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Crossover from two to three dimensions in the layered xy-model

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Abstract. Using Monte-Carlo simulations we studied the layered xy-model. The decrease of the transition temperature T_c with reduced thickness and the behavior of the specific heat are estimated. In an approximate Ginzburg-Landau treatment we find that the drop of T_c and the associated dimensional crossover is a combined effect of fluctuations and boundaries.

Introduction

As a model to study the crossover between two and three dimensions we investigate the layered xy-model defined by

$$H = -J_{\|} \sum_{<ij>_{\|}} \vec{S}_i \vec{S}_j - J_{\perp} \sum_{<ij>_{\perp}} \vec{S}_i \vec{S}_j, \tag{1}$$

where $J_{\|}$ ($J_{\perp}$) is the intra- (inter-) layer coupling strength, $\vec{S}_i = (\cos\varphi_i, \sin\varphi_i)$ are the xy-spins on a simple cubic lattice of $N = L^2 M$ spins and $< ij >_{\|,\perp}$ denote nearest neighbors within and perpendicular to the planes. To mimic a real system of finite thickness we adopt periodic boundary conditions parallel to the layers and free boundaries perpendicular to them.

Numerical method

Using a Metropolis algorithm and the single-cluster algorithm [1] together with the multihistogram technique [2], we estimate the transition temperature $T_c(M)$ by the intersection point of the fourth-order cumulant [3]

$$U_L(T) = 1 - \frac{\langle(\vec{m}^2)^2\rangle_T}{3\langle\vec{m}^2\rangle_T^2} \tag{2}$$

for different sizes L of the layers. Here $\vec{m} = \frac{1}{N}\sum_{i=1}^{N} \vec{S}_i$ denotes the magnetization and $\langle\rangle_T$ the thermal average.

Approximate treatment

By using a Hubbard-Stratanovich transformation and a mean-field description perpendicular to the layers we can partly take the 2d fluctuations in the layers into account and approximate the free energy of model (1) up to quartic terms in a Ginzburg-Landau form as

$$F \approx \int d^2r \{T_c^\circ(1 - \frac{T_c^\circ}{T})|\psi|^2 + J_{\|}(\frac{T_c^\circ}{T} - \frac{1}{2})|\nabla_{\|}\psi|^2 + \frac{1}{(M+1)^2}\sum_{n=1}^{M} \sin^4(\frac{\pi}{M+1})\frac{(T_c^\circ)^4}{T^3}|\psi|^4\} \tag{3}$$

with the mean-field transition temperature $T_c^\circ(M) = 2J_{\|} + J_{\perp}\cos(\frac{\pi}{M+1})$. Using the Kosterlitz-Thouless transition of this effective 2d xy-model we obtain an upper bound $T_{KT}^{>}(M)$ for the transition temperature [4]

$$T_{KT}^{>}(M) = T_c^\circ(M)\left(\frac{3}{2} - \frac{1}{2}\sqrt{1 + 16\frac{M}{(M+1)^2}\frac{\langle S^4\rangle}{\pi J_{\|}}T_c^\circ(M)}\right), \tag{4}$$

where $\langle S^4\rangle \equiv \frac{1}{M}\sum_{n=1}^{M}\sin^4(\frac{\pi}{M+1})$.

Results and Conclusions

Figure 1 depicts the numerical estimates $T_c(M)$. The limits for $M = 1$ and $M \to \infty$ agree with previous estimates [5], but we notice a steep increase of $T_c(M)$ for small M values. This can be understood by invoking finite-size scaling to our system: the correlation length $\xi = b\left(\frac{T_c^{3d}-T}{T_c^{3d}}\right)^{-\nu_{3d}}$ of the 3d system cannot exceed the finite thickness M, so that

$$T_c(M) = T_c^{3d}\left(1 - \left(\frac{b}{M}\right)^{\frac{1}{\nu_{3d}}}\right), \quad (5)$$

where b is a measure of the interaction range corresponding to the zero temperature correlation length. Eq. (5) fits the data very well for $M \geq 4$ and yields $\nu_{3d} = 0.70 \pm 0.08$ and $b = 1.3 \pm 0.5$, in agreement with previous estimates of ν_{3d} [5,6].

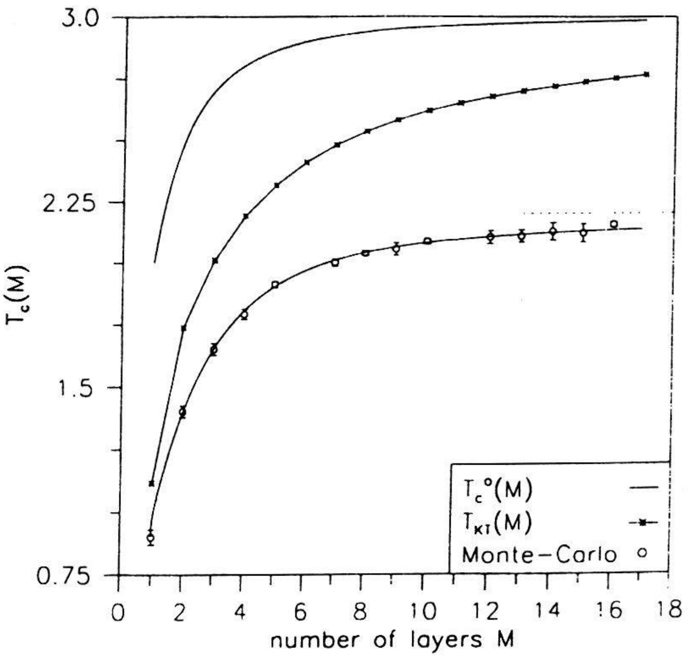

Figure 1. $T_c^o(M)$, $T_{KT}^{>}(M)$ and the numerical estimates $T_c(M)$. The short dashed line indicates the transition temperatur of the 3d xy-model.

Because the interaction range b is of the order 1, the drop of T_c is appreciable only for small M. For comparison we also included the results of our approximate treatment. Here the decrease of T_c with reduced thickness is traced back to the presence of boundaries incorporated in $T_c^o(M)$ and a further reduction due to the 2d fluctuations, becoming dominant for small M values. A related crossover phenomenon occurs in the specific heat: a broad peak well above T_c for $M = 1$, which sharpens and shifts towards T_c with increasing M to approach a sharp cusp at T_c in the bulk.

To summarize: our Monte-Carlo study of the layered isotropic xy-model revealed the drop of the transition temperature as a function of thickness for rather small M. This can be understood in terms of the short interaction range b of order one. With our approximate treatment we find two important contributions to this behavior: the free boundary conditions and the 2d fluctuations.

References

[1] U. Wolff, Phys. Rev. Lett. **62**,361 (1989); Nucl. Phys. B **322**, 759 (1989)

[2] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989)

[3] K. Binder, Phys. Rev. Lett. **47**, 693 (1981); Z. Phys. B **43**, 119 (1981)

[4] A. Schmidt and T. Schneider: preprint

[5] R. Gupta et al. , Phys. Rev. Lett. **61**, 1996 (1988) W. Janke, Phys. Lett. A **148**, 306 (1990)

[6] J. C. Le Guillou, J. Zinn-Justin, Phys. Rev. B, **21**, 3976 (1980)