First-order commensurate-incommensurate magnetic phase transition in the coupled FM spin-1/2 two-leg ladders

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We consider the spin-1/2 two-leg ladders with ferromagnetic (FM) interactions along legs and rungs. Using the stochastic series expansion QMC method, we study the low-temperature magnetic behavior of the system. An isolated spin-1/2 FM two-leg ladder is in the gapped saturated FM phase at zero temperature. As soon as the spin-1/2 FM two-leg ladders are connected with antiferomagnetic (AFM) inter-ladder interaction, a first-order commensurate-incommensurate quantum phase transition occurs in the ground state magnetic phase diagram. In fact a jump in the magnetization curve is observed. We found that, coupled spin-1/2 FM two-leg ladders are in a nonmagnetic phase at zero temperature. Applying a magnetic field, the ground state of coupled spin-1/2 FM two-leg ladders remains in the nonmagnetic phase up to a quantum saturate critical field.

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I. INTRODUCTION

Recently, spin-1/2 two-leg ladder systems have devoted considerable growth to itself experimentally and theoretically. The main interest to study of these systems is related to this fact that the high-Tc superconductivity phenomenon occurs in these systems and also they have a gap in the spin excitation spectrum.

In the study of spin-1/2 two-leg ladder systems with antiferromagnetic (AFM) leg and rung interactions, the formation of spin singlets located on each rung open the spin gap in the energy spectrum which is called the gaped spin liquid phase. These kind of AFM two-leg ladder systems are observed in the nature. The effect of a magnetic field on the physical properties of these compounds has been a field of intense studies. It is found that there are two quantum critical fields in the ground state phase diagram of these kind of spin-1/2 two-leg ladders. Generally, at low magnetic fields \( (h < h_c^1) \), there is a spin liquid phase (a gapped phase) at low temperatures. Both magnetic susceptibility and the magnetization go up first with cooling, then decay exponentially to zero at low temperatures. Also, the specific heat has a single peak at low temperature due to transition from disordered phase to the spin singlet gapped phase. The Tomonaga-Luttinger liquid (TLL) gapless phase is found in \( h_{c_1} < h < h_{c_2} \) regime at low temperatures. One of the spin liquid \( (h < (h_{c_1} + h_{c_2})/2) \) or spin polarized \( (h > (h_{c_1} + h_{c_2})/2) \) phases at higher temperature is expected. The thermodynamic properties like magnetization and the susceptibility have a finite value at low temperature which show the vanishing of the energy gap in the TLL phase. Specific heat shows a second peak and goes down linearly with lowering temperature in the TLL regime.

The spin-1/2 two-leg ladder systems with AFM legs and FM rungs are also observed from experimental point of view. By means of the specific heat and the magnetocaloric effect measurements, a phase boundary between the spin liquid phase and the ordered phase is determined. We have to mention that, the ladders with FM leg and AFM rung exchange interactions found experimentally during last two years.

Recently, Nagashiwa and coworker synthesized chlorido-bridged dinuclearcopper(II) complex with 2-methyloxothiazol-3(2H)-one with chemical formula \( [\text{Cu}^{II} \text{Cl(O-mi)}_2(-\text{Cl}_2)] \). This compound is a quasitwo-leg ladder system with FM exchange interaction in legs and rungs. The Weiss temperature is estimated about 8.7 K, indicating ferromagnetic behavior. Also no exotic phenomena due to spin frustration were observed within the measured temperature range. From theoretical point of view, spin-1/2 two-leg ladders with FM legs and rungs are much less studied. In a very recent work, the temperature dependence of the magnetic susceptibility and the magnetic structure factors is studied using the modified spin wave theory and the numerical exact diagonalization technique. They have showed that in an intermediate temperature range, their analytical results are consistent with the numerical exact diagonalization results. The need for investigation of AFM inter-ladder coupling in FM ladders ( FM exchange interaction in both legs and rungs ) is also motivated by synthesizing the 3-Cl-4-F-V, 3-Br-4-F-V and 3-I-V crystals recently which are the candidates for two-leg ladders with FM legs and AFM rungs.

