Original contributions

Dimensional crossover in the layered xy-model

A. Schmidt and T. Schneider
IBM Research Division, Zurich Research Laboratory, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland
Received January 14, 1992

Using the Monte-Carlo technique we studied the isotropic layered xy-model. We concentrate on the fall of the transition temperature $T_c$, the behavior of the specific heat and the vortex density with reduced thickness. Our approximate Ginzburg-Landau treatment suggests that the drop of $T_c$ resulting from the dimensional crossover is a combination of fluctuation and boundary effects.

1. Introduction

A relevant model to simulate the phase transition between normal and superconducting states as well as the superfluid transition in $^4$He [1] is the xy-model defined by

$$H = -J_{||} \sum_{\langle ij \rangle ||} S_i S_j - J_{\perp} \sum_{\langle ij \rangle \perp} S_i S_j,$$

where $J_{||}$ and $J_{\perp}$ are the coupling constants within and perpendicular to the layers. $S_i = (\cos \varphi_i, \sin \varphi_i)$ denotes xy-spins on a simple cubic lattice and the sum runs over all (ordered) pairs of nearest neighbors in or perpendicular to the layers.

It is well known that the properties of physical systems near and at a continuous phase transition depend strongly on dimensionality. Recently this issue became particularly relevant because superconducting [2, 3] and $^4$He-films [4] of finite thickness have been produced and experimentally investigated. This has opened the possibility of exploring the crossover from three (3d) to two-dimensional (2d) behavior as the thickness of the film is reduced.

In this paper we investigate the layered xy-model (1) consisting of $M$ planes, coupled in terms of $J_{\perp}$.

2. Approximate treatment

The relationship between the xy-model and the Ginzburg-Landau formalism of superconductors is disclosed as follows: we rewrite (1) as

$$-\beta H = K_{||} \sum_{\langle ij \rangle ||} \cos (\varphi_i - \varphi_j) + K_{\perp} \sum_{\langle ij \rangle \perp} \cos (\varphi_i - \varphi_j)$$

$$= \frac{1}{2} v^T P v - K_N,$$

where $\beta = 1/k_B T$, $v_i = e^{i \varphi_i}$, $P_{ij} = K_{ij} + \delta_{ij} \sum_{\parallel} K_{\parallel}$, $K_N = \frac{1}{2} \sum_{ij} K_{ij}$ and $K_{ij}$ is the matrix of the couplings:

$$K_{ij} = \begin{cases} 
K_{||} = J_{||} / T & \text{if nearest neighbors in the xy-layer,} \\
K_{\perp} = J_{\perp} / T & \text{if nearest neighbors perpendicular to the layers,} \\
0 & \text{otherwise}.
\end{cases}$$

To simplify the notation we set $a = k_B = 1$, where $a$ denotes the lattice constant.

Because $P$ is positive definite we can transform the partition function

$$Z = \int_\varphi D\varphi \exp (-\beta H)$$

using the Hubbard-Stratanovich transformation [5] into

$$Z \propto \int_\varphi Dz Dz^* \exp \left( -\frac{1}{2} z^T P^{-1} z \right) \prod_i I_0(|z_i|),$$

where $I_0$ is the modified Bessel function.

Introducing an external field that couples to $v$ in the partition function $Z$ we obtain the relation

$$\langle z \rangle ' = P \langle v \rangle ,$$

where $\langle \ldots \rangle$ represents the statistical averages with the partition function $Z$ in the form of (4) or (5). For the physical interpretation of the transformed partition function $Z$ it is therefore useful to change to new variables $P^{-1} z$. To diagonalize matrix $P$ simultaneously we define the new variables $\tilde{\psi} = S^T P^{-1} z$, where $S$ is unitary and $S^T P S = A$, with $A$ diagonal.
With the expansion \( I_0(x) = \exp(\frac{1}{4}x^2 - \frac{1}{6}x^4 + \ldots) \) the partition function reduces to

\[
Z \propto \int D\psi D\bar{\psi} \exp(-\beta F)
\]

\[
\beta F = \frac{1}{2} \psi^+ A (1 - \frac{1}{2} \triangle) \psi + \frac{\lambda}{4\pi} \sum_i |(S_i A \bar{\psi}_i)|^4.
\]

