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Approximate Calculations for the Two-Dimensional Ising Model

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A self-consistent molecular field approximation for the two-dimensional, square-lattice Ising model is used to calculate the energy and magnetization. Agreement with the exact calculations is good except near the critical temperature, which differs from the exact critical temperature by 4%. The specific heat has no anomalous behavior as T approaches T_c from above, and the magnetization follows the incorrect Weiss $(T_c - T)^{1/2}$ law as T approaches T_c from below.

KEY WORDS: Two-dimensional, square lattice; Ising model; self-consistent molecular field approximation; magnetization.

The two-dimensional, square-lattice Ising model is a good model to try approximations on because its thermodynamic properties are known exactly and a phase transition is found. If one could make a good approximate calculation on this model in the region of the critical temperature, then one might gain an insight into phase transitions applicable to other systems. Many such approximations have been made[1] and several have been in the spirit of a molecular field, including the Weiss and Bethe–Peierls models. This is a refinement of molecular field models essentially suggested by Brout[2].

In the Ising model, each site i, $i = 1,..., N$, has a spin S_i which can take on the values ± 1. Nearest-neighbor sites contribute an energy $-\epsilon_0 S_i S_j$, so that, if there is no external field, the total Hamitonian is

$$H = -\tfrac{1}{2}\epsilon_0 \sum_i \sum_j S_i S_j$$

where the sum on j is over the nearest neighbors of i. The thermodynamic quantities we will calculate are the energy per site,

$$E = (1/N)\,\mathrm{Tr}(He^{-\beta H})/\mathrm{Tr}(e^{-\beta H})$$

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and the average spin (magnetization) per site,

$$M = (1/N)\,\mathrm{Tr}\left[\left(\sum_i S_i\right) e^{-\beta H}\right] \Big/ \mathrm{Tr}(e^{-\beta H})$$

where $\beta = 1/kT$ and

$$\mathrm{Tr} = \sum_{S_1=-1}^{1} \sum_{S_2=-1}^{1} \cdots \sum_{S_N=-1}^{1}$$

To calculate E and M, we make a self-consistent calculation of $\epsilon(S_1)$, the average energy stored in the nearest-neighbor bond 1–2 when site 1 has spin S_1. If the exact (but unknown) relative probability of site 2 having spin S_2 when site 1 has spin S_1 is $P(S_1, S_2)$, then

$$\epsilon(S_1) = -\epsilon_0 \left[\sum_{S_2=-1}^{1} S_1 S_2 P(S_1, S_2)\right] \Big/ \sum_{S_2=-1}^{1} P(S_1, S_2) \tag{1}$$

The self-consistent molecular field approximation to $P(S_1, S_2)$ is the following: the bond 1–2 contributes a factor $\exp(+\beta\epsilon_0 S_1 S_2)$ and each of the other three bonds connected to site 2 is assumed to have its average energy (for given S_2) and hence contributes a factor of $\exp(-\beta\epsilon(S_2))$. Thus,

$$P(S_1, S_2) = \exp[\beta\epsilon_0 S_1 S_2 - 3\beta\epsilon(S_2)] \tag{2}$$

The expressions (1) and (2) give two equations to be solved for the two unknowns $\epsilon(+1)$ and $\epsilon(-1)$. These were solved by computer[2] using a combination of extrapolation in $\beta\epsilon_0$ and Newton's method. When $\epsilon(S)$ is known, E and M are calculated from

$$E = 2\left[\sum_{S_1=-1}^{1} \epsilon(S_1)\, e^{-4\beta\epsilon(S_1)}\right] \Big/ \sum_{S_1=-1}^{1} e^{-4\beta\epsilon(S_1)}$$

$$M = \left[\sum_{S_1=-1}^{1} S_1 e^{-4\beta\epsilon(S_1)}\right] \Big/ \sum_{S_1=-1}^{1} e^{-4\beta\epsilon(S_1)}$$

This gives approximation 1 of Figures 1 and 2.

Approximation 2 is the same as approximation 1 except that a square of four sites is now considered to be one hyperspin site. The energy in a bond (which is just two normal bonds) between hyperspin sites is calculated self-consistently (there are now four equations in four unknowns), and E and M are evaluated to give the approximation 2 curves.

