ランダム強磁性—反強磁性スピン鎖のエネルギースケールの分離に関するモンテカルロ法による研究

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包括的なランダム・ボンドの模型で、$Sr_3CuPt_{1-x}Ir_xO_6$ を記述する現実的な模型の熱力学的性質を量子モンテカルロ・ループ・アルゴリズムを用いて数値的に調べた。まずは、近似を用いない数値的に厳密な方法で元々のハミルトニアンを取り扱い、3つの異なる温度領域に分離されることを示した。特に中間領域は、比熱と磁化率の両方で、はっきりと定義されて、観測可能であることを示した。次に、一般化したスタッガード磁化率と磁化の、低温での温度依存性を調べ、それらを記述する二つの新しいユニバーサルなスケーリング指数を提出した。

MC study of the separation of energy scales of random FM/AF spin chains

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We have investigated numerically the thermodynamic properties of a generic random bond model and of a realistic model of $Sr_3CuPt_{1-x}Ir_xO_6$ by the quantum Monte Carlo loop algorithm. For the first time we demonstrate the separation into three different temperature regimes for the original Hamiltonian based on an exact treatment, especially we show that the intermediate temperature regime is well-defined and observable in both the specific heat and the magnetic susceptibility. In a second part we investigate the low-temperature temperature dependence of the the generalized staggered susceptibility and magnetization, and we propose two new universal scaling exponents in order to describe them.

One-dimensional (1D) quantum spin chains are typical examples of many-body systems with a very rich variety of physical properties. Disorder effects play a particularly important role in quasi-1D systems, because even small deviations from regularity often destabilize the pure phases [1]. A peculiar example of a disordered spin chain is the alloy $Sr_3CuPt_{1-x}Ir_xO_6$ [2]; a spin system with randomly distributed ferromagnetic (FM) ($J_F < 0$) and antiferromagnetic (AF) ($J_A > 0$) bonds. There is a correlation among the bonds in the sense that FM bonds always occur in sequences of even numbers, since each Ir-ion makes such bonds with its two neighboring Cu-ions. A generic model neglecting these correlations is given by $\mathcal{H}_{gen} = \sum_i J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$ [3], with a bond probability distribution $P(J_i) = p\delta(J_i + J_F) + (1-p)\delta(J_i - J_A)$.

Three different temperature regimes are present in this system [3, 4]. The low temperature regime has been investigated [4, 5] for an effective Hamiltonian with a broad random distribution of couplings J_i, in contrast to the discrete distribution in $Sr_3CuPt_{1-x}Ir_xO_6$. Here we demonstrate that the intermediate temperature regime is well-defined and observable in both the specific heat and the susceptibility by an exact treatment of the original Hamiltonian. Further we investigate for the first time effect of the correlations among the FM bonds in $Sr_3CuPt_{1-x}Ir_xO_6$ in an experimentally accessible temperature range [6], providing a sensitive test for the randomness of the distribution of the Pt- and Ir-ions in $Sr_3CuPt_{1-x}Ir_xO_6$.

In the second part we concentrate on the low-temperature regime of the generalized staggered susceptibility, correlation and magnetization [7] for a box-distribution of couplings J_i. Besides the scaling exponent α we propose two other new universal scaling exponents for the scaling of the generalized staggered susceptibility and magnetization.

The numerical simulations are performed by the continuous time Quantum Monte Carlo (QMC) loop algorithm [8, 9]. For both studies we have used chains of the length of 400 sites each and considered 400 different random distributions for the discrete distributions and 100 for the box-distributions.

Let us start with the discussion of the results for the discrete distributions. We have studied $\mathcal{H}_{gen}$ without correlations and $|J_F| = |J_A|$ for the case of $p = 0.5$, what we call the "unconstrained model". In a "constrained model" we include the additional restriction that the FM

