Néel Temperature of Quasi-Low-Dimensional Heisenberg Antiferromagnets

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The Néel temperature, $T_N$, of quasi-one- and quasi-two-dimensional antiferromagnetic Heisenberg models on a cubic lattice is calculated by Monte Carlo simulations as a function of inter-chain (inter-layer) to intra-chain (intra-layer) coupling $J'/J$ down to $J'/J \approx 10^{-3}$. We find that $T_N$ obeys a modified random-phase approximation-like relation for small $J'/J$ with an effective universal renormalized coordination number, independent of the size of the spin. Empirical formulae describing $T_N$ for a wide range of $J'$ and useful for the analysis of experimental measurements are presented.

While genuinely one-dimensional (1D) and two-dimensional (2D) antiferromagnetic Heisenberg (AFH) models cannot display long-range order (LRO) except at zero temperature\textsuperscript{1}, weak inter-chain or inter-layer couplings, $J'$, which always exist in real materials, lead to a finite Néel temperature $T_N$. So far, the $J'$-dependence of $T_N$ was calculated by exactly treating effects of the strong interaction $J$ in the 1D or 2D system, but using mean-field approximations for the inter-chain and inter-layer coupling $J'$. Recently, more advanced theories of the latter effects have been proposed for quasi-1D (Q1D)\textsuperscript{2} and quasi-2D (Q2D)\textsuperscript{3} systems, and the results have been compared with the experimental observations on Q1D antiferromagnets, e.g., Sr\textsubscript{2}CuO\textsubscript{3}\textsuperscript{4} and quasi-2D antiferromagnets, e.g., La\textsubscript{2}CuO\textsubscript{4}\textsuperscript{5}. In view of the importance of experimentally well-studied Q2D antiferromagnets as undoped parent compounds of the high-temperature superconductors, accurate and unbiased numerical results for Q1D and Q2D AFH models are strongly desired. In a recent work along this line, Sengupta \textit{et al.}\textsuperscript{6} have demonstrated peculiar temperature dependences of the specific heat in the quantum Q2D AFH model.

Here we calculate the Néel temperature $T_N$ as a function of $J'$ in fully three-dimensional (3D) classical and quantum Monte Carlo (MC) simulations of coupled-chains and coupled-layers. Our MC results on the quantum spin-$S$ and classical $S = \infty$ AFH models are analyzed by a modified random-phase approximation (RPA) with a renormalized coordination number defined by

$$
\zeta(J') = \frac{1}{J' \chi_s(T_N(J'))},
$$

where $\chi_s(T)$ is the staggered susceptibility of the 1D or 2D model at temperature $T$.

In a simple RPA calculation\textsuperscript{7}, this quantity is just the coordination number $z_d$ in the inter-chain or inter-layer directions: $z_1 = 4$ and $z_2 = 2$ for the Q1D and Q2D systems, respectively. Our main result is that $\zeta(J')$ evaluated by Eq. (1) with our numerically obtained $T_N(J')$ and $\chi_s(T)$ becomes constant

$$
\zeta(J') \approx \zeta_d = k_d z_d
$$

for $J' < J'_c \approx 0.1J$, with the constants $k_1 = 0.695$ and $k_2 = 0.65$. These constants $k_d$ differ from the simple RPA result $k_d = 1$, but the value of $k_1$ is consistent with the modified self-consistent RPA theory for the quantum Q1D ($q$-Q1D) model of Irkhin and Katanin (IK)\textsuperscript{8}. Furthermore we find, that, within our numerical accuracy, the value of $k_d$ is the same for the $S = 1/2, S = 1, S = 3/2$ and $S = \infty$, and we conjecture that $k_d$ is universal and independent of the spin $S$ for small $J'/J$.

We also propose empirical formulae for $T_N(J')$ for all values of $J'$ examined in the present work up to $J' = J$ where corrections to the modified RPA are significant quantitatively. These formulae are useful in analyzing experimental results on infinite-layer antiferromagnets such as Ca\textsubscript{13}Sr\textsubscript{15}CuO\textsubscript{28}\textsuperscript{9}, (5CAP)\textsubscript{2}CuBr\textsubscript{4} and (5MAP)\textsubscript{2}CuBr\textsubscript{11}\textsuperscript{11}, where they allow to determine the strength of the inter-chain or inter-layer coupling $J'$ from experimental measurements of $T_N$.