There are several remarks to be made about the results. Both approximation 1, with $kT_c = 2.595\epsilon_0$, and approximation 2, with $kT_c = 2.362\epsilon_0$ have a critical temperature closer to the exact value of $kT_c = 2.269\epsilon_0$ than the Weiss ($kT_c = 4$)

[2] The calculations were carried out at the Computing Center of the University of Rochester, which is supported in part by NSF Grant GJ-828.

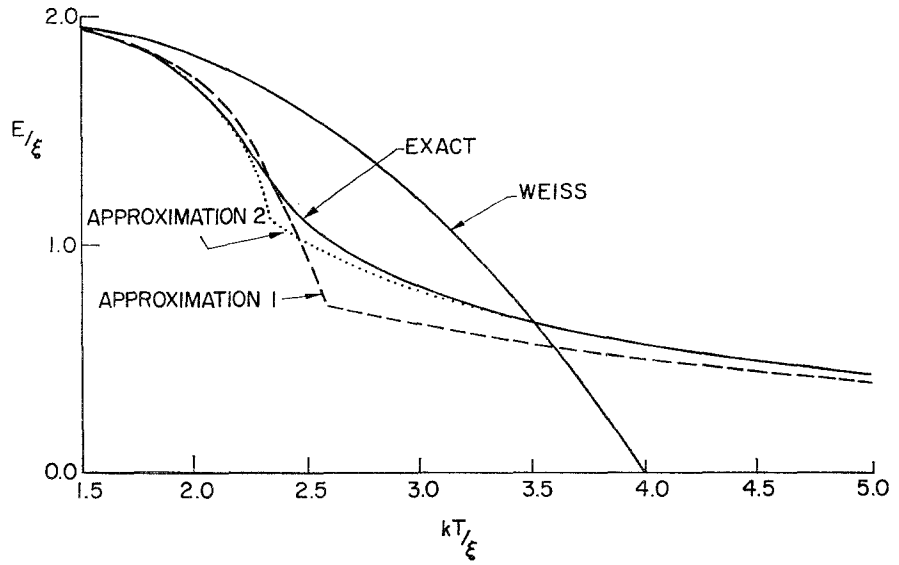

Fig. 1. Energy vs temperature ($\xi = \epsilon_0$).

and Bethe–Peierls ($kT_c = 2.885$) results, and both have better E and M curves. Also, both approximations 1 and 2 give an infinite specific heat as T approaches T_c from below, although it is difficult to determine the exact analytic form because the calculations are numerical.

On the other hand, both approximations have an M-curve which approaches T_c as $(T_c - T)^{1/2}$, just as in the Weiss model, but in contradiction to the exact $(T_c - T)^{1/8}$

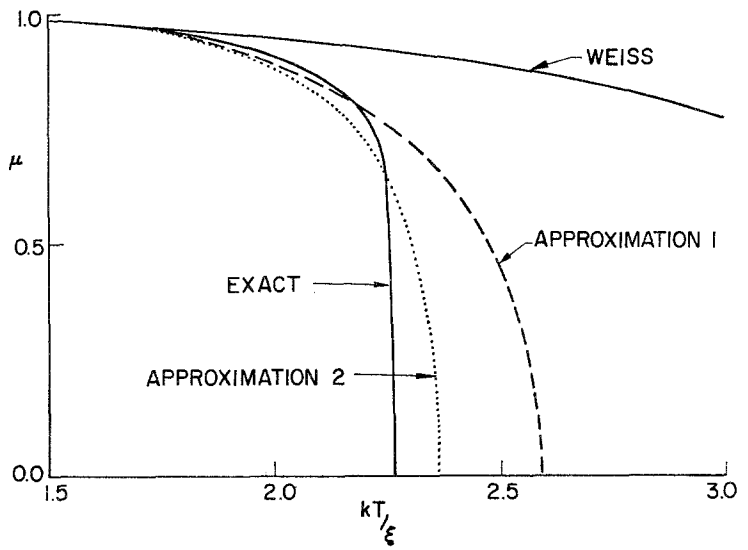

Fig. 2. Magnetization vs temperature ($\xi = \epsilon_0$).

approach. Also, neither curve has any anomaly (let alone an infinity) in the specific-heat curve as T approaches T_c from above.

Although approximation 2 gives reasonably good agreement with the exact theory for T not near T_c, the failure near $T = T_c$ indicates that the self-consistent calculation does not take long-range correlations near $T = T_c$ into account in the proper manner. Thus, this type of approximation is not capable of giving a good description of the phase transition in the Ising model with short-range forces.

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