Quantum Monte Carlo Simulations on S=1/2 Antiferromagnetic-Ferromagnetic Random Alternating spin chain

Peng Zhang, Zhaoxin Xu∗, Heping Ying and Jianhui Dai
Zhejiang Institute of Modern Physics, Zhejiang University,
Hangzhou, 310027, P.R. China
(Dated: March 23, 2022)

The S=1/2 Heisenberg chain with bond alternation and randomness of antiferromagnetic (AFM) and ferromagnetic (FM) interactions is investigated by quantum Monte Carlo simulations of loop/cluster algorithm. Our results have shown interesting finite temperature magnetic properties of this model. The relevance of our study to the observed results of the material (CH$_3$)$_2$CHNH$_3$Cu(Cl$_x$Br$_{1-x}$)$_3$ is discussed.

PACS numbers: 75.10.Jm, 75.10.Nr, 75.40.Cx, 75.40.Mg

Keywords: bond randomness; antiferromagnetic; ferromagnetic.

I. INTRODUCTION

Randomness induced quantum phase transitions have attracted intensive interests in the past decades. Putting enough strong bond randomness, analyses of real space renormalization group (RSRG) method have shown that RG flows of spin S=1 and S=1/2 quantum antiferromagnetic Heisenberg chains [1, 2, 3] go to a stable fixed point called the random singlet (RS) phase in which spins far apart in space randomly form weakly bound singlet pairs. This property induces universal behaviors of ground states and low temperature thermodynamics, e.g. the energy spectrum is gapless, the temporal correlation length $\xi_t$ and spatial correlation length $\xi_L$ diverge at zero temperature, and there is a non-universal infinite dynamical exponent $z$ which comes from the relation $\xi_t^z \sim \xi_L$. More important, the uniform susceptibility diverges universally in the RS phase as

$$\chi \sim \frac{1}{T \ln^2 \left( \Omega/T \right)}$$

at low temperature, where $\Omega$ is a non-universal constant. On the other hand, the S=1/2 dimerized AFM chain was found to be extremely stable against strong bond randomness [4]. In this case, the system is in a quantum Griffiths-McCoy (QG) phase when the bond randomness is strong enough. This phase is characterized by gapless excitations and finite correlation length. In the QG phase, the uniform susceptibility behaves as

$$\chi \sim T^{-\gamma}$$

at low temperature, where $\gamma$ is a non-universal exponent. On the experiments, the bond randomness effects have been found in several antiferromagnetic quasi-1D materials [5, 6, 7]. Especially, a recent experiment on BaCu$_2$(Si$_{0.5}$Ge$_{0.5}$)$_2$O$_7$ [7] clearly show typical scaling relations of RS phase predicted by theory [8]. Moreover, there is another kind of bond randomness whose bonds can be both AFM and FM. In such systems, the RSRG analyses [9, 10] predicted a universal fixed point different from the RS phase because the spins correlate to form effective spins whose average size grows with lowering of the energy scale, and the magnetic susceptibility is Curie-like $\chi_u \sim 1/T$. Materials with such randomness is also fabricated [11].

Besides the above mentioned two kinds of bond randomness, Manaka and coworkers recently found that the compound (CH$_3$)$_2$CHNH$_3$Cu(Cl$_x$Br$_{1-x}$)$_3$ [12] can be considered as a bond randomness S=1/2 AFM and FM alternating Heisenberg chains. The isomorphous compounds (CH$_3$)$_2$CHNH$_3$CuCl$_3$ [13] is regarded as quasi-1D S=1/2 FM-AFM alternating material, and (CH$_3$)$_2$CHNH$_3$CuBr$_3$ [14] is a S=1/2 AFM dimerized material. Mixing these two compounds, they observed that a gapless phase appeared in the regime of the intermediate concentration $0.44 < x < 0.87$ of FM bonds by measuring magnetic susceptibility and specific heats. In order to describe the properties of this material, Hida [15] and Nakamura [16] suggested a 1D model

$$H = \sum_{i=1}^{N} J S_{2i-1} \cdot S_{2i} + \sum_{i=1}^{N} J_x S_{2i} \cdot S_{2i+1},$$

