Field-induced gap in the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain: A density-matrix renormalization-group study

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We study the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain in both uniform and (perpendicular) staggered magnetic fields using the density-matrix renormalization-group method. This model has been shown earlier to describe the physics of the copper benzoate materials in magnetic field. In the present work, we extend the study to more general case for a systematic investigation of the field-induced gap and related properties of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain. In particular, we explore the high magnetic field regime where interesting behaviors in the field-induced gap, magnetization, and spin correlation functions are found. Careful examination of the low energy properties and magnetization reveals interesting competing effects of the staggered and uniform fields. The incommensurate behavior in the spin correlation functions is demonstrated and discussed in detail. The present work reproduces earlier results in good agreement with experimental data on copper benzoate and predicts new interesting field-induced features at very high magnetic field.

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I. INTRODUCTION

The quasi-one-dimensional magnetic materials have attracted considerable experimental and theoretical interest since Haldane's pioneering work[1] that pointed out the difference between the integer spin Heisenberg antiferromagnetic (HAFM) chains and the half-integer spin chains. By mapping the Heisenberg spin chains onto the $O(3)$ nonlinear sigma model,[2] Haldane conjectured that the low-energy excitation spectrum displays a finite energy gap for the integer spin systems while for half-integer spin chains it is gapless. These conjectures have been verified by later detailed studies.

In the linear chain HAFM family, the spin-$\frac{1}{2}$ chain is of particular interest since most of its properties can be obtained exactly. These exact results serve as benchmarks in testing the validity of various approximation schemes. The low energy excitation spectrum in this system has no gap; the elementary excitations are spin-$\frac{1}{2}$ spinons; the ground state is quasi-long-range ordered, and the spin-spin correlations display power law decay.

The effect of an applied magnetic field on the spin-$\frac{1}{2}$ Heisenberg chain has also been studied to gain more insight into the physics of such a system. When the external magnetic field is present, the Hamiltonian of the system is written as

$$H = J\sum_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1} - h_u S_i^z), \tag{1}$$

where J is the coupling constant, $\mathbf{S}_i$ the spin-$\frac{1}{2}$ operator on site i, S_i^z the z component of $\mathbf{S}_i$, $h_u = g\mu_B H/J$ is the effective dimensionless uniform field, g the average effective gyromagnetic ratio, and H the applied magnetic field. When $h_u = 0$, the critical wave vector of the gapless excitation is located at 0 and π. The applied field will shift the critical wave vector of the gapless excitation away from 0 (for transverse spin correlations) and π (for longitudinal spin correlations) to incommensurate values while the excitation remains gapless until the field is larger than its saturation value $h_u = 2.0$.[6] When $h_u = 2.0$, the magnetization is saturated with all spins on the lattice sites oriented parallel to the applied uniform field. Further increase in the applied field leads to the opening of a gap in the low energy spectrum with its magnitude changing almost linearly with the applied field, corresponding to flipping one spin to its opposite direction.

The field-induced incommensurate state was first observed in the neutron scattering measurements on copper benzoate $Cu(C_6D_5COO)_2 3D_2O$.[3] Copper benzoate is a linear chain spin-$\frac{1}{2}$ AFM[4] with coupling constant $J \sim 1.57$ meV.[5] In this material, the effective spin-$\frac{1}{2}$ Cu^{2+} ions form a linear chain structure, but the two neighboring copper sites are not totally equivalent. Because of the small value of the coupling constant J, it is possible to study the high field (large h_u) properties of Hamiltonian (1) and investigate how the induced incommensurate soft mode behaves with the changing magnetic field.

In the copper benzoate experiment,[3] in addition to the field-dependent incommensurate low energy modes, an unexpected nonzero energy gap induced by the magnetic field was detected. The value of the gap varies with the magnitude and the relative orientation of the applied magnetic field.[3] It was first suggested[3] that the unexpected gap is caused by the inequivalence of the Cu sites leading to an effective staggered g tensor, which in turn gives rise to an effective staggered field in addition to the applied uniform magnetic field. Later, detailed analysis[7] shows that an additional staggered Dzyaloshinskii-Moriya[8,9] interaction term provides similar contribution along with the staggered g tensor, and both have the same order in magnitude. The Dzyaloshinskii-Moriya interaction together with the staggered g factor can account for the observed nonzero energy gap in copper benzoate. After

making some assumptions and ignoring the small exchange anisotropy, the effective Hamiltonian to describe the copper benzoate in the magnetic field can be written as[7]

$$H = J\sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - h_u S_i^z - (-1)^i h_s S_i^x\right], \tag{2}$$

where h_s is the induced effective dimensionless staggered field, which is the key term to account for the observed nonzero energy gap. The magnitude of h_s depends on the magnitude and relative direction of the applied uniform field h_u with respect to the sample.

