdot \mathbf{S}_{i+n\hat{z}}| \rangle \quad , \tag{33}$$

where z = x or y and  $i + n\hat{z}$  is the nth site from the site i in the x or y direction. We calculate  $M_z(L)$  for each lattice size and extrapolate to the thermodynamic limit using the finite-size scaling:

$$M_z(L) = M_z(\infty) + \mu L^{-1} + \cdots, \tag{34}$$

where  $\mu$  is a constant. This scaling agrees with the prediction of the spin-wave theory and arguments given by Huse.<sup>21</sup> The obtained  $M_z(\infty)$  is the staggered magnetization.

Since the variational function is a Gutzwiller-projected mean-field solution, the properties of the latter wave function are inherited by it. The mean-field wave function, which shows the long-range order gives a finite staggered magnetization even after the Gutzwiller projection, while that which shows no long-range order gives vanishing staggered magnetization after the projection. We find that, for any anisotropy, the optimized parameter  $\alpha_p$  is larger than 0.1356 for any  $\alpha$  and, as a result, our variational state always has a long-range order. Furthermore, we find that the magnetizations in the x and y directions coincide, which is consistent with the mean-field solution. The  $\alpha$  dependence of the staggered magnetization is shown in Fig. 4. The staggered magnetization and hence the antiferromagnetic long-range order remains down to  $\alpha = 0$ .

#### **V. DISCUSSIONS**

In this paper we first solved the Hamiltonian by the Schwinger-boson mean-field theory, and then the solution is Gutzwiller projected to obtain the variational wave function, which we used to investigate the order-disorder transition. Our Gutzwiller-projected wave function is very suitable for studying the order-disorder transition.

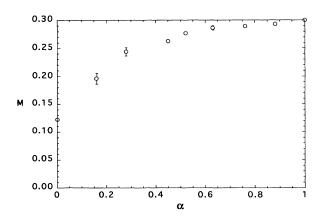


FIG. 4. Staggered magnetization  $M=M_x(\infty)=M_y(\infty)$  as a function of  $\alpha$ .

Since it is rewritten as a RVB state, it can represent a disordered spin state as well as an ordered state. As shown by Liang, Douçot and Anderson,  $^{17}$  when the weight of the singlet RVB bond,  $a_{i,j}$ , has a power-law behavior, the RVB state has a long-range order. On the other hand, when  $a_{i,j}$  is short ranged, the RVB state becomes a disordered state with a spin gap, and it has a short-range spin-spin correlation.

By solving the Schwinger-boson mean-field theory for the anisotropic Heisenberg model, we construct an anisotropic  $a_{i,j}$ , which is suitable for the anisotropic case. Furthermore, we can compare the variational energy for the ordered state ( $\alpha_p > 0.1356$ ) and the disordered state  $(\alpha_p < 0.1356)$  by regarding  $\alpha_p$  as a variational parameter. The critical state where spin-spin correlation decays algebraically is also included as a trial state with  $\alpha_n = 0.1356$ . We have found that the optimized parameter  $\alpha_p$  is always larger than  $\alpha$  and, moreover, larger than  $\alpha_c = 0.1356$ . (Even at  $\alpha \to 0$ , we get  $\alpha_p = 0.205$ .) This means that the ground state is stabilized if it develops a long-range order for all parameters,  $0 \le \alpha \le 1$ . Although both the spin-wave theory discussed by Parola, Sorella, and Zhong<sup>9</sup> and the Schwinger-boson mean-field theory predict a disordered phase for small  $\alpha$ , our result supports the existence of a long-range order even for small  $\alpha$  in accordance with other mean-field theories.<sup>7,8</sup>

We believe the phase transition obtained in the spinwave theory and in Sec. II at a finite value of  $\alpha$  is an artifact of the poorness of the mean-field solutions. It is known that in the one-dimensional limit even though there is no long-range order, the excitation spectrum is gapless and the spin-spin correlation decays not exponentially but algebraically. This algebraic decay lies at the base of our belief that an infinitesimal coupling between one-dimensional chains causes a long-range order in the entire system, although the magnitude of the staggered magnetization is infinitesimally small. On the other hand, our mean-field solution at  $J_y = 0$  gives a massive excitation spectrum, and the spin-spin correlation shows an exponential decay. This qualitative difference between the mean-field and the exact solution does not persist in our variational wave function, since we use  $\alpha_p > 0.205$ . We remark here that the massive excitation and the exponential decay of the spin-spin correlation are properties of the integer spin-antiferromagnetic Heisenberg chain, and the order-disorder transition in the presence of the interchain coupling has been successfully discussed by Azzouz and Douçot<sup>22</sup> using the Schwingerboson mean-field theory.