* E-mail: zxxu@zimp.zju.edu.cn
where $S_i$ presents a spin $S=1/2$, $J > 0$, $J_i = J_F(< 0)$ with a probability $p = x^2$ and $J_i = J_A(> 0)$ with $1 - p$. This model has two limits: (i) when $p = 1$, it is a S=1/2 AFM-FM alternating Heisenberg spin chain. When $|J_i/J| > 1$ its ground state is the Haldane phase with gapped energy spectrum; (ii) when $p = 0$, it is a dimerized AFM Heisenberg spin chain, its ground state is the singlet dimer phase with gapped spectrum. By density matrix renormalization group (DMRG) method, Hida [15] considered the case $p > 0.6$ with $J = 1.0$ and $|J_i| = 2.0$ or $4.0$, and confirmed that there exists QG singularity when $p \leq 0.7$. Nakamura [16] studied the model by non-equilibrium relaxation analysis of the quantum Monte Carlo (QMC) simulation in the whole parameter space of concentration $0 \leq x \leq 1$ with $J = 1.0$ and $|J_i| = 2.0$, and found the gap vanishes in the regime $0.44 < x < 0.87$ consistent with the experimental results [12]. However, in all these numerical works, the finite temperature magnetic properties in the whole parameter space of $x$ are absent. In order to directly compared with the experimental results [12], we perform the finite temperature QMC simulations extensively on this model in this paper.

II. QMC SIMULATION RESULTS

We investigate the magnetic and thermodynamic properties of the model defined by eq. (3) with $J = 1.0$ and $|J_i| = 2.0$ using QMC simulations of continuous imaginary time loop/cluster algorithm. The weak AFM coupling $J = 1.0$ is fixed on all odd position bonds. For even position bonds, the strong AFM or FM bonds $|J_i| = 2.0$ are chosen randomly according to the probability $p$. We perform simulations for $100 \sim 200$ bond arrangement configurations. For each bond configuration, after 2000 Monte Carlo steps (MCS) for thermalization, we further update 2000 MCS for Monte Carlo average. The temporal and spatial periodic boundary conditions are chosen for all simulations. In order to convince us of the code validity, we study $S=1/2$ dimerized AFM chain in weak dimerization, and find our results for the energy gap consist well with recent DMRG results [15].

We first investigate the ground state properties on the system size $L = 128$ for temperatures as low as $\beta = 1/T = 200$. At low temperature, the energy gap $\Delta$ is estimated by

$$\Delta = \lim_{L \to \infty} \frac{1}{\xi_\tau},$$

(4)

where $\xi_\tau$ is the imaginary time correlation length obtained by second-moment method [17]. Then the valence-bond-solid (VBS) order parameter [18]

$$Z_L = \langle e^{i \frac{2\pi}{L} \sum_{j=1}^{L} j S^z_j} \rangle .$$

(5)

is measured to

The results obtained are shown in Fig. 1.

![FIG. 1: The energy gap $\Delta$ and VBS order parameter $Z_L$ versus the probability $p$.](image1)

It is interesting to find that energy gap $\Delta$ exists for the Haldane phase at $p = 1$ point. It gradually approaches to zero at $p \approx 0.7$, and it opens again at very small $p \approx 0.02$. It’s hard to locate accurately the vanishing point of $\Delta$ because our $\Delta$ results are not exact zero value due to finite-size effects. But our calculations show that the gap should close at $p_{c1} \approx 0.02$ and $p_{c2} \approx 0.7$. As a result, we presume that the system stays in the gapless phase in the regime of $p_{c1} < p < p_{c2}$, which is consistent with the previous results [16].

In Fig. 1 we also observe that $Z_L \approx 1.0$ at the limit $p = 1$, keeps at finite in the regime $0.35 < p < 1.0$, changes its sign at $p \approx 0.35$, and then turns down to $-1.0$ when $p < 0.35$. The values of $Z_L \approx \pm 1.0$ characterize the two limits of different ordered phases presented in Fig. 2.