**Model and numerical methods.**— The Hamiltonian of the Q1D and Q2D AFH models is defined on an anisotropic simple cubic lattice:

$$
\mathcal{H} = \sum_{i,j,k} \left( J_x S_{i,j,k} \cdot S_{i+1,j,k} + J_y S_{i,j,k} \cdot S_{i,j+1,k} + J_z S_{i,j,k} \cdot S_{i,j,k+1} \right),
$$

where the summation $\sum_{i,j,k}$ runs over all the lattice sites on an $L_x \times L_y \times L_z$ cubic lattice and $S_{i,j,k}$ is the spin operator at site $(i,j,k)$. We put $J_x = J_y = J'$ and $J_z = J$ for the Q1D model and $J_x = J_y = J$ and $J_z = J'$ for the Q2D model with $J > 0$ and $0 \leq J' \leq J$. For comparison, we also examine the classical limit $S = \infty$ of Eq. (3). Note that $JS(S+1)$ sets the energy scale in the classical
In practice, we simulate a system of unit vectors, which is equivalent to fixing $JS(S + 1)$ to unity.

The MC simulations have been performed using the continuous-imaginary-time loop algorithm [11] for the classical model (CMC). The AF correlation length $\xi_\alpha$ in each of the directions $\alpha = x, y, z$ is evaluated by the second-moment method [13] on lattices whose aspect ratio is chosen such that $\xi_\alpha/L_\alpha$ does not depend on $L_\alpha$ in the vicinity of $T_N$. Explicitly, for the $S = 1/2$ q-Q1D systems with $J'/J = 0.01, 0.05, 0.1$, and $0.5$, we set $L_x/L_z = 36$ ($L_z \leq 504$), $12$ ($384$), $4$ ($200$), and $2$ ($128$), respectively, while for the $S = 1/2$ quantum Q2D (q-Q2D) systems with $J'/J = 0.001, 0.005, 0.01$, and $0.02$, we set $L_x/L_z = 48$ ($L_z \leq 288$), $20$ ($240$), $16$ ($192$), and $1$ ($80$), respectively. Then we determine $T_N$ from finite-size scaling, looking for the best data collapse of $\xi_\alpha/L_\alpha$ plotted versus $(T-T_N)L^{1/\nu}$ for different system sizes. We have fixed the exponent $\nu = 0.71$ [14] to the value of the 3D classical Heisenberg universality class. The values of $T_N$ obtained for the $S = 1/2$ q-Q1D and classical Q1D (c-Q1D) systems, and the $S = 1/2$ q-Q2D and classical Q2D (c-Q2D) systems are listed in Table I.

### Table I: Néel temperatures of the $S = 1/2$ q-Q1D, c-Q1D, S = 1/2 q-Q2D, and c-Q2D AFH models, normalized by $JS(S + 1)$. The result for the classical system with $J'/J = 1$ is taken from Ref. [13].

| $J'/J$ | $T_N/JS(S + 1)$ |
|--------|----------------|
| q-Q1D  | c-Q1D | q-Q2D | c-Q2D |
| 1      | 1.2589(1) | 1.4429(1) | 1.2589(1) | 1.4429(1) |
| 0.5    | 0.78997(8) | 0.9317(1) | 1.0050(4) | 1.1733(1) |
| 0.1    | 0.22555(3) | 0.39551(8) | 0.6553(4) | 0.8526(1) |
| 0.05   | 0.12171(5) | 0.28377(4) | 0.5689(2) | 0.7797(1) |
| 0.02   | 0.05258(1) | 0.18361(3) | 0.48463(8) | 0.7115(1) |
| 0.01   | 0.02768(1) | 0.13157(2) | 0.43515(6) | 0.6731(2) |
| 0.005  | 0.09393(2) | 0.39513(4) | 0.6419(2) |
| 0.001  | 0.042547(6) | 0.32571(8) | 0.5858(4) |

#### 1D systems

The classical 1D (c-1D) model shows LRO at $T = 0$, while the ground state of the $S = 1/2$ and $S = 3/2$ quantum 1D (q-1D) model is gapless and has no LRO [12]. Correspondingly, the staggered susceptibility $\chi_s$ for the classical model, given exactly by [16]

$$\chi_s(T) = \frac{x}{3} \frac{1 + 1/\tanh x - 1/x}{1 - 1/\tanh x + 1/x}$$

(4)

with $x = JS(S + 1)/T$, diverges as $T^{-2}$ in the limit $T \to 0$, while the one for the $S = 1/2$ model, asymptotically given by [17]

$$\chi_s(T) \approx \frac{c_1}{T} \left[ \ln \frac{\Lambda J}{T} + \frac{1}{2} \ln \ln \frac{\Lambda J}{T} \right],$$

(5)

exhibits only a $1/T$ divergence with logarithmic corrections. Here we note that the quantitative accuracy of this expression is limited to a very low temperature range. In fact Eq. (5) with the constants $c_1$ and $\Lambda$ derived field-theoretically [17] does not fit well to $\chi_s$ calculated numerically at $T \geq 0.003J$. This indicates the limits of applicability of analytical results and that one has to use instead numerical data in this temperature range.