Hamiltonian (2) has been studied using the bosonization approach, mapping on the sine-Gordon model, and form-factor techniques. The gap and magnetization behavior,[7,10] the dynamical magnetic susceptibility,[11,10] the specific heat,[12] and the electron spin resonance[13] experiments have been analyzed using the sine-Gordon quantum field theory. There have also been numerical studies of the excitation energy and transition amplitudes in the staggered magnetic field, based on the Bethe ansatz solutions.[14] These studies focus mainly on the parameter range corresponding to the reported copper benzoate magnetic field experiment.[3] The field-induced gap and related magnetization, as well as spin correlations in generic spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chains are of great interest but yet to be fully understood. Of particular interest is the study of a wider range of parameter and very high magnetic field conditions beyond those probed by the experiment and previous theoretical work, which may prove to be of significant importance in understanding the entire range of field-induced phenomena and the underlying physics in this interesting system.

In this paper, we report results of our numerical calculations of the ground state and the low energy excitations of Hamiltonian (2) using the density matrix renormalization group (DMRG) method.[15] We study the most general case and take h_u and h_s as independent variables in our calculations. We find that the critical (saturation) uniform field $h_u^c = 2.0$ serves as an important reference point in understanding the obtained results. When fixed h_u is lower than or equal to h_u^c, the induced energy gap increases with h_s as a power with exponent $\sim\frac{2}{3}$, and for fixed h_u larger than h_u^c, the small h_s dependence is exponential. On the other hand, when h_s is fixed, the h_u dependence of the gap displays a minimum around h_u^c. When h_u and h_s increase simultaneously with a fixed ratio, the gap increases with the field when the ratio is small but develops a minimum around h_u^c at larger ratios. The magnetization results are consistent with the intuitive expectation in general. The most interesting features are obtained for fixed $h_u < h_u^c$ and in small fixed h_s cases. When h_u is lower than h_u^c and fixed, the existence of a small staggered field enhances the uniform magnetization instead of suppressing it; similar effects are also observed for small fixed h_s case, where the staggered magnetization increases until h_u approaches h_u^c. The uniform field induced incommensurate behavior is also studied, and the results show competing effects of the uniform and staggered fields, with the staggered field frustrating the incommensurate state. In the following, the numerical DMRG results will be presented in Sec. II and a summary given in Sec. III.

II. DMRG RESULTS

The DMRG method[15] is a powerful tool for the calculation of low lying states of quasi-one-dimensional systems and has been developed to calculate other properties of many strongly correlated systems.[16] The accuracy of the DMRG calculations on spin chains is generally high. This has also been verified in the $S=1$ (Ref. 17) and $S=2$ (Ref. 18) Heisenberg chain calculations. In the present work, we employ the periodic boundary conditions (PBC's) and use the infinite chain length algorithm of DMRG. We retain as many as 500 optimal states and compute up to chain length $N = 100$ in each calculation. The largest truncation errors are of the order of 10^{-9} for zero uniform field calculations and 10^{-6} for nonzero uniform field calculations. To simplify the discussion, we set the coupling constant J as the energy unit, h_u as the effective uniform field, and h_s as the effective staggered field.

For the Hamiltonian considered here, the effect of the uniform field is to induce a uniform magnetization and shift the critical wave vector from π (in this paper we will concentrate on this case for the pitch vector, where a peak in the static structure factor is expected), and the staggered field will induce a nonzero energy gap between the ground state and the lowest excited state. A nonzero staggered magnetization will also be expected for finite staggered fields. The nature of the ground state depends on the competition of the uniform and the staggered field. We will discuss the energy spectrum of the Hamiltonian first, and then show the ground-state magnetization behavior and investigate the incommensurate behavior of the spin correlation functions.

A. Energy gap

When the staggered field is present alone in the spin-$\frac{1}{2}$ chain, that is, $h_u = 0$ in Hamiltonian (2),

$$H = \sum_i \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - (-1)^i h_s S_i^x\right] \tag{3}$$

the x component of the total spin S_{tot}^x is conserved. This property can be used in DMRG calculations to reduce the dimension of the Hilbert space to be considered.

The spin-1 case of Hamiltonian (3) has been studied in detail.[19] For the standard spin-1 Heisenberg chain, the low energy spectrum is gapful, and the lowest excited state is a spin triplet known as Haldane triplet. The presence of a staggered field will split the Haldane triplet into two branches, the transverse branch and the longitudinal branch. Both branches are gapful and the gap increases with the staggered field.

For the spin-$\frac{1}{2}$ case, the excitation spectrum for zero-field chain is gapless, and the presence of the staggered field may also open a finite gap between the ground state and the low-energy continuum. It is expected that the gapful excitations