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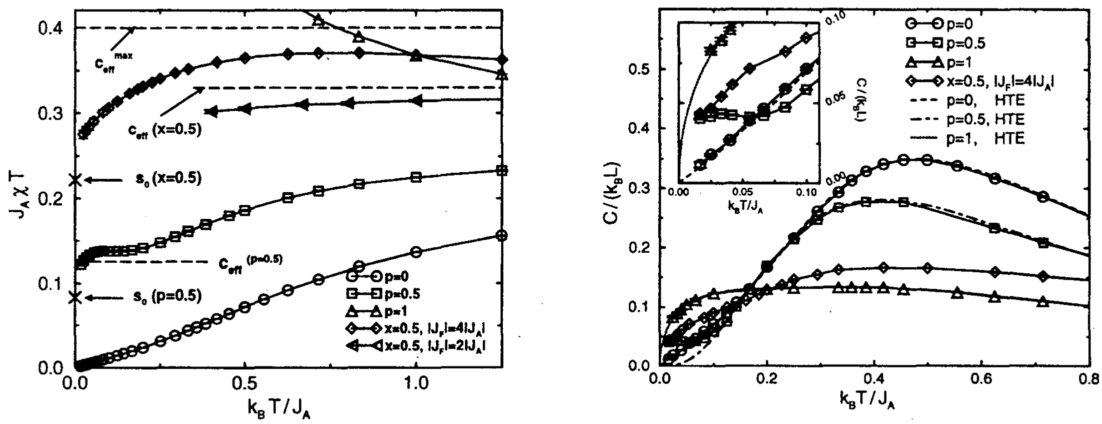

図 1: (left): QMC simulations of the uniform magnetic susceptibility χ times temperature T. (right): QMC and high-temperature expansions (HTE) [3] results for the specific heat per spin c_V.

bonds always occur pairwise and that the FM couplings are stronger than the AF couplings $|J_F| = 4|J_A|$, as it is expected for $Sr_3CuPt_{1-x}Ir_xO_6$.

In the intermediate temperature regime $J \propto T$ we expect the formation of correlated spin segments and the susceptibility following $\chi = \frac{\mu^2 C_{\text{eff}}}{k_B T}$, where C_{eff} is an effective Curie-constant [3]. This Curie-law can be seen as a plateau in Fig. 1, where we show χJT. From our QMC simulations we get $C_{\text{eff}} = 0.138 \pm 0.003$ [6]. In the case of $Sr_3CuPt_{1-x}Ir_xO_6$ the FM bonds start to correlate at higher temperatures due to the stronger coupling. If all the spins within the segments are completely correlated, we find a lower bound of $C_{\text{eff}} = 0.33 \pm 0.017$ by a statistical analysis. An upper bound of $C_{\text{eff}}^{\max} = 0.40 \pm 0.02$ is obtained for the case where all AF spins remain uncoupled due to their weaker couplings. From our QMC data we get $C_{\text{eff}} \approx 0.36$ [6].

The crossover between different temperature regimes should be visible by two peak-like structures in the specific heat, one for the correlation of the original $S = 1/2$, and a second peak where segments of the effective spins start to correlate. We show the first calculations [6] where this can actually be seen in Fig. 1. The large peak around $T = 0.5J$ corresponds to the first peak, and in the inset one can clearly see the second peak at low temperatures for the unconstrained model. Because of the different coupling strengths in the constrained model, the peaks are washed out in this case, but we can interpreted the cusp-like structure near $T \approx 0.05J$ as the onset of correlations among the effective spins.

Next we would like to discuss the low-temperature behavior of the generalized staggered susceptibility. In this part we start with the bond distribution $P(J) = \begin{cases} \frac{1}{2J_0} & -J_0 < J < J_0 \\ 0 & \text{otherwise,} \end{cases}$ where J_0 is the maximal coupling setting the energy scale. The low energy behavior of the random FM-AF chain is independent of the initial for regular distributions [10].

The generalized staggered susceptibility is defined here as the linear response of the spin chain to a staggered field H_{st} whose sign on site j is given by $\tau_j = \prod_{m=0}^{i-1} \text{sgn}(-J_m)$ in analogy to the regular AF staggering. Nagaosa et al. [11] suggested that each cluster forms a (classical) staggered spin $s_{\text{st}} = \zeta l$ proportional to the cluster length l and $\zeta = \text{const}$. From this we obtain by a statistical cluster analysis [7] $\chi_{\text{st}} = \frac{\zeta^2 \lambda^2}{3} T^{-(1+2\alpha)} + \frac{\zeta - 2\zeta^2}{3} T^{-1} + O(T^{-1+2\alpha})$. However, from the QMC data we rather find a different leading powerlaw $\chi_{\text{st}} \propto T^{-\gamma}$ with $\gamma = 1.17 \pm 0.01$ down