Due to the different functional forms of the quantum and classical susceptibilities, we observe in Fig. 1 that, at small $J'/J$, $T_N(J') \propto \sqrt{J'/J}$ for the classical model, while $T_N(J') \propto J'/J$ with logarithmic corrections for the quantum model. Comparing the RPA result (Eq. (2) with $k_1 = 1$) with the modified RPA one (Eq. (2) with $k_1 \simeq 0.70$, denoted by IK), one can easily see that the latter describes $T_N(J')$ much better and is a fairly good description of $T_N(J')$ in the range $J'/J \lesssim 0.3$. Comparing our results to the next leading order finite-temperature perturbation theory [1] (NLO in Fig. 1 which is based on Eq. (5), however, we do not find good agreement, because, as pointed out above, Eq. (5) is inappropriate in the considered temperature range.

The agreement with the modified RPA theory is directly shown in Fig. 2 where the $J'$-dependence of $\zeta(J')$ in Eq. (1) is shown. The $\chi_s(T_N(J'))$ are obtained from QMC simulations interpolated near $T = T_N$ for the $S = 1/2$ model and from Eq. (4) for the $S = \infty$ model. For $J'/J \leq 0.1$ we reach Eq. (2) with $k_1 \simeq 0.695$ for the $S = 1/2$ model as well as for the classical limit $S = \infty$ model and conclude that, within the numerical accuracy of our simulation, the modified RPA with $J'$-independent $\zeta(J')$ is an appropriate quantitative description of the models with $J'/J$ in this range.

Interestingly the result mentioned above seems to hold for quantum models with other values of $S$. As also shown in Fig. 2 within our numerical accuracy, this is
well confirmed for the $S = 3/2$ model with $J'/J \geq 0.02$. For the $S = 1$ case we find agreement in the range $J'/J \geq 0.05$, where $T_N$ is larger than the Haldane gap \cite{18} of the isolated chain. Below this temperature the finite size scaling of the QMC data becomes less reliable and we cannot draw definitive conclusions. Even if the result for the $S = 1$ model is restricted to this temperature range, the present result is surprising, given the different behavior of $\chi_s(T)$ in the c-1D and q-1D models.

**Q2D systems.**— In both classical 2D (c-2D) and quantum 2D (q-2D) models, AF-LRO appears at $T = 0$, together with an exponential divergence of $\chi_s(T)$ at $T \to 0$. In the c-2D system, $\chi_s$ is proportional to $T^3 \exp(4\pi J/T)$ at low temperatures \cite{15} and our numerical results agree with previous simulations \cite{20}. For the q-2D models, there is a similar exponential divergence at $T \to 0$. In the renormalized classical regime of the non-linear $\sigma$ model \cite{21}, for example, $\chi_s(T)$ is written as

$$\chi_s(T) J = c_2 T / J \exp(4\pi \rho_s / T),$$

where $\rho_s$ is the spin stiffness and $c_2$ a constant.

The $J'$-dependence of $T_N$ for the Q2D models is shown in Fig. 3. We see that $T_N(J') \propto -1/\ln(J'/J)$ at small $J'/J$ in the $S = 1/2$, $S = 1$ and $S = \infty$ models due to the similar exponential forms of $\chi_s$ at $T \to 0$ of the classical and quantum models. Figure 3 shows that again for $J'/J \lesssim 0.05$ the values of $\zeta(J')$ are universal for the quantum and the classical models: $k_2 = 0.65$ in Eq. \ref{6} independent of the spin size $S$. This confirms the validity of our modified RPA scenario represented by Eqs. \ref{1} and \ref{2} also for the Q2D systems.

If we insert Eq. \ref{6} into Eq. \ref{1} with $\zeta(J') = \zeta_2$, we obtain the following expression of $T_N$ for $J'/J \ll 1$,

$$T_N = 4\pi \rho_s / (b - \ln(J'/J) - \ln(T_N / J)),$$

with $b = -\ln(\zeta_2 c_2)$. This result is compatible with that of the $1/N$-expansion theory of $T_N(J')$ due to Irkhin et al. \cite{4} for the $S = 1/2$ model in the same limit. Various estimations of $b$ and $\rho_s$ can be obtained analytically \cite{4} according to the different approximation schemes used. Unfortunately, we cannot judge which approximation is most relevant in general since higher order corrections in $T/4\pi \rho_s$ over the leading asymptotic expression Eq. \ref{4} are known to be necessary \cite{22} to reproduce the numerically obtained $\chi_s$ in the temperature range $T/4\pi \rho_s \gtrsim 0.1$ simulated. In fact, corrections of this type and uncertainty on $T_N$ due to the different possible estimates of $b$ are comparable. We expect, on the other hand, that the constancy of the normalization factor $k_2$, which is found numerically to be within $2\%$ in $0.001 \leq J'/J \leq 0.05$ and $0.32 \leq T_N / J S(S + 1) \leq 0.57$ (Fig. 4), holds in the limit $J'/J \to 0$ as well.