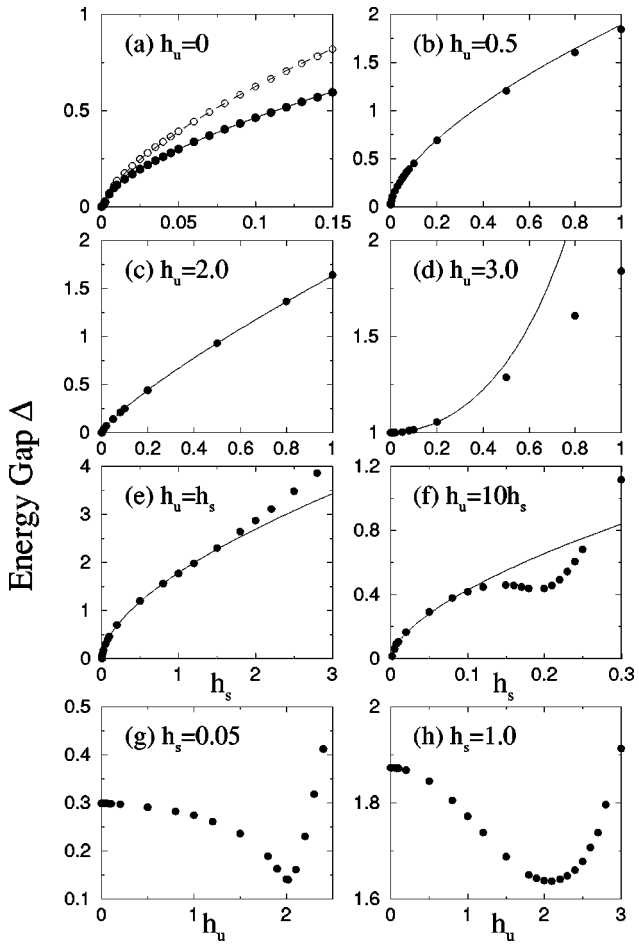

FIG. 1. Field dependence of the induced energy gap for Hamiltonian (2) with different h_u and h_s relations. The DMRG results are shown by circle, the lines denote the fitting curves. In (a), the filled circles denote the transverse branch, while the empty circles the longitudinal branch. It should be noted that in several cases [(d), (g), and (h)] the y axis does not start from $\Delta=0$ as in other cases.

will also split into two branches, with the x component of total spin $S^x_{\rm tot}=0$ (longitudinal branch) and 1 (transverse branch).

The field dependence of the gap of the longitudinal and transverse branches for Hamiltonian (3) is shown in Fig. 1(a). It is clear that the low energy spectrum becomes gapful as soon as the staggered field is present. The magnitude of both longitudinal and transverse modes increases when the staggered field becomes larger with the longitudinal mode goes up faster than the transverse one. This behavior is exactly the same as for the spin-1 chain. But for the spin-1 chain in the staggered field, the increase of the longitudinal gap is about three (two) times faster than the transverse one for small (large) staggered field. For the spin-$\frac{1}{2}$ chain case, this ratio is smaller. The two gaps are fitted using the equation

$$\Delta = a h_s^b, \tag{4}$$

where a and b are fitting parameters. The least square fitting gives

$$\Delta_L = a_L h_s^{b_L} = 2.97 h_s^{0.678},$$

$$\Delta_T = a_T h_s^{b_T} = 1.97 h_s^{0.63}, \tag{5}$$

where Δ_L and Δ_T denote the longitudinal and transverse gap, respectively. The ratio of the gap increase coefficient of the longitudinal mode to the transverse mode a_L/a_T is about 1.5. The fitting curves Eq. (5) are also shown in Fig. 1(a). For larger staggered field, the fitting is almost perfect, while it is not very good for very small staggered field. [This deviation is not visible in Fig. 1(a).] It should be noted here that the numerical error of DMRG results for small staggered field is much bigger than that for large field.

When the uniform field in Hamiltonian (2) is not vanishing, the competition of the uniform and the staggered field needs to be taken into account. The presence of the uniform field will affect the behavior of the energy gap. In the nonzero uniform field case, the calculation is more difficult, since now even $S^x_{\rm tot}$ is not conserved any more. There is no good quantum number which can be used to reduce the relevant Hilbert space dimension. To investigate the gap behavior, the ground state and the lowest excited state must be calculated at the same time, and at least two states must be targeted in each calculation.

To study the effect of the uniform field on the gap behavior, we first calculate the staggered field dependence of the gap when uniform field h_u is a nonzero constant. As described above, when the uniform field is present alone, there is a critical point $h_u^c=2.0$, where the magnetization is saturated. We need to perform calculations at different values of h_u, one in each part of the h_u phase space. We choose $h_u=0.5$ for the small uniform field case and $h_u=3.0$ for the large field case. We also calculate the h_s dependence of the gap at the uniform field critical point $h_u^c=2.0$.

The results for $h_u=0.5$, 2.0, and 3.0 are shown in Figs. 1(b), 1(c), 1(d), respectively. For $h_u=0.5$ and 2.0, the spectrum is gapless when $h_s=0$, and an energy gap opens up when the staggered field is present. The gap increases with the staggered field h_s following the same function Eq. (4) as in the $h_u=0$ case, although with different parameters. Least square fitting gives $a=1.89$, $b=0.624$ for $h_u=0.5$ and $a=1.63$, $b=0.81$ for $h_u=2.0$. Comparison with results in Fig. 1(a) shows that both the coefficient and the exponent in the $h_u=0.5$ case differ only slightly from those of the transverse branch for $h_u=0$; for $h_u=2.0$, the difference becomes more pronounced. The calculated results show that in the uniform field gapless phase ($h_u \leqslant 2.0$), the induced gap is affected by the uniform field only when the uniform field is strong enough. For $h_u=3.0$, the gap dependence is different. The energy spectrum is gapful even when $h_s=0$. With the application of the staggered field, the gap increases. The increase of the gap is nearly exponential when the staggered field is not very strong, following $\Delta=\exp(a h_s^b)$ with parameters $a=1.186$ and $b=1.939$. When the staggered field is large enough, the gap increase deviates from the exponential behavior.