![FIG. 2: The illustration of spin ordered phases with the probability $p = 0$ and 1.0.](image2)
Recent QMC study \cite{20} on S=1 random bond-alternating Haldane chain has shown that the VBS order parameter $Z_L$ is not effected by QG singularity, and it is an effective parameter to locate the RS critical point. Combining the results of $Z_L$ and $\Delta$, we find that in the regime of $0.02 < p < 0.35$ where $\Delta$ vanishes and $Z_L$ approaches zero from finite values, the system belongs to a critical phase. At the point $p \approx 0.35$, as $Z_L$ changes its sign, a phase transition happens. In the regime of $0.35 < p < 0.7$, $\Delta$ vanishes and $Z_L$ increases from zero to finite values. This fact reveals the system enters to other critical phase. In the regime of $0.7 < p < 1.0$, where both $\Delta$ and $Z_L$ are finite, the system keeps in an ordered phase.

In order to distinguish the upper mentioned different phases, we calculate the uniform magnetic susceptibility $\chi_u$ over the whole parameter space $0 < p < 1.0$ at finite temperatures. The results are summarized as following.

**I.** As shown in Fig. 3, in the regime $0.02 < p < 0.35$, the system keeps in gapless phase, where $\chi_u$ diverges when $T \to 0$, and every $\chi_u$ curve appears a valley, that is the typical feature of eq. (1) for denoting RS phase. We fit the curves of $p = 0.04$ and $p = 0.15$ by eq. (1), and find they can be very well fitted as plotted in Fig. 4. Thus we believe that the phase in this regime belongs to RS phase.

**II.** The regime of $0.35 < p < 0.7$ is also a gapless regime, where $\chi_u$ curves diverge too, but they are obviously different from those in the regime of $0.02 < p < 0.35$. Instead, as plotted in Fig. 5, these curves are very similar as those in the QG phase, where the typical feature is described by eq. (2). In Fig. 6, we fit our low temperature results of $\chi_u$ by $T^{-\gamma}$, and find again the fitness are quite good. It is interesting to note that the behavior of $\chi_u$ is not Curie-like, so one can believe the phase is not belong to the universal class of AFM and FM bonds randomness \cite{9}. We thus conjecture that the system is now in QG phase.

**III.** For the regime of $0.7 < p < 1.0$, the system enters to a gapped phase because all $\chi_u$ curves appear the tendencies going to zero when $T \to 0$. Our results are plotted in Fig. 7.

**IV.** At last, we consider the two limit cases $p = 0$ and $p = 1$, and our results are plotted in Fig. 8. Obviously, the system belong to the gapped Haldane phase and dimerized AMF phase on these two points, respectively.
III. CONCLUSION AND DISCUSSION

From our QMC calculations, we can conclude that this S=1/2 AFM-FM alternating bond randomness chain has four different phases with respect to the probability p: (i) p = 0, the system is a dimerized AFM chains with gapped energy spectrum; (ii) in the regime of 0.02 < p < 0.35, the system enters to the RS phase, whose energy spectrum is gapless and the uniform magnetic susceptibility $\chi_u$ obeys the eq. 14; (iii) in the regime of 0.35 < p < 0.7, the system turns to the QG phase where the energy gap vanishes and the curves of $\chi_u$ consist with eq. 23; (iv) in the regime of 0.7 < p ≤ 1.0, the system is again in a gapped phase. Finally, the case p = 1 corresponds to the gapped AFM-FM alternating spin chain.

Consequently, there should be three phase boundaries between these different phases: (i)→(ii), because there is no effective quantities to locate the exact position of this boundary, we only say that the transition from the dimerized phase to the RS phase happens at very small p = 0.02; (ii)→(iii), the phase boundary between RS phase and the QG phase resides at p = 0.35, where both the results of VBS order parameter $Z_L$ and susceptibility $\chi_u$ consist reciprocally. $Z_L$ changing its sign at the point p = 0.35 also implies that it is a good quantity to indicate the transition from RS phase to other phase, which confirm the previous argument. 20; (iii)→(iv), the location of the boundary between QG phase and the gapped phase at p ≈ 0.7 is hard to be determined by results of energy gap $\Delta$ because of the finite-size-effects, but it can be extracted from the behaviors of $\chi_u$ at different temperature. In the QG phase, $\chi_u$ diverges as T → 0, but in a gapped phase, $\chi_u$ approach zero when T → 0. Thus there should be a cross point of $\chi_u$ at different temperature which correspond to the boundary. We investigate the case of same system size $L = 128$ at different temperature $1/T = \beta = 10, 50, 100, 200$, and analyze the results by finite-size-scaling of imaginary time 21. Our results, plotted in Fig. 9 have $\chi_u(T)$ diverges also for 0.56 < x < 0.83 at low temperature. Especially, we find the critical point $p_c2 = 0.71$ corresponding to x = 0.84 is very close to the experimental x = 0.83. As the critical point $p_c1 \approx 0.02$ corresponding to x ≈ 0.14 is different from the experimental x = 0.56, it implies the current single chain model eq. 3 is failed to describe the results of experiment for small p, and some additional terms such as