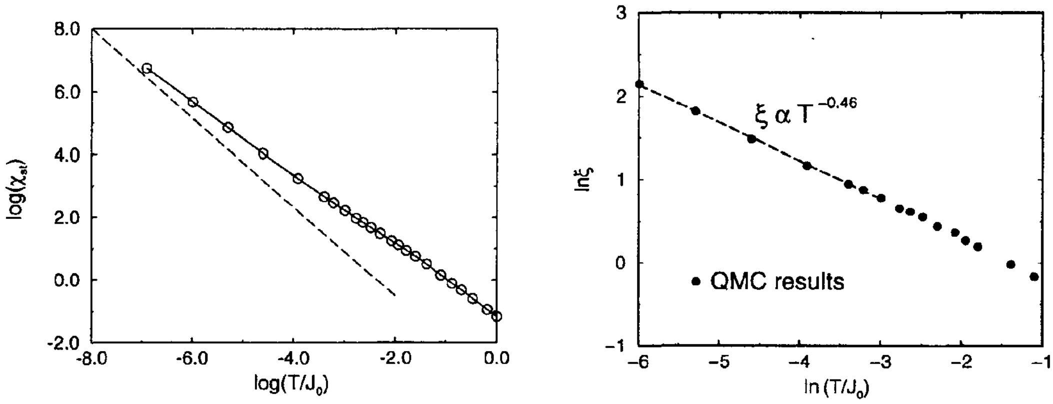

図 2: (left:) Double logarithmic plot of the generalized staggered susceptibility as a function of temperature. The dashed line shows a divergence with $T^{-(1+2\alpha)}$.
(right): Double logarithmic plot of the correlation length ξ as function of temperature T. $\xi(T)$ diverges approximately with $T^{-0.46}$ (dashed line) for $T \to 0$

to temperatures as low as $T = J_0/1000$.

We treat the application of the staggered field as a perturbation to the Hamiltonian and assume that the generalized staggered correlation function of a single cluster is bounded by $\sum_{i,j} \tau_i \tau_j \langle \Psi_0(S,M)|S_i^z S_j^z|\Psi_0(S,M)\rangle \leq g_2 l^\rho$, where $g_2 =$ const. and ρ a scaling exponent. Thus we find upper bounds for the correlation function for large r within a correlated cluster $\Gamma_0(r) = \sum_i \tau_i \tau_{i+r} \langle \Psi_0(S,M)|S_i^z S_{i+r}^z|\Psi_0(S,M)\rangle \propto r^{-\eta}$ with $\rho = 2-\eta$. From this we find that $\chi_{\rm st}$ per spin in a correlated cluster to scales as $\chi_{\rm st} \propto T^{-(1+2\alpha(\rho-1))}$. From the QMC result $\gamma = 1.17 \pm 0.01$ (Fig. 2) we can give an upper bound for the exponent $\eta \leq 1 - \frac{\gamma-1}{2\alpha} \approx 0.62 \pm 0.02$ We conclude that the correlation is much longer ranged than in a regular AF spin-1/2 chain where the exponent is 1. However, the exponent of $\chi_{\rm st}$ is smaller than $1+2\alpha$, inconsistent with the assumption that the ground state of the random FM-AF chain has long range order.

Finally, we calculate the correlation function $\Gamma(r) = \langle \frac{1}{L}\sum_{i=1}^{L} S_i^z S_{i+r}^z \left(\prod_{m=i}^{i+r-1} {\rm sgn}(-J_m)\right)\rangle$. For large r and at fixed temperature T, the correlation function $\Gamma(r,T)$ is found to be rather well described by a pure exponential form $\Gamma(r,T) = R(T)e^{-r/\xi(T)}$ for $r \gg \xi(T)$, where $\xi(T)$ is the correlation length and the prefactor $R(T)$ is r independent. From the QMC data we obtain $\xi(T) \propto T^{-0.46}$ (Fig. 2), in agreement with the scaling $\xi \propto \bar{l} \propto T^{-2\alpha} = T^{-0.42\pm0.04}$.