The diagonalization of \( P \) (with diagonal elements equal to zero [6]) yields for the eigenvalues \( \lambda \) and the matrix elements of \( S \):

\[
\lambda_{\rho i} = 2K|| \cos(\rho_x \xi_i + \rho_y \eta_i) + 2K_\perp \cos\left(\frac{\pi l}{M+1}\right)
\]

\[
\{S\}_{\rho i, \rho i'} = \sqrt{\frac{2}{L^2(M+1)}} \exp\left(-i(\rho_x x_i + \rho_y y_i)\right)
\times \sin\left(\frac{\pi l}{M+1} \xi_i\right)
\]

with \( \rho = (\rho_x, \rho_y) \) and \( l = 1, \ldots, M \). For this we invoked periodic boundary conditions with a period of \( L \) in the \( x \)- and \( y \)-direction and free boundaries perpendicular to them.

Next we treat the \( z \)-direction in the mean-field approximation. This is equivalent to considering in (8) the \( (l = 1) \) mode only. Changing back to the Fourier transform \( \psi(x_i, y_i, l) \) of \( \tilde{\psi}(\rho, l) \), with this approximation and in the continuum limit, \( F \) is given by

\[
F \approx \int d^2r \left[ T^0_e \left( 1 - \frac{T_e^0}{T} \right) |\psi|^2 \right.
+ J || \left( \frac{T_e^0}{T} - \frac{1}{2} \right) |V|| \psi|^2
+ \frac{1}{(M+1)^2} \sum_{n=1}^{M} \sin^2\left(\frac{\pi n}{M+1}\right) \left( T^0_e \frac{\psi^2}{T^3} \right) |\psi|^4 \right],
\]

with \( V || = (\tilde{\partial}_{x_i}, \tilde{\partial}_{y_i}) \) and the mean-field transition temperature

\[
T^0_e(M) = 2J || + J \perp \cos\left(\frac{\pi}{M+1}\right).
\]

Comparing this with the free energy of a \( 2d \) \( xy \)-model in the same limit, we find that we reduced the layered \( xy \)-model with \( M \) planes to an effective \( 2d \) \( xy \)-model with

\[
J_{\text{eff}} = J || \left( \frac{T_e^0(M)}{T} - 1 \right) |\psi^0|^2.
\]

Here \( |\psi^0|^2 \) follows from \( \frac{\delta F}{\delta \psi} \big|_{\psi^0} = 0 \) and we used \( |V|| \psi(r)| = |\psi||V|| \delta(r) \).

An estimate of the Kosterlitz-Thouless transition temperature [7] is obtained from

\[
\frac{J_{\text{eff}}(T_{KT})}{T_{KT}} \approx \frac{2}{\pi}
\]

yielding

\[
T^0_e(M)
\]

\[
\equiv T^0_e(M) \left( \frac{\frac{3}{2} - \frac{3}{2}}{1 + 16 \frac{M}{(M+1)^2}} \frac{\langle S^4 \rangle}{\pi J ||} \right),
\]

with \( \langle S^4 \rangle \equiv (1/M) \sum_{n=1}^{M} \sin^4(\pi n/(M+1)) \). This expression reveals that with reduced \( M \) there are two contributions to the fall of \( T_e \): a boundary effect, yielding in the mean-field approximation \( T^0_e(M) = 2J || + J \perp \cos(\pi/(M+1)) \) and a further reduction due to the \( 2d \) fluctuations becoming more important with reduced \( M \).

3. Numerical results and discussion

To obtain numerical estimates for the transition temperature and other observables we performed Monte-Carlo simulations of model (1), adopting a vectorized Metropolis algorithm by using a checker board-like decomposition of the system, and the recently proposed single-cluster algorithm [8] together with the multihistogram technique [9].

To estimate the transition temperature we used the fourth-order cumulant [10]

\[
U_L(T) = 1 - \frac{\langle (m^2)^2 \rangle_T}{3 \langle m^2 \rangle_T^2},
\]

where \( m = (1/N) \sum_i S_i \) denotes the magnetization, \( N = L^2 M \) the total number of spins and \( \langle \ldots \rangle_T \) the ther-