Our wave function is much improved from the mean-field solution using the Gutzwiller projection and by the optimum choice of the variational parameter  $\alpha_p$ . However, the energy and the magnetization in the limit of  $\alpha \to 0$  clearly indicate that there is ample room for improvement of our wave function. Our results show discontinuity in the staggered magnetization at  $\alpha=0$ : with infinitesimal  $\alpha$  the magnetization jumps from zero to  $0.1227 \pm 0.023$ . This will not be correct. When the ordered state persists down to the limit of  $\alpha=0$ , the most natural behavior would be a continuous growth of the magnetization from zero as  $\alpha$  increases, power de-

pendence on  $\alpha$  being quite plausible. We expect that improvement of the ground-state energy at  $\alpha < 1$  will decrease the value of magnetization. At present we do not know if such an improvement will cause the magnetization vanish even at finite value of  $\alpha$  or not. However, our results show a strong tendency toward the existence of a long-range order even for infinitesimally small  $\alpha$ .

In conclusion we have investigated the two-dimensional anisotropic Heisenberg model using the Schwinger-boson Gutzwiller-projection method. Our results show the existence of the long-range order in the whole range of the anisotropic parameter  $\alpha$ . This is in agreement with Sakai and Takahashi, and with Azzouz, but in disagreement with the work by Parola, Sorella, and Zhong. We think the order-disorder transition at a finite value of  $\alpha$  is still an open question. This question is too delicate to be answered by mean-field theories. Our present investigation is one attempt to go beyond the mean-field theory, but more elaborate work will certainly be necessary to draw a definite conclusion. We can and will try to improve the

wave function by treating  $a_{i,j}$  as variational parameters. We have found that the choice of  $a_{i,j}$ , which decays inversely proportional to  $r_{i,j}$ , the distance between the *i*th and *j*th sites, gives much better ground-state energy for the one-dimensional system. This is in contrast to our mean-field  $a_{i,j}$ , which decays either exponentially (for  $\alpha_p < 0.1356$ ) or proportional to  $r_{i,j}^{-3}$  (for  $\alpha \geq 0.1356$ ). The results will be reported in the near future.

#### ACKNOWLEDGEMENTS

The authors thank H. Yokoyama and K. Higuchi for helpful comments on the Monte Carlo algorithm. This work was supported by a Grant-in-Aid for Scientific Research on Priority Area "Computational Physics as a new Frontier in Condensed Matter Research" (Grant No. 04231105) from the Ministry of Education, Science and Culture.

<sup>&</sup>lt;sup>1</sup> R.R.P. Singh and D.A. Huse, Phys. Rev. B 40, 7247 (1989).

<sup>&</sup>lt;sup>2</sup> K.J. Runge, Phys. Rev. B **45**, 12 292 (1992).

<sup>&</sup>lt;sup>3</sup> N. Trivedi and D.M. Ceperley, Phys. Rev. B **40**, 2737 (1989).

<sup>&</sup>lt;sup>4</sup> K.J. Runge, Phys. Rev. B 45, 7229 (1992).

<sup>&</sup>lt;sup>5</sup> H.A. Bethe, Z. Phys. **71**, 205 (1931).

<sup>&</sup>lt;sup>6</sup> D.J. Scalapino, Y. Imry, and P. Pincus, Phys. Rev. B **11**, 2042 (1975).

<sup>&</sup>lt;sup>7</sup> T. Sakai and M. Takahashi, J. Phys. Soc. Jpn. **58**, 3131 (1989).

<sup>&</sup>lt;sup>8</sup> M. Azzouz, Phys. Rev. B **48**, 6136 (1993).

<sup>&</sup>lt;sup>9</sup> A. Parola, S. Sorella, and Q.F. Zhong, Phys. Rev. Lett. **71**, 4393 (1993).

<sup>&</sup>lt;sup>10</sup> A. Parola, Phys. Rev. B **40**, 7109 (1989).

<sup>&</sup>lt;sup>11</sup> P.W. Anderson, Mater. Res. Bull. 8, 153 (1973).

<sup>&</sup>lt;sup>12</sup> P.W. Anderson, Science **235**, 1196 (1987).

<sup>&</sup>lt;sup>13</sup> D.P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988).

<sup>&</sup>lt;sup>14</sup> A. Auerbach and D.P. Arovas, Phys. Rev. Lett. **61**, 617 (1988).

<sup>&</sup>lt;sup>15</sup> D. Yoshioka, J. Phys. Soc. Jpn. **58**, 32 (1989).

<sup>&</sup>lt;sup>16</sup> D. Yoshioka, J. Phys. Soc. Jpn. **58**, 3733 (1989).

<sup>&</sup>lt;sup>17</sup> S. Liang, B. Douçot, and P.W. Anderson, Phys. Rev. Lett. 61, 365 (1988).

<sup>&</sup>lt;sup>18</sup> Y.C. Chen and K. Xiu, Phys. Lett. A **181**, 373 (1993).

<sup>19</sup> It is known that the energy per site is -1.0058J in the isotropic case (Refs. 15 and 16), which is about 1.5 times larger than the best estimate value -0.6696J (Ref. 21).

<sup>&</sup>lt;sup>20</sup> E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991).

<sup>&</sup>lt;sup>21</sup> D.A. Huse, Phys. Rev. B **37**, 2380 (1988).

<sup>&</sup>lt;sup>22</sup> M. Azzouz and B. Douçot, Phys. Rev. B 47, 8660 (1993).