In the experiment on Cu benzoate,[3] the magnitude of the induced staggered field depends on the applied uniform field.

Roughly speaking, when the relative orientation of the applied field is fixed, the induced staggered field increases linearly with the applied uniform field. To compare with experiment directly, we have also considered the case when h_s and h_u increase at the same time with the ratio h_s/h_u being fixed. In Figs. 1(e) and 1(f), we present the calculated results of the energy gap with the staggered field for the cases of $h_u=h_s$ and $h_u=10h_s$. In both cases, the field dependence of the gap for smaller staggered field can also be fitted with function (4). For $h_u=h_s$, the fitting holds at $h_s=h_u<2.0$ with $a=1.786$ and $b=0.594$, while for $h_u=10h_s$, it holds for $h_s<0.1$ with $a=1.755$ and $b=0.613$. The gap for $h_u=h_s$ case increases monotonically but that for $h_u=10h_s$ exhibits a minimum near $h_s\sim0.2$ ($h_u\sim2.0$), and then increases rapidly. The largest induced staggered field produced in experiment[3] is about $h_s\sim0.05$, and it is not big enough to detect the gap minimum shown in Fig. 1(f). Experiments at higher magnetic field are needed to test this predicted phenomenon. Here we can see again that the critical point $h_u^c=2.0$ plays an important role in separating different regions where the scaling behavior of the field-induced gap shows qualitative difference.

The effect of the uniform field on the spin gap induced by the staggered field can be studied directly by calculating the uniform field dependence of the gap at fixed staggered field. From the above results, we have learned that the system stays in one single gapful phase when the staggered field is present alone, so we just choose two sets of h_s, $h_s=0.05$ as the small staggered field limit and $h_s=1.0$ as the large staggered field limit. In Figs. 1(g) and 1(h), we show the gap behavior with the change of the uniform field for the two cases. It is clearly seen that in both cases the gap decreases when the uniform field increases from zero and reaches its minimum near $h_u\sim2.0$, followed by a rapid increase with further increase in the uniform field. The increase of the gap after the minimum is approximately linear for both cases.

Detailed calculations around the gap minimum provide more information on the gap behavior. For $h_s=0$, the system is gapless until the uniform field reaches the saturation point $h_u^c=2.0$. When h_s is not zero, the system has a finite energy gap, and the presence of a small uniform field may suppress the gap. However, for small uniform fields, the suppression of the gap is negligible; it becomes visible only when the uniform field is large enough. The gap minimum for nonzero h_s occurs when the uniform field h_u is slightly larger than 2.0. It occurs at $h_u\sim2.02$ for $h_s=0.05$ and $h_u\sim2.1$ for $h_s=1.0$. This means that the minimum gap uniform field value $h_u^{\min}$ increases slowly with h_s. After the gap minimum, its behavior is dominated by the uniform field, and the gap increases almost linearly with h_u. We should emphasize here that the minimum gap for both cases is not zero, and for the $h_s=1.0$ case the decrease in magnitude is a little bigger than that for the $h_s=0.05$ case.

B. Magnetization

The existence of a nonzero uniform field will induce a magnetization in the system, and the existence of a nonzero staggered field will induce an additional staggered magnetization. The staggered magnetization $M_s(N)$ and the uniform magnetization $M_u(N)$ of the system with a finite chain length N are defined as

$$M_s(N)=\frac{1}{N}\sum_i (-1)^i\langle S_i^x\rangle,$$

$$M_u(N)=\frac{1}{N}\sum_i \langle S_i^z\rangle. \tag{6}$$

The results for the thermodynamic limit

$$M_s=\lim_{N\to\infty} M_s(N),$$

$$M_u=\lim_{N\to\infty} M_u(N) \tag{7}$$

can be obtained by studying different chain-length systems. The results of the magnetization and the staggered magnetization for the eight parameter sets (h_u,h_s) used in the previous subsection are shown in Fig. 2.