![FIG. 7: The uniform susceptibility at 0.7 < p < 1.0 versus temperature $T = 1/\beta$.](image1)

![FIG. 8: The uniform susceptibility at p = 0 and p = 1.0 versus temperature $T = 1/\beta$.](image2)

![FIG. 9: Finite size scaling by $T = 1/\beta$ of the uniform susceptibility near $p_c = 0.71$.](image3)
the weak inter-chain coupling should be taken into account. Furthermore, we believe that the behavior of $\chi_u(T)$ in the regime $0.56 < x < 0.87$ for the experiment should successively exhibit first the QG-type divergence $T^{-\gamma}$, then the RS-type divergence $\ln^{-2}(\Omega/T)/T$ at low temperatures. Our further simulations are under consideration, and interesting results are expected in the near future.

Acknowledgments

Xu thanks for valuable discussion with Dr. H. Huang and Dr. P. Crompton. This work was supported in part by the NNSF of China and NSF of Zhejiang province.

[1] C. Dasgupta and S.-K. Ma, Phys. Rev. B 22 1305(1980).
[2] D.S. Fisher, Phys. Rev. B, 50, 3799(1994).
[3] R.A. Hyman and K. Yang, Phys. Rev. Lett. 78, 1783(1997).
[4] R.A. Hyman, K. Yang, R.N. Bhatt and S.M. Girvin, Phys. Rev. Lett. 76, 839(1996).
[5] Y. Uchiyama, Y. Sasago, I. Tsukada, K. Uchinokura, A. Zheludev, T. Hayashi, N. Miura, and P. Boni, Phys. Rev. Lett. 84, 632(1999).
[6] M. Azuma, Y. Fujishiro, M. Takano, M. Nohara and H. Takagi, Phys. Rev. B 55, R8658(1997).
[7] T. Masuda, A. Zheludev, K. Uchinokura, J.-H. Chung and S. Park, cond-matt/0404688.
[8] O. Motrunich, K. Damle and D.A. Huse, Phys. Rev. B 63, 134424(2001).
[9] E. Westerberg, A. Furusaki, M. Sigrist and P.A. Lee, Phys. Rev. Lett. 75, 4302(1995).
[10] B. Frischmuth, M. Sigrist, B. Ammon and M. Troyer, cond-matt/9808027.
[11] T.N. Nguyen, P.A. Lee, and H.-C. zur Loye, Science 271, 489(1996).
[12] H. Manaka, I. Yamada and H.A. Katori, Phys. Rev. B 63, 104408(2001).
[13] H. Manaka, I. Yamada and K. Yamanagi, J. Phys. Soc. Jpn. 66, 564(1997).
[14] H. Manaka, I. Yamada, J. Phys. Soc. Jpn. 66, 1908(1997).
[15] H. Hida, J. Phys. Soc. Jpn. 72, 688(2003).
[16] T. Nakamura, J. Phys. Soc. Jpn. 72, 789(2003).
[17] S. Todo and K. Kato, Phys. Rev. Lett. 87, 047203(2001).
[18] M. Nakamura and S. Todo, Phys. Rev. Lett. 88, 167208(2002).
[19] T. Papenbrock, T. Barnes, D.J. Dean, M.V. Stoitsov, and M.R. Strayer, Phys. Rev. B 68, 024416(2003).
[20] T. Arakawa, S. Todo and H. Takayama, cond-mat/0410755
[21] S. Sachdev, Quantum Phase Transition(1999), Cambridge University Press.