PHYSICAL REVIEW B VOLUME 27, NUMBER 9 1 MAY 1983

Probability density function of the double-Gaussian model

Paul D. Beale*
Laboratory of Atomic and Solid State Physics and Materials Science Center, Cornell University, Ithaca, New York, 14853
(Received 10 January 1983)

An exact factorization of the partition function of the double-Gaussian model into Gaussian and Ising components is exploited to derive an exact factorization of the block probability density function. The block probability density function factors into a Gaussian, which describes the phonons in the problem, and a block probability density function of a long-ranged Ising model. This quantity is shown to be consistent with scaling assumptions near criticality. As long as the correlation length and the block size are much larger than the phonon correlation length, the scaling assumptions are satisfied.

The class of double models of structural phase transitions[1] is defined by the potential energy

$$\beta U_N=\sum_j \beta V(x_j)+\sum_{(ij)}\frac{\beta C}{2}(x_i-x_j)^2 \ , \tag{1}$$

where $\beta=1/k_BT$, $\{x_j\}$ is the set of displacements of N particles measured relative to the lattice sites of a d-dimensional hypercubic lattice, and $\{(ij)\}$ is the set of all nearest-neighbor pairs on the lattice. The site potential βV has a double-well structure. The limit where the well depth vanishes is called the displacive limit. In the limit that the well depth diverges, the model is equivalent to a nearest-neighbor Ising model. I will be discussing the double-Gaussian model[2] which is defined by

$$\beta V(x)=\frac{1}{2}\left(\frac{x}{w}\right)^2-\ln\left[\cosh\left(\frac{xv}{w^2}\right)\right] \ . \tag{2}$$

The partition function for this model factorizes[2,3] exactly into the partition function for the Gaussian model[4] and the partition function for an Ising model with long-range interactions.[5] This factorization has been exploited to derive bounds on the critical line T_c, and to locate the region where the Ising to Gaussian crossover occurs.[3]

One quantity which is useful for describing the ordering process in the double-well models is block probability density function (PDF). It is defined by[6,7]

$$P_L(s)=\left\langle\delta\left[s-\sum_j f(r_j)x_j\right]\right\rangle . \tag{3}$$

The angular brackets denote a thermal average over a canonical ensemble, δ is Dirac's δ function, $\{r_j\}$ is the set of all lattice sites, and $f(r)$ is a normalized nonnegative function which is sizable on roughly L^d lattice sites in a region of linear dimension L. $P_L(s)\,ds$ is the probability that $\sum_j f(r_j)x_j$ has a value between s and $s+ds$. P_L describes the character of configurations on the lattice when viewed with a linear resolution of order L. The Fourier transform of P_L is called the block characteristic function and is given by

$$S_L(y)=\left\langle\exp\left[iy\sum_j f(r_j)x_j\right]\right\rangle . \tag{4}$$

For L sufficiently large so that P_L embraces many lattice sites, scaling theories[6,7] indicate that the functions P_L and S_L assume universal limiting forms.[5] For temperatures $T>T_c$, independent of the well depth of the system, the distribution of the block-spin variables tend to a Gaussian form as $L\to\infty$. For L much greater than the correlation length, ξ, S_L takes the form[7]

$$S_L(y)\approx\exp\left[\frac{-k_BT\chi_Ty^2}{2L^d}\right] \ , \tag{5}$$

where χ_T is the isothermal susceptibility:

$$k_BT\chi_T=N^{-1}\sum_{(ij)}\langle x_ix_j\rangle \ . \tag{6}$$

The reason for this is that regions of volume L^d contain roughly $(L/\xi)^d$ regions of independently fluctuating variables, and by the mean value theorem the probability density is Gaussian.

For T very close to T_c, scaling arguments[6,7] imply that S_L tends to a universal form for $L \gg R$ and $\xi \gg R$ where R is the largest noncritical length in the problem:

$$S_L(y)\approx\tilde{S}(\sigma L^{-\beta/\nu}y,L/\xi) \ . \tag{7}$$

$\tilde{S}$ is a universal function for the double-well models and depends only on the dimensionality. The variable σ is a nonuniversal number which describes the scale of variation in the order parameter $\langle x_j\rangle$. The variables β and ν are, respectively, the exponents which describe the power-law singularities of the order parameter and the correlation length as $T\to T_c$.

The shapes of $\tilde{S}$ have been determined for $d=2,3$ by Bruce *et al.*[6] and by Binder.[7] In $d=2$ the block PDF is doubly peaked but is singly peaked for $d \geqslant 3$.

In this paper I calculate certain features of the block PDF for the double-Gaussian model by exploiting the partition function factorizability. By using the Fourier-transform variables

$$z_q = N^{-1} \sum_j e^{iqr_j} x_j \ , \tag{8}$$

$S_L(y)$ can be written

$$S_L(y) = \left\langle \exp\left[iy \sum_q f_q^* z_q \right] \right\rangle , \tag{9}$$

where f_q is the Fourier transform of $f(r)$. The asterisk denotes complex conjugation. Now, by using the partition function factorization technique described in detail in Ref. 3, I arrive at the result

$$S_L(y) = \frac{1}{Z_N^{\text{Ising}}} \sum_{\{\mu\}} \exp\left[-\tfrac{1}{2} w^2 y^2 \sum_j \sum_k [f(r_j) f(r_k) G(r_j - r_k)] \right] \exp\left[iyv \sum_j \sum_k [f(r_j) G(r_j - r_k) \mu_k + K_{jk} \mu_j \mu_k] \right] , \tag{10}$$

where $\{\mu\}$ is a set of Ising spin variables, Z_N^{Ising} is the partition function for the associated Ising model, K_{jk} is the (long-ranged) Ising interaction energy, and