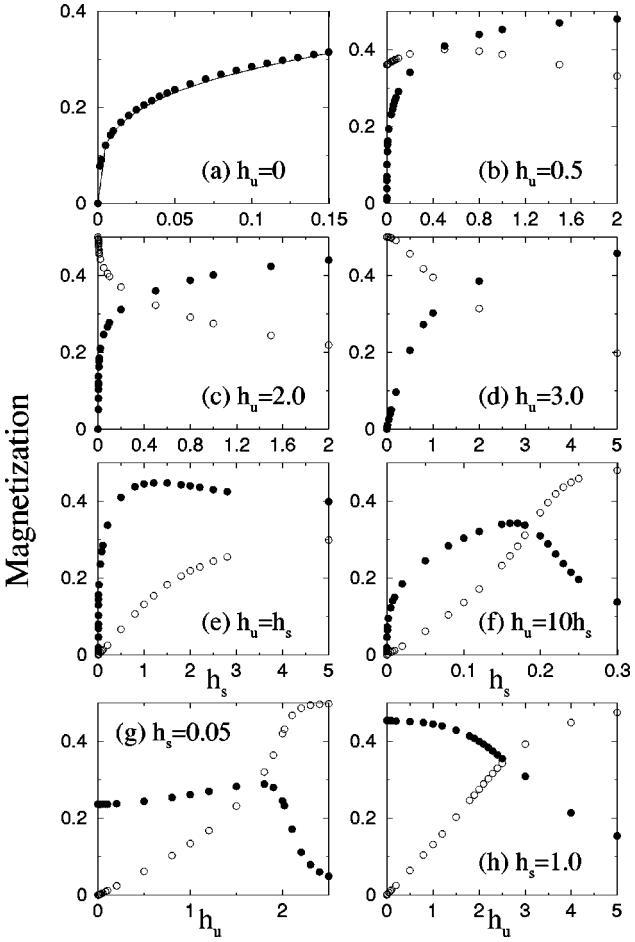

FIG. 2. Magnetization curves for eight parameter sets of h_u and h_s. The filled (empty) circles are for the staggered (uniform) magnetization. The solid line in (a) is the fitting curve described in text. For the $h_u=0.5$ case in (b), the uniform magnetization is amplified 6 times to bring it up to the same scale with the other panels.

When the uniform magnetization is absent ($h_u=0$), the induced staggered magnetization increases with the staggered field and approaches the saturation value 0.5 when $h_s \to \infty$. From the field dependence of the staggered magnetization, we can extract the staggered magnetic susceptibility $\chi^{(s)}=\partial M_s/\partial h_s$. In Fig. 2(a), we can see clearly that the staggered magnetic susceptibility goes to infinity when the staggered field $h_s \to 0$ instead of approaching a constant as in the case of the spin-1 chain. This is because the spin-$\frac{1}{2}$ chain is gapless for zero staggered field while it has a finite gap in the spin-1 case. The magnetization curves are fitted using the following function:

$$M_s = a h_s^b \tag{8}$$

with $a=0.527$ and $b=0.277$. The fitting line is also shown in Fig. 2(a). In the h_s range shown in Fig. 2(a), the fitting is good, but it should be noted that the fitting Eq. (8) will not be valid for very large h_s, since it diverges when $h_s \to \infty$ instead of approaching the finite value 1/2 which is the strong staggered field limit of Hamiltonian (3).

When h_u is finite and fixed, the staggered magnetization increases monotonically with the staggered field and approaches the saturation value $M_s=0.5$ when h_s goes to infinity, the same as in the $h_u=0$ case. The magnetizations for $h_u=0.5$, 2.0, and 3.0 are shown in Figs. 2(b), 2(c), and 2(d), respectively. Because the zero staggered field energy spectrum for $h_u=0.5$ and $h_u=2.0$ is gapless, the zero-field staggered magnetic susceptibility at $h_s=0$ is still divergent. For $h_u=3.0$, the $h_s=0$ system is gapful, so the zero-field staggered magnetic susceptibility has a finite value $\chi^{(s)}(0)=0.299$. For $h_u=2.0$ and 3.0, the uniform magnetization is saturated when the staggered field is absent; it decreases from the saturation value 0.5 when a staggered field is applied. When the staggered field is weak, the way the magnetization changes is different for the two cases. It decreases rapidly for $h_u=2.0$ but slowly for $h_u=3.0$. For $h_u=0.5$, at zero staggered field, the uniform magnetization has a finite value but is not saturated; when the staggered field increases, the uniform magnetization will also increase and reach a maximum when $h_s \sim 0.5$ before decreasing with further increasing staggered field.

In Figs. 2(e) and 2(f), we show the field dependence of the magnetization for the $h_u=h_s$ and $h_u=10h_s$ cases, respectively. When the uniform and staggered fields increase simultaneously from zero, both staggered and uniform magnetizations increase. For both cases, the zero-field staggered susceptibility is divergent and the zero-field uniform susceptibility is zero. We should note here that the zero-field uniform susceptibility is not shown clearly in Figs. 2(e) and 2(f) due to the large field scale used. Its zero value was obtained by analyzing results for very small field. When $h_u=h_s$, the effect of the staggered field rises rapidly and is dominating at small fields. When the field increases, the effect of the uniform field becomes more important and must be taken into account. At $h_s=h_u \sim 1.2$, the staggered magnetization reaches its maximum, and it decreases with further increasing field. The uniform magnetization increases monotonically with the increasing fields. Both staggered and uniform magnetizations approach finite but nonsaturated values when the field goes to infinity. For $h_u=10h_s$, the effect of the staggered field is also dominating at small field. But at large field, the effect of the uniform field becomes dominant. The staggered magnetization decays fast to a small finite value ~ 0.05 after reaching its maximum. The uniform magnetization increases monotonically and approaches a nearly saturated value 0.498 at high enough field.