In this paper we study the AFM inter-ladder interaction effect between FM two-leg ladders in the presence of a magnetic field (see Fig. 1). This system for large inter-ladder interaction can be considered as the ladders with FM legs and AFM rungs by FM coupling. We used the recently developed stochastic series expansion (SSE) QMC method to provide numerical simulation results. The magnetization, the susceptibility and the specific heat are calculated for large enough finite size systems. Our simulation results show that isolated FM two-leg ladders are in an ordered phase at zero temperature. As soon as the AFM inter-ladder interaction is added, a first-order commensurate-incommensurate quantum phase transi-
FIG. 1: The schematic picture of FM two-leg ladders with AFM inter-ladder interaction. The size of coupled ladders is $10 \times 30$.

The Hamiltonian of the system is written as

$$H = J_{\text{leg}} \sum_{n,\alpha} S_{n,\alpha} \cdot S_{n+1,\alpha} - g\mu_B h \sum_{n,\alpha} S_{n,\alpha}^z + J_{\text{rung}} \sum_{n} S_{n,1} \cdot S_{n,2}$$

where $S_{n,\alpha}$ is the spin $S = 1/2$ operator on rung $n$ ($n = 1, ..., L$) and leg $\alpha$ ($\alpha = 1, 2$). An applied magnetic field $h$ in the $Z$ direction leads to zeeman term. The rung and leg exchanges are denoted by $J_{\text{rung}}$ and $J_{\text{leg}}$, respectively.

It is found that the rung exchange $J_{\text{rung}} = -9.68 K$ is about four times larger than $J_{\text{leg}} = -2.068 K$. In the following, we consider these values in our QMC simulation approach. We have used the ALPS code which is known as one of the best codes in this field. We have considered two-leg ladders with the maximum size $N = 2L = 2 \times 100$ and periodic boundary conditions. The QMC simulation is performed for the maximum 1000000 equilibration sweeps and 2000000 measurement steps.

Fig. 2 presents the magnetization as a function of the temperature in the absence of the magnetic field. Induced thermal fluctuations by increasing temperature cause in decreasing the magnetization and it reaches zero for high enough temperatures. The magnetic susceptibility is also shown in the inset of Fig. 2. It only goes up first with lowering temperature until it reaches to a maximum value, then decreases exponentially down to zero at low temperatures. This exponential fall of susceptibility indicates that there is a gap in the excitation spectrum of the FM two-leg ladder system in the presence of a magnetic field. With decreasing the magnetic field the peak of susceptibility curve increases and thus

FIG. 2: The spontaneous magnetization as a function of the temperature for isolated spin-1/2 FM two-leg ladders. As it is seen, at zero temperature the ground state of the system is in a saturated FM phase. By increasing the temperature the induced thermal fluctuations decrease the magnetization of the system. In the inset, the magnetic susceptibility in the absence of the magnetic field is plotted as a function of the temperature. QMC simulation has been carried out for Heisenberg model. The size of two-leg ladder is $2 \times 100$. 

As shown in Fig. 3(a), the magnetic susceptibility goes up first with lowering temperature until it reaches to a maximum value, then decreases exponentially down to zero at low temperatures. This exponential fall of susceptibility indicates that there is a gap in the excitation spectrum of the FM two-leg ladder system.
FIG. 3: (a) Magnetic susceptibility $\chi(T)$ versus temperature for isolated spin-1/2 FM two-leg ladders at different values of the magnetic field. QMC simulation has been carried out for Heisenberg model. (b) Magnetic specific heat per site versus temperature results and found an exponential behavior for isolated spin-1/2 FM two-leg ladders at different values of the magnetic field. QMC simulation has been carried out for Heisenberg model. QMC simulation has been carried out for isolated spin-1/2 FM two-leg ladders at different values of the magnetic field. QMC simulation has been carried out for isolated spin-1/2 FM two-leg ladders at different values of the magnetic field. We have also calculated the specific heat, $C_m(T)$. Our numerical results are presented in Fig. 3(b) for different values of the magnetic field. As it is seen, at zero temperature the specific heat is zero, by increasing the temperature it remains almost zero up to a threshold temperature which is known as the indication of the spin gap. We have also checked the low temperature results and found an exponential behavior which is also an indication of the gapped phase.

III. COUPLED FM TWO-LEG LADDER SYSTEM

High-field nuclear magnetic resonance and inelastic neutron scattering measurements in some quasi-two-leg ladder systems\textsuperscript{11,12,25,26} show that weak coupling between ladders induces 3D phase transition at low temperature region. In these compounds, phase transition between quantum phases and the 3D gapless-Neel ordered phase occurs at very low temperatures.