For for ($\frac{r}{\xi} \gg 1$) and $T \to 0$ we propose the scaling behavior $\Gamma(r) = \xi^\nu \tilde{\Gamma}(r/\xi)$ for the correlation function of random FM-AF spin chains, where $\tilde{\Gamma}(x)$ is a universal (temperature independent) function. As a consequence the prefactor $R(T)$ should behave as $\xi(T)^\nu$ at low temperatures, leading to $\ln R(T) - \ln R(T_0) = \nu \ln \xi - \nu \ln \xi_0 = -2\nu\alpha \ln T + 2\nu\alpha \ln T_0$. From the QMC data in Fig. 3 we get estimate of $\nu = -0.61 \pm 0.06$. Another possibility to estimate the exponent ν is to consider the low-temperature behavior of the square of the generalized staggered magnetization defined by $M_{\rm st}^2 = \langle \left(\frac{1}{L}\sum_{i=1}^{L} \tau_i S_i^z\right)^2 \rangle = \frac{2}{L}\left(\sum_{r>0} \Gamma(r) + \frac{\Gamma(0)}{2}\right) \approx \frac{2}{L}\int_0^\infty dr \Gamma(r)$ for $L \gg \xi \gg 1$. Using our proposed scaling for $\Gamma(r)$ we obtain $M_{\rm st}^2 = \frac{2}{L}\xi^\nu \int_0^\infty dr \tilde{\Gamma}(r/\xi) = \frac{2}{L}\xi^{\nu+1}\int_0^\infty dx \tilde{\Gamma}(x) \propto \xi^{\nu+1} \propto T^{-2\alpha(\nu+1)}$. From the QMC data in Fig. 3 we obtain $M_{\rm st}^2 \propto T^{-0.180\pm0.002}$, and thus $\nu \approx -0.61$ in good agreement with the previous result.

In conclusion we have presented the first exact numerical treatment of the original Hamil-

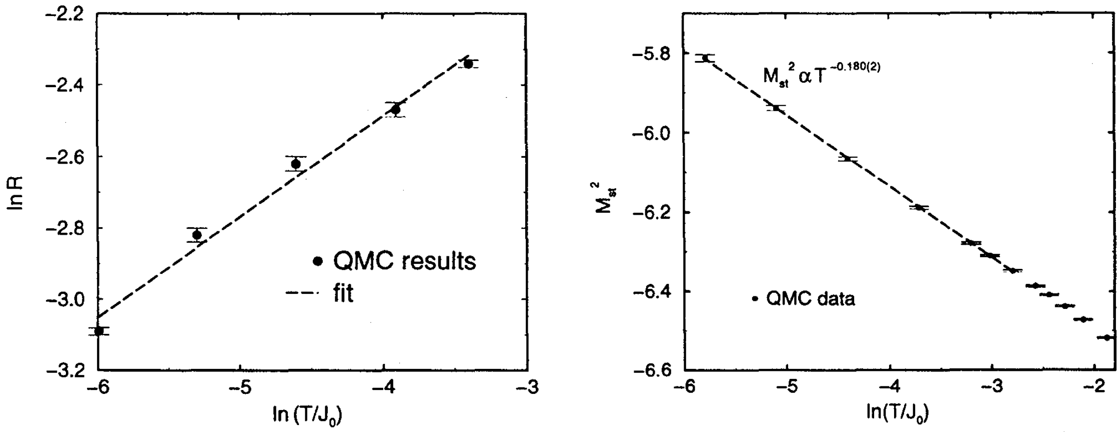

図 3: (left): Double logarithmic plot of the prefactor of the correlation function R as function of temperature T. From the slope $-2\nu\alpha = 0.28 \pm 0.02$ we get $\nu = -0.61 \pm 0.06$.
(right): Double logarithmic plot of the square of the generalized staggered magnetization M_{st}^2.

tonian showing a clear separation into three different temperature regimes. This separation can be seen by two marked peaks in the specific heat and two Curie laws in the magnetic susceptibility. In a realistic model of $Sr_3CuPt_{1-x}Ir_xO_6$, the different magnitudes of the FM and AF couplings lead to overlapping energy scales and the crossover between the three regimes is rather continuous. We have given upper and lower bounds for the effective Curie-constants C_{eff}. Non-random distributions in actual experiments will give much larger values of C_{eff}.

In the second part we have studied the low temperature behavior of the generalized staggered susceptibility. We introduce a new exponent $\gamma \approx 1.17$ describing $\chi_{\mathrm{st}} \propto T^{-\gamma}$. A further exponent $\nu \approx 0.61$ arises from the scaling form of the correlation function. We have shown that ν is connected with the ground state correlation function which probably exhibits a powerlaw decay over long distances, $\Gamma_0(r) \propto r^{-\eta} < r^{-\nu}$. Both exponents are assumed to be universal like α. There is no obvious relation between γ, ν and α.

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