When the staggered field is fixed, at $h_u=0$ the staggered magnetization is finite while the uniform magnetization is zero. The uniform field dependence of the magnetization for $h_s=0.05$ and $h_s=1.0$ is shown in Figs. 2(g) and 2(h). For $h_s=0.05$, the staggered magnetization increases with the uniform field first, reaches its maximum at $h_u \sim 1.8$, and then decays to zero rapidly. For $h_s=1.0$, the staggered magnetization decreases with the uniform field monotonically. But the decrease is not rapid for small h_u. In both cases, the uniform magnetization increases with the uniform field. At small uniform field, the uniform magnetization increases linearly with the uniform field. We have obtained zero-field uniform magnetic susceptibility $\chi^{(u)}(0)=0.1185$ for $h_s=0.05$ and $\chi^{(u)}(0)=0.1283$ for $h_s=1.0$.

For the $h_u=0.5$ ($h_s=0.05$) case, the existence of a small staggered (uniform) field enhances the corresponding uniform (staggered) magnetization instead of suppressing it. This phenomenon can be explained intuitively. In these cases, when a small uniform (staggered) field is applied, the coupling between neighboring spins is weakened. While this uniform (staggered) field is not strong enough to destroy the effect of the stronger staggered (uniform) field, it enhances the ratio between the effective uniform (staggered) field and the effective coupling constant and, consequently, the induced uniform (staggered) magnetization.

C. Correlation function and incommensurate behavior

We define three ground-state spin correlation functions for chain length L, (i) $\mathcal{C}_u$ parallel to the uniform magnetic field, (ii) $\mathcal{C}_s$ parallel to the staggered field, and (iii) $\mathcal{C}_y$ along the remaining (y) axis, as

$$\mathcal{C}_u(i-j)=\langle S_i^z S_j^z \rangle,$$

$$\mathcal{C}_s(i-j)=\langle S_i^x S_j^x \rangle,$$

$$\mathcal{C}_y(i-j)=\langle S_i^y S_j^y \rangle. \tag{9}$$

The correlation function $\mathcal{C}_y$ is expected to display exponential decay because of the existence of the spin gap induced by the staggered field. $\mathcal{C}_s$ and $\mathcal{C}_u$ do not decay exponentially because of the effects of the nonzero staggered and uniform magnetization, respectively. $\mathcal{C}_u$ is also expected to show incommensurate behavior due to the existence of the uniform field. These correlation functions have the following form:[20]

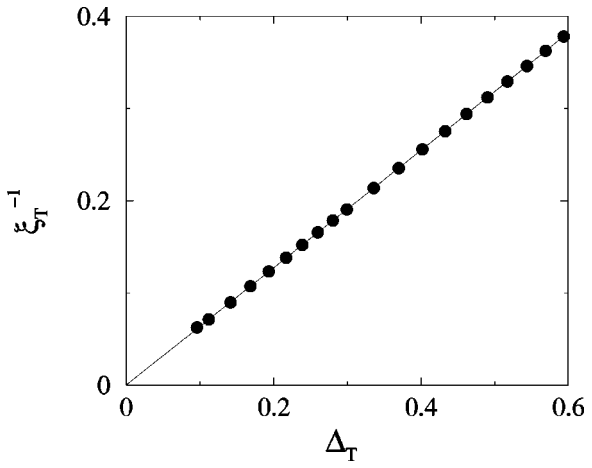

FIG. 3. The inverse correlation length for the transverse branch of the zero uniform field case vs the transverse gap at different staggered fields. The solid fitting line is $\xi_T^{-1}=0.6364\Delta_T$.

$$\mathcal{C}_u(l)=M_u^2+(-1)^l A_1\frac{e^{-l/\xi}}{\sqrt{l}}\cos(al+\theta_0),$$

$$\mathcal{C}_s(l)=(-1)^l M_s^2+(-1)^l A_2\frac{e^{-l/\xi}}{\sqrt{l}},$$

$$\mathcal{C}_y(l)=(-1)^l A_3\frac{e^{-l/\xi}}{\sqrt{l}}, \tag{10}$$

where M_u and M_s are the uniform and staggered magnetization, respectively, A_1, A_2, A_3, a, θ_0, are l independent constants, and ξ is the correlation length. It should be noted here that the length ξ may not be the same along three different directions.

From the spin correlation functions Eq. (10), we can extract the corresponding correlation length. When $h_u=0$, the obtained correlation length is a function of the staggered field. The product of the correlation length and the spin gap gives the spin wave velocity of the system. In Fig. 3, we show the relation between the inverse correlation length and the transverse gap. It is seen that the curve goes linearly which means that the spin wave velocity does not change with the magnitude of the staggered field. The linear fitting of the line gives the spin wave velocity $v=\Delta_T\xi_T=1/0.6364=1.5713$, in good agreement with the exact spin wave velocity for the spin-$\frac{1}{2}$ chain $\pi/2\approx 1.5708$. As in the spin-1 chain case,[19] this also serves as an independent check of the self-consistency of our calculations. From the figure, we can see for zero stagger field spin-$\frac{1}{2}$ chain, the spectrum is gapless, $\Delta=0$, so the correlation length is infinite. For other cases in our calculations, the correlation length is difficult to obtain, because the chain length is short and the numerical error is bigger for those cases. But we can conclude from our results that in general the spin wave velocity is not a constant anymore, and, instead, it changes with the applied uniform field.