To the best of our knowledge, the effect of the inter-ladder coupling in spin-1/2 two-leg ladders with FM legs and rungs has not been studied so far. Interesting results are not expected for the inter-ladder AFM coupling. For this reason, we have considered the inter-ladder AFM coupling. We have performed the QMC simulations on the AFM coupled FM two-leg ladder systems for different values of the inter-ladder exchange $J_{\text{in}}$ and in the presence of a magnetic field. The scheme of coupled ladders is illustrated in Fig. 4. The numerical results are calculated for coupled ladders with $J_{\text{rung}} = -9.68 \, K$, $J_{\text{leg}} = -2.068 \, K$, $J_{\text{in}}/J_{\text{leg}} = -0.1, -0.2, ..., -0.5$ and different sizes up to $5 \times 2L = 5 \times (2 \times 30)$.

Fig. 4(a) shows the magnetization, $M$, of the coupled system as a function of the magnetic field in the vicinity of the zero temperature and $J_{\text{in}}/J_{\text{leg}} = -0.2$. It is clearly seen that the magnetization is zero in the absence of the magnetic field which shows that the induced quantum fluctuations by inter-ladder interaction destroy the long-range FM order of the ground state of isolated FM two-leg ladders. It means that in the ground state phase diagram of the coupled FM ladders, the line $J_{\text{in}}/J_{\text{leg}} = 0$ must be a quantum critical line. By applying the magnetic field, the magnetization starts to increase and will be saturated in a critical magnetic field, which depends on the value of the inter-ladder exchange interaction. So, such behavior of magnetization upon contribution of AFM inter-ladder interaction suggests, the existence of a nonmagnetic phase.

Now let us see what happens when we attempt to change the inter-ladder interaction at zero temperature and in the absence of the magnetic field. Fig. 4(b) presents the magnetization versus inter-ladder $J_{\text{in}}$ interaction in the absence of the magnetic field. The inter-ladder interaction effects embedded in the coupled ladders drastically change the value of magnetization. There is a sharp drop of magnetization in the low inter-ladder coupling about $0.01J_{\text{leg}}$. This behavior is known as the main indication of a first-order phase transition. Therefore it suggests the existence of a first-order commensurate-incommensurate quantum phase transition in the ground state phase diagram of the model. Moreover, to confirm the type of the mentioned quantum phase transition in our model, we have also implemented the Lanczos algorithm to find the ground state energy of the system. A very important indication of the first order phase transition is the discontinuity in the first derivative of the ground state energy at the quantum
critical point. Using the numerical Lanczos method, we have calculated the ground state energy for system sizes $2 \times (2 \times L) = 16, 20$ and plotted the first derivative of the ground state energy per site as a function of the inter-ladder interaction in the bottom inset of Fig. 4(b). The results show a clear discontinuity in the first derivative of ground state energy which is in agreement with our QMC results. To find out the effect of inter-ladder AFM interaction, we have also presented the QMC results for the specific heat, $C_m$, in the top inset of Fig. 4(b). In this figure, we observe a second peak at very low temperatures which can be considered as an indication of the mentioned nonmagnetic phase.

It is interesting to discuss the thermodynamic properties of coupled ladders in the gapless phase $J_{in} = -0.2 J_{leg}$ for different magnetic fields. In general there is a similarity between isolated FM ladders and the AFM coupled FM ladders for high magnetic fields. But, the differences can be noticed within the range of $0 < h < 0.5 T$. Fig. 5(a) shows the magnetization versus the temperature for $h = 0.2 T$, $h = 0.3 T$, $h = 0.45 T$, and $h = 0.5 T$. The magnetization is not saturated for $h < 0.45 T$ at zero temperature. To find the critical magnetic field $h_c$, we have performed the calculation for other magnetic fields within the range of $0 < h < 0.5 T$. The size of coupled ladders is $10 \times 30$.

FIG. 4: (a) The magnetization of spin-1/2 FM two-leg ladders with inter-ladder AFM interaction as a function of the magnetic field in the vicinity of the zero temperature and $J_{in}/J_{leg} = -0.2$. QMC simulation has been carried out for Heisenberg model. The size of coupled ladders is $10 \times 30$. (b) The magnetization versus inter-ladder $J_{in}$ interaction in the absence of the magnetic field. The size of coupled ladders is $10 \times 30$. The effect of AFM inter-ladder interaction causes the system undergoes a first-order phase transition. QMC calculation has been carried out for Heisenberg model. In the above inset, specific heat per site was plotted as a function of the temperature in the absence of the magnetic field by using QMC simulation. In the bottom inset, using numerical lanczos algorithm, the first derivative of energy per site versus $J_{in}$ was plotted.

