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COMMENT

Low-temperature expansion of the planar spin model

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Abstract. We present new low-temperature series results for the 2D planar spin model. High- and low-temperature series results for the energy density are shown to reproduce Monte Carlo simulation results for $T \leqslant 0.6$ and $T \geqslant 1.3$ to within one per cent.

The planar spin model exhibits an infinite-order Kosterlitz-Thouless type transition (Kosterlitz and Thouless 1973, Kosterlitz 1974). Monte Carlo simulations (Tobochnik and Chester (1979), Metropolis algorithm; Kogut and Polonyi (1986), microcanonical ensemble) yield results consistent with the KT picture. Whilst series expansions at high temperature have been performed (Camp and Van Dyke (1975), susceptibility to tenth order; Bowers (1969), free energy to eighth order) at low temperatures, the conventional spin-wave approximation considers only the lowest-order terms. In the following calculation, we consider the simplest observable, the energy density, and obtain the next three corrections to the spin-wave result.

The 2D planar spin model is defined by the following action:

$$S = -\frac{1}{T}\sum_{\langle i,j\rangle}[\cos(\theta_i - \theta_j) - 1].$$

The variables θ_i are angles lying between 0 and 2π, the indices i, j label sites on a 2D square lattice of unit spacing, and the summation is over nearest-neighbour sites, each pair counted only once. In the limit of an infinite lattice, we have the following Fourier transform:

$$\theta_i = \int \mathrm{d}\tilde{p}\, \theta(p) \exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}_i)$$

where

$$\int \mathrm{d}\tilde{p} = \int_{-\pi}^{\pi} \frac{\mathrm{d}^2 p}{(2\pi)^2}$$

and $\boldsymbol{r}_i$ is the position vector of site i. Following Luck (1982), we expand the cosine in the action and transform to momentum space to obtain the spin-wave action:

$$S_2 = \frac{1}{2T}\int \mathrm{d}\tilde{p}\, \theta(p)\pi^{-1}(p)\theta^*(p)$$

and the higher-order corrections:

$$S_m = -\frac{2^m}{Tm!}\int \mathrm{d}\tilde{p}_1 \ldots \mathrm{d}\tilde{p}_m\, \theta(p_1)\ldots\theta(p_m)(2\pi)^2\delta(p_1 + \ldots + p_m)$$
$$\times \sum_\mu (\sin\tfrac{1}{2}p_1^\mu)\ldots(\sin\tfrac{1}{2}p_m^\mu) \qquad m = 4, 6, 8, \ldots$$

where

$$\pi(p)=\left(2\sum_{\mu}(1-\cos p^{\mu})\right)^{-1}.$$

The Fourier transform of $\pi(p)$ is the usual 2D lattice Green function $G(\boldsymbol{r})$. We define the normalised Green function $\tilde{G}(\boldsymbol{r})$

$$\tilde{G}(\boldsymbol{r})=G(\boldsymbol{r})-G(\boldsymbol{0}).$$

Consider the energy per site,

$$E=2[1-\langle\exp[\mathrm{i}(\theta_i-\theta_j)]\rangle] \qquad i,j=\text{arbitrary fixed link.}$$

If we introduce the following source term:

$$J(p)=\tfrac{1}{2}[1-\exp(\mathrm{i}p^{\nu})] \qquad \nu=\text{direction of link } i,j$$

then

$$E=2[1-\Gamma[J]] \qquad \Gamma[J]=Z[J]/Z[0]$$

where $Z[J]$ is the source-dependent generating functional

$$Z(J)=\int[\mathrm{d}\theta(p)]\exp\left(-S[\theta(p)]-\mathrm{i}\int\mathrm{d}\tilde{p}\,\theta(p)J^*(p)+\theta^*(p)J(p)\right).$$

$\ln\Gamma[J]$ is then the sum over all J-dependent connected diagrams. The power of T is given by the number of propagators minus the number of vertices. All diagrams to $\mathrm{O}(T^4)$ are given in figure 1;

$$\tilde{G}(1)=-\tfrac{1}{2}\int\mathrm{d}\tilde{p}\frac{4\sin^2\frac{1}{2}p^{\nu}}{4(\Sigma_{\mu}\sin^2)\frac{1}{2}p^{\mu}}=-\tfrac{1}{4}$$

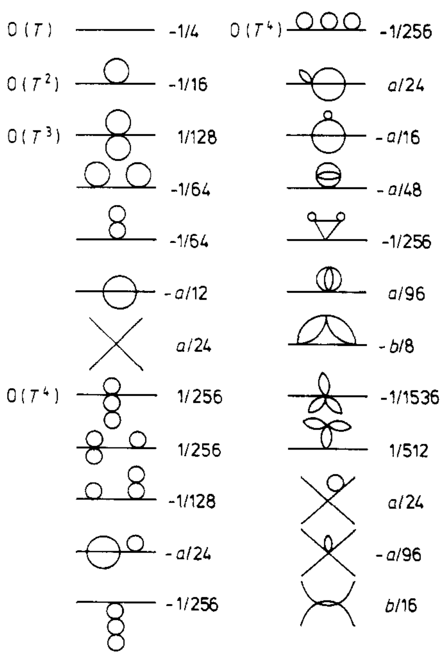

Figure 1. All J-dependent connected diagrams to $\mathrm{O}(T^4)$.