The cosine function in $\mathcal{C}_u$ comes from the incommensurate behavior induced by the uniform field. Because of the existence of the staggered field, the net incommensurate behavior is a result of competition between h_u and h_s. In Fig. 4, we present $\phi(l)=\sqrt{l}e^{l/\xi}[\mathcal{C}_u(l)-M_u^2]$ at chain length 100 as a function of l for $h_u=0.5$ and $h_s=0.05$, where M_u is obtained by the magnetization calculation discussed above. This clearly shows the existence of incommensurability in the system. In this case, the correlation length $\xi\approx 4.05$.

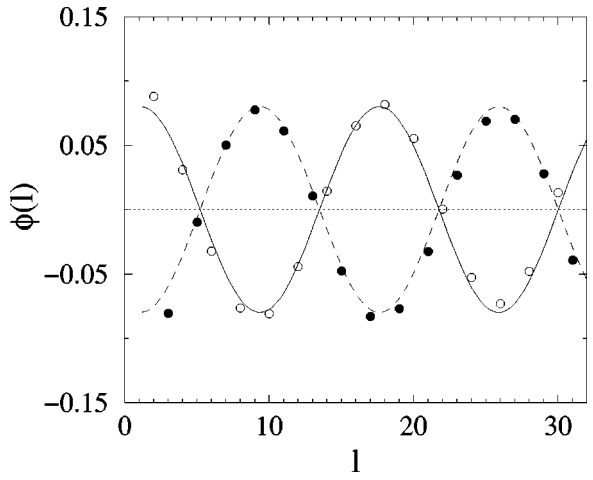

FIG. 4. Incommensurate behavior in $\phi(l)=\sqrt{l}e^{l/\xi}[\mathcal{C}_u(l)-M_u^2]$ for $h_u=0.5$, $h_s=0.05$ and chain length $L=100$ system. The correlation length $\xi\approx 4.05$. The odd and even l are denoted by filled and empty circles, respectively. The solid and dashed fitting lines are $\pm 0.08\cos(0.38l-0.407)$.

The incommensurate behavior in the correlation function leads directly to the peak shift from π in the static structure factor $\mathcal{S}(q)$ which can be obtained from the correlation functions. For the uniform field (z) axis and the staggered field (x) axis, we can write

$$\mathcal{S}_u(q)=\frac{1}{L}\sum_l e^{iql}\mathcal{C}_u(l), \tag{11}$$

$$\mathcal{S}_s(q)=\frac{1}{L}\sum_l e^{iql}\mathcal{C}_s(l). \tag{12}$$

Since we use the periodic boundary conditions in our calculations, the wave vector q is well defined, $q=2\pi n/L, n=1,\ldots,L$.

In Fig. 5, we present the static structure factor $\mathcal{S}_u$ at $h_u=0.5$ and $h_s=0.05$ for the even chain length from 60 to 100. The results for different chain length systems fall onto the same curve. This success is due to the small correlation length of the system considered ($\xi\sim 4.05$). The chain lengths used here are much larger than the correlation length, and the finite size effect is very weak. Figure 5 shows a two peak structure symmetric about π which is obtained by Eq. (11). For this case, we have obtained the critical wave vector shift $\delta q=|q-\pi|\sim 0.224\sim 0.07\,\pi$. The accuracy of δq obtained from the peak deviation of $\mathcal{S}_u(q)$ is good; it is mainly limited by the finite chain lengths used in the calculations and the error is estimated to be less than 1%.

For all parameters studied in these calculations, using the peak position of the static structure factor $\mathcal{S}_u(q)$ to determine the existence of the incommensurate state, we found the critical wave vector shift in three sets of parameters, $h_u=0.5$, $h_u=10h_s$, and $h_s=0.05$. The critical wave vector

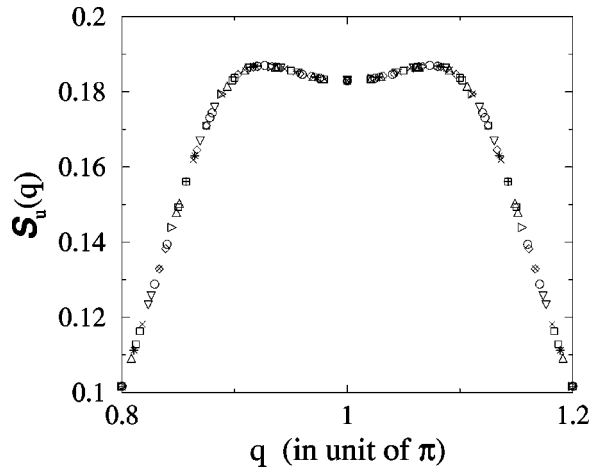

FIG. 5. Static structure factor $\mathcal{S}_u(q)$ for $h_u=0.5$ and $h_s=0.05$. The results for chain length from 60 to 100 are shown.

shift δq versus field in these cases is shown in Fig. 6. Since the largest total chain length in our calculations is $N=100$, we cannot detect the incommensurate state if $\delta q<2\pi/100=0.02\pi$. For the $h_u=0.5$ case, the critical wave vector shift becomes smaller when the staggered field h_s increases from zero. It is expected to go to zero when the staggered field is large enough. In other words, the existence of the staggered field will frustrate the incommensurate state. For the other two cases $h_u=10h_s$ and $h_s=0.05$, the critical wave vector