$$G(r) = N^{-1} \sum_q \left[\frac{e^{iqr}}{1 + 2Kw^2 \left(d - \sum_{n=1}^{d} \cos(q_n) \right)} \right] \tag{11}$$

is the lattice Green's function. The sum on q is over the first Brillouin zone, and q_n refers to the nth Cartesian coordinate of q. S_L can then be evaluated as

$$S_L(y) = \exp\left[-\frac{w^2 y^2}{2} \sum_j f(r_j) \tilde{f}(r_j) \right] \times \left\langle \exp\left[iyv \sum_j \tilde{f}(r_j) \mu_j \right] \right\rangle^{\text{Ising}} , \tag{12}$$

where

$$\tilde{f}(r) = \sum_j f(r_j) G(r - r_j) \tag{13}$$

is the convolution of f with the lattice Green's function and the angular brackets with superscripts "Ising" is a thermal average over the Ising variables. The function $\tilde{f}$ is normalized, non-negative, and defines a *different* block size $\tilde{L}$ on the Ising variables.

The result of this analysis is that the block characteristic function for the double-Gaussian model is (for all dimensions) *exactly* the product of a Gaussian (coming from the phonons in the problem) and a *block characteristic function for the associated Ising model,* which describes the nonlinear ordering features in the Hamiltonian. The Green's function $G(r)$ is exponentially decaying for large r and has a range of $R=(Kw^2)^{1/2}$, where R is the range of phonon correlations.[2,3]

If $L \ll R$ then the Ising-model block size is $\tilde{L} \approx R$:

$$S_L(y) = \exp\left[-\frac{w^2 y^2}{2R^d} \right] S_R^{\text{Ising}}(vy), \quad \text{for } L \ll R \ . \tag{14}$$

If $L \gg R$ then $\tilde{L} \approx L$:

$$S_L(y) = \exp\left[-\frac{w^2 y^2}{2L^d} \right] S_L^{\text{Ising}}(vy), \quad \text{for } L \gg R \ . \tag{15}$$

Now it can be shown that the block characteristic function is consistent with the scaling assumptions of Bruce *et al.*[6] near criticality and in the high-temperature ($L \gg \xi$) limit.

For $L \gg \xi$, assuming the validity of Eq. (5), I arrive directly at the result

$$k_B T \chi_T^{\text{DG}} = w^2 + k_B T \chi_T^{\text{Ising}} \ , \tag{16}$$

which is exactly the result which can be obtained directly from the partition function.

Near criticality, for $L \gg R$, Eq. (15) gives [assuming the validity of the scaling form (7)]

$$\tilde{S}\left[\sigma^{\text{DG}} L^{-\beta/\nu} y, \frac{L}{\xi} \right] \approx \exp\left[-\frac{w^2 y^2}{2L^d} \right] \times \tilde{S}\left[\sigma^{\text{Ising}} L^{-\beta/\nu} vy, \frac{L}{\xi} \right] . \tag{17}$$

For this to be valid, σ^{DG} and $v\sigma^{\text{Ising}}$ must be equal and the Gaussian prefactor must be slowly varying with respect to the variation of $\tilde{S}$. The variance of the Gaussian is clearly L^d/w^2, whereas the variance of the other factor is[7]

$$\frac{L^d}{v^2 k_B T \chi_L} ,$$

where

$$k_B T \chi_L = L^{-d} \sum_{j \in L^d} \sum_{k \in L^d} \langle \mu_j \mu_k \rangle$$

is the susceptibility of a block of size L on the Ising lattice. Therefore scaling will be valid as long as

$$k_B T \chi_L \gg 1 \ . \tag{18}$$

This is trivially true if $\xi \gg L \gg R$. For the case

$L >> \xi$, inequality (18) is identical to the criterion

$$\xi >> \xi_+ \chi_+^{-\nu/\gamma} , \tag{19}$$

where ν and γ are, respectively, the exponents of the power-law divergence of ξ and χ_T as T_c is approached from above, and ξ_+ and χ_+ are the amplitudes of those divergences. For large R, one would expect that χ_+ does not scale with R because it is a measure of the coupling of the spins to an external field. On the other hand, ξ_+ is a measure of lengths on the lattice, and therefore one would expect that $\xi_+ \approx R$ as R increases. Therefore scaling is valid if both $\xi >> R$ and $L >> R$. This is, of course, what one would have expected from the start. The phonon correlation range R is the longest noncritical length in the double-well models. Near the displacive limit on the critical line the phonon correlation range is very long, diverging in the displacive limit.[3] Nonlinear ordering effects begin to predominate only when the correlation length is large compared to the phonon correlation length.

ACKNOWLEDGMENTS

I wish to thank J. A. Krumhansl, A. R. Bishop, and A. D. Bruce for several useful conversations. This work was supported by the National Science Foundation under Grant No. DMR-80-20429 to the Laboratory of Atomic and Solid State Physics and under Grant No. DMR-79-24008 to the Cornell University Materials Science Center.

*Present address: Department of Theoretical Physics, 1 Keble Road, University of Oxford, Oxford, OX1 3NP England

[1]A. D. Bruce, Adv. Phys. 29, 111 (1980).
[2]G. A. Baker and A. R. Bishop, J. Phys. A 15, L201 (1982); J. H. Chen, M. E. Fisher, and B. G. Nickel, Phys. Rev. Lett. 48, 630 (1982).
[3]G. A. Baker, Jr., A. R. Bishop, K. Fesser, P. D. Beale, and J. A. Krumhansl, Phys. Rev. B 26, 2596 (1982).
[4]T. H. Berlin and M. Kac, Phys. Rev. 86, 821 (1952).
[5]C. Domb, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1974), Vol. 3, p. 357.
[6]