**Empirical formulae.**— Finally, we propose empirical formulae for $T_N(J')$ based on our QMC results. For the $S = 1/2$ q-Q1D system we propose a modified RPA form based on Eqs. \ref{6} and \ref{4} with a constant $\zeta(J')$,

$$J' = T_N/(4e \sqrt{\ln(\lambda J / T_N) + 1/2 \ln(\lambda J / T_N))},$$

but with modified values of the constants with $e = 0.233$ and $\lambda = 2.6$. These values are chosen to reproduce not $\chi_s(T)$ but $T_N(J')$ in a wide range of $J'$. This formula describes $T_N(J')$ very well in the whole range of $J'/J$ as shown in Fig. 4 and it can be used to analyze experimental results, e.g. to obtain $J' / J \approx 0.0007$ for Sr$_2$CuO$_3$ from $T_N / J \approx 0.002$.\cite{R2}

For the q-Q2D systems, we find that instead of Eq. \ref{4}, the following simpler expression describes $T_N$ better in
The Néel temperatures of various infinite-layer compounds. The Néel temperatures $T_N$ of infinite-layer materials with $S=1/2$ can be well described by an anisotropic non-linear $\sigma$-model (NL$\sigma$M) in the renormalized classical regime, we conjecture universal corrections to RPA also for the NL$\sigma$M.

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FIG. 4: $J'$-dependence of $\zeta(J')/z_2$ for the Q2D systems. In all cases $\zeta(J')/z_2$ approaches a constant ($\approx 0.65$), denoted by the dotted line, at small $J'/J$. The error bar of each point is smaller than the symbol size unless given explicitly.

TABLE II: Inter-layer coupling $J'$ estimated by Eq. 4 for various infinite-layer compounds. The Néel temperatures $T_N$, the intra-layer couplings $J$, and their ratio estimated by the experiments are also listed.

| Compound       | $T_N$ (K) | $J'/J$ | $T_N/J'/J$ |
|----------------|-----------|--------|------------|
| $\text{Cu}_8\text{Sr}_{15}\text{CuO}_2$ [9] | 537 | 0.35 | 0.016 |
| (5CAP)$_2\text{CuBr}_4$ [10] | 5.08K | 8.5 | 0.6 | 0.24 |
| (5MAP)$_2\text{CuBr}_4$ [10] | 3.8K | 6.5 | 0.58 | 0.22 |
| (5CAP)$_2\text{CuCl}_4$ [10] | 0.74K | 1.14K | 0.64 | 0.33 |
| (5MAP)$_2\text{CuCl}_4$ [10] | 0.44K | 0.76K | 0.57 | 0.21 |

with $\rho_s/J = 0.183$ and $b = 2.43$ for $S = 1/2$, and $\rho_s/J = 0.68$ and $b = 3.12$ for $S = 1$. Table III shows inter-layer couplings $J'$ estimated using this equation for a number of infinite-layer materials with $S = 1/2$.

To conclude, we have determined, by high-precision Monte Carlo simulations, the Néel temperatures of quantum and classical Q1D and Q2D Heisenberg antiferromagnets. Besides finding empirical formulae for $T_N(J')$, we observe that, using numerically accurate values of the staggered susceptibility a modified RPA with the $J'$-independent renormalization coordinate number $\zeta_J$ succeeds in quantitatively describing the relation between $T_N$ and $J'/J$ for $J'/J' < J'/J$.

An intriguing result of our simulations is the independence of $\zeta_J$ on the value of the spin $S$, suggesting a universality of corrections to RPA for $J' < S$. Since in this temperature regime the physics of all these models should be well described by an anisotropic non-linear $\sigma$-model (NL$\sigma$M) in the renormalized classical regime, we conjecture universal corrections to RPA also for the NL$\sigma$M.

The range $0.001 \leq J'/J \leq 1$ (see Fig. 4):

$$T_N = 4\pi\rho_s/(b - \ln (J'/J)),$$

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