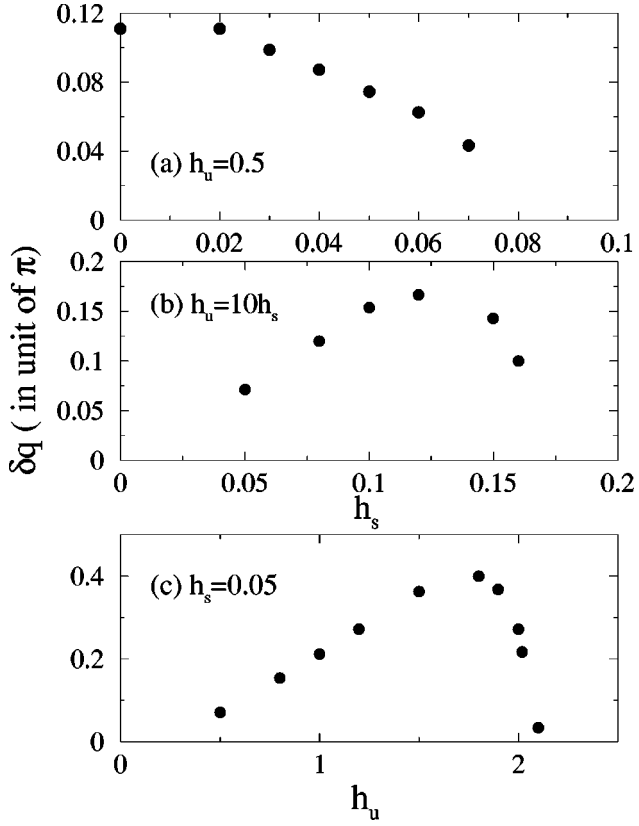

FIG. 6. The field dependence of the critical wave vector shift δq for (a) $h_u=0.5$, (b) $h_u=10h_s$, and (c) $h_s=0.05$.

shifts away from π with increasing uniform field but eventually returns to π around h_u^c.

For comparison, we examine our calculated results with parameters corresponding to the reported experimental case on Cu benzoate.[3] The highest magnetic field reached in the experiment is about 7 T which corresponds to $h_u\approx 0.52$. The energy gap observed at this field is $\Delta\sim 0.4$ meV, considering the coupling constant for the material $J=1.57$ meV, $\Delta/J\sim 0.255$. From our calculated results for $h_u=0.5$, we estimate that the induced staggered field $h_s\sim 0.04$. The critical wave vector shift δq for $h_u=0.5$, and $h_s=0.04$ is $\delta q\sim 0.274\sim 0.09\pi$. The critical wave vector shift for $h_u=0.52$, $h_s=0.04$ will be slightly larger than 0.09π. In the experiment, the largest wave shift for $H=7$ T is about 0.12π. This comparison shows that the calculated results are in good agreement with the experiment.

III. SUMMARY

We have carried out systematic calculations using the density matrix renormalization group method to study the behavior of the energy gap, magnetization, and spin correlation functions of spin-$\frac{1}{2}$ antiferromagnetic Heisenberg chain in the presence of a uniform and a perpendicular staggered magnetic field. An extensive examination of the parameter space has revealed many interesting features beyond those reported in previous studies. In particular, results at very high magnetic field show quantitatively and even qualitatively different behaviors in the energy gap and magnetization, from those found for lower fields. For the $h_u=10h_s$ case, which is close to the real parameters in the Cu benzoate experiment, we can see from Figs. 1 and 2 that the competition of the staggered and uniform field is visible when $h_s>0.15$, or $h_u>1.5$. In Cu benzoate, $h_u=1.5$ corresponds to an applied field $H\sim 21$ T. Further experimental investigation at such high magnetic fields is needed to test these predictions.

The field-induced energy gap is dominated by the staggered field when the uniform field is smaller than the standard spin-$\frac{1}{2}$ chain saturation field $h_u^c=2.0$. When the uniform field is comparable or larger than h_u^c, the effect of the uniform field becomes important and must be taken into account. The uniform field introduces frustration effects and creates a local minimum in the energy gap near h_u^c in several cases.

The magnetization results clearly reveal the competition of the uniform and staggered fields. However, for some uniform (staggered) field, the existence of a small staggered (uniform) field enhances the uniform (staggered) magnetization instead of suppressing it. The competition of the two kinds of field can also be seen from the incommensurate behavior with the staggered field suppressing the incommensurate state and moving the critical wave vector closer to the zero-field value π.

The specific heat experiment on Cu benzoate[3] shows that the field-induced gap scales with approximately 2/3 power of the applied magnetic field. The analytic results[7,10] yield the same power law dependence for Hamiltonian (2). In our numerical results, for $h_u=0$ case, the scaling power $b_L=0.678$ for the longitudinal gap and $b_T=0.63$ for the trans-

verse gap. They are in good agreement with the experiment and the analytic value. The existence of the nonzero uniform field modifies the power law relation. When the uniform field is small, the modification is almost negligible. Further high field experiments are needed to examine the predicted effect of the applied uniform field on the scaling behavior of the induced gap.

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