by symmetry, and for all size lattices. If we define

$$A_{\mu\nu}(x)=\int \mathrm{d}\tilde{p}\,\pi(p)\exp(\mathrm{i}p\cdot x)[1-\exp(\mathrm{i}p^{\mu})][1-\exp(-\mathrm{i}p^{\nu})]$$

then the coefficients a and b are given by

$$a=\tfrac{1}{2}\sum_{\mu,\nu}\sum_{x}A^{4}_{\mu\nu}(x)$$

$$b=\sum_{\alpha,\mu,\nu}\sum_{x,y}A^{2}_{\mu\alpha}(x+y)A^{2}_{\nu\alpha}(y)A^{2}_{\mu\nu}(x).$$

The values of a and b can then be computed for a finite lattice.

To $\mathrm{O}(T^4)$, we obtain the following series for E:

$$E=\tfrac{1}{2}T+\tfrac{1}{16}T^2+(\tfrac{1}{48}+\tfrac{1}{12}a)T^3+(\tfrac{9}{1024}+\tfrac{1}{16}a+\tfrac{1}{8}b)T^4.$$

Calculating the coefficients a and b on lattices of increasing size, the values were found to converge towards the limits

$$a=0.0684(1)\qquad b=0.0206(1).$$

The series of E up to $\mathrm{O}(T^3)$ has been recalculated, using an x-space expansion of $Z[0]$ on a finite periodic lattice. This gives identical coefficients, indicating that the above series is valid for finite lattices, as well as for the infinite lattice limit. This can also be seen by considering the above calculation with momentum integrals replaced by discrete sums, and δ functions by periodic δ functions.

In figure 2, the spread of the Padé approximants to the above series, calculated at $L=60$, is plotted together with data from a Monte Carlo simulation of a 3600 spin system (Tobochnik and Chester 1979). Also shown is the spread of the Padé approximants to the high-temperature series, derived from expressions given by Bowers (1969) and Domb (1960):

$$E=2-\frac{1}{T}-\frac{3}{8}\frac{1}{T^3}-\frac{1}{48}\frac{1}{T^5}+\frac{31}{3072}\frac{1}{T^7}+\mathrm{O}(T^{-9}).$$

The error bars on the data are comparable in size to the plotted symbols. The Padé approximants agree with the data to within one per cent over the range $T\leqslant 0.6$ and

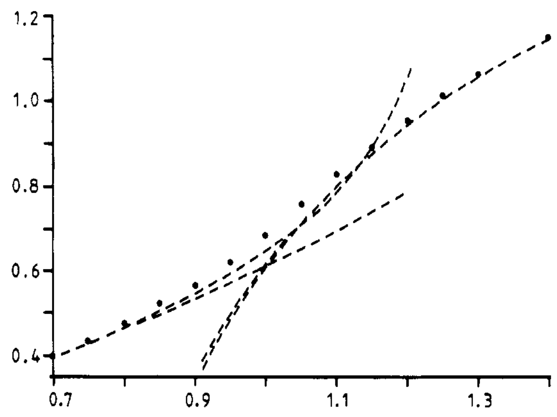

Figure 2. Spread of Padé approximants (broken curves) to high- and low-temperature series, together with Monte Carlo data (dots).

$T \geqslant 1.3$. This represents, at low temperatures, a distinct improvement over the spin-wave result, and a more reliable check on possible approximation schemes or new numerical algorithms.

The calculation illustrates the difficulties in continuing the series to higher orders. Further coefficients, arising from graphs with n non-trivial δ functions, will involve $O(L^{2n})$ operations, which soon becomes prohibitively large.

The method can be generalised to calculate the susceptibility χ, where

$$\chi = \sum_x \langle \exp[i(\theta(\boldsymbol{x}) - \theta(\boldsymbol{0}))] \rangle = \sum_x \Gamma[J_x]$$

and J_x is the source term,

$$J_x(p) = \tfrac{1}{2}[1 - \exp(-i\boldsymbol{p} \cdot \boldsymbol{x})].$$

Although the diagrammatics is identical and the calculation to $O(T^2)$ is straightforward, it is again the δ functions which complicate matters at $O(T^3)$ and higher.

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References

Bowers R G 1969 *PhD thesis* Kings College, London, p 172
Camp W J and Van Dyke J P 1975 *J. Phys. C: Solid State Phys.* **8** 335
Domb C 1960 *Adv. Phys.* **9** 245
Kogut J and Polonyi J 1986 *Nucl. Phys.* B **265** [FS15] 313
Kosterlitz J M 1974 *J. Phys. C: Solid State Phys.* **7** 1046
Kosterlitz J M and Thouless D J 1973 *J. Phys. C: Solid State Phys.* **6** 1181
Luck J M 1982 *J. Phys. A: Math. Gen.* **15** L169
Tobochnik J and Chester G V 1979 *Phys. Rev.* B **20** 3761