FIG. 5: (a) Magnetization versus temperature for spin-1/2 FM two-leg ladders coupled with AFM inter-ladder interaction at different values of the magnetic field. QMC simulation has been carried out for Heisenberg model. (b) the magnetic susceptibility versus the temperature for different values of the magnetic field above and below quantum critical field. QMC simulation has been carried out for Heisenberg model. The size of coupled ladders is $10 \times 30$. This figure, we observe a second peak at very low temperatures which can be considered as an indication of the mentioned nonmagnetic phase.

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At low temperatures within the range of low magnetic fields $h < h_c = 0.42 \, T$, the magnetic specific heat per site is plotted for values of the field more than the quantum critical field $h$. In the inset, above the quantum critical field $h_c$, the magnetic specific heat $C_m(T)$ is depicted. It can be clearly seen that below the quantum critical field, a second peak appears at low temperatures, whereas in the inset, above the quantum critical field $h_c$, the second peak disappears. These results indicate that the system undergoes a cross-over from a gapped phase in the low magnetic fields to a non-magnetic phase at zero temperature. In principle, the ground state of the coupled ladders is in the saturated FM phase.

As soon as the inter-ladder AFM exchange interaction is added, a first-order commensurate-incommensurate quantum phase transition occurs in the ground state phase diagram. Numerical results of magnetization and specific heat showed that the gapped FM phase is replaced by a nonmagnetic phase. In the presence of a magnetic field, the ground state of the coupled ladders remains in this nonmagnetic phase up to a critical field $h_c$. The value of the mentioned critical field depends on the value of the inter-ladder AFM interaction. Although in the case of $[\text{Cu}^{II} \, \text{Cl(O-mi)}_2(-\text{Cl}_2)]_2$, the compound consists of isolated two-leg ladder, but such an enhancement of coupled interaction may occur upon chemical substitution.

In summary, we have calculated the thermodynamic properties of FM two-leg ladder like $[\text{Cu}^{II} \, \text{Cl(O-mi)}_2(-\text{Cl}_2)]_2$. We have performed stochastic series expansion QMC using ALPS code to investigate spin-1/2 isolated FM two-leg ladders and the effect of the AFM inter-ladder exchange interaction on the low-temperature behavior of these type of ladders. For an isolated spin-1/2 FM two-leg ladder, a gapped behavior was observed at zero temperature. In principle, the ground state of an isolated spin-1/2 FM two-leg ladder is in the saturated FM phase.

In Fig. 6, the magnetic susceptibility is plotted for different magnetic fields in the ratio of $J_{\text{in}}/J_{\text{leg}} = -0.2$. There are indications that the FM two-leg ladder spin systems under this weak AFM inter-ladder interaction undergo to a nonmagnetic phase in the low magnetic fields. $\chi(T)$ goes to finite values at low temperatures within the range of $h < h_c$. Also this behavior suggests that the coupled ladders should be in gapless phase, whereas the exponential fall-off of $\chi(T)$ above critical field is a signature of existence of gap in this system.

In conclusion, we have calculated the thermodynamic properties of FM two-leg ladder like $[\text{Cu}^{II} \, \text{Cl(O-mi)}_2(-\text{Cl}_2)]_2$. We have performed stochastic series expansion QMC using ALPS code to investigate spin-1/2 isolated FM two-leg ladders and the effect of the AFM inter-ladder exchange interaction on the low-temperature behavior of these type of ladders. For an isolated spin-1/2 FM two-leg ladder, a gapped behavior was observed at zero temperature. In principle, the ground state of an isolated spin-1/2 FM two-leg ladder is in the saturated FM phase.

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Existence of the non-magnetic phase in this model is very similar to what can be probably observed in the coupled spin-1/2 two-leg ladders with FM leg and AFM rung exchange interactions in the presence of a magnetic field. In fact, two-leg ladders with FM leg and rung interactions consisting of weak AFM inter-ladder coupling can also be considered as the two-leg ladders with FM leg and weak AFM rung exchange interactions which are FM coupled. The observation of non-magnetic phase in these new type of coupled ladders is stimulating for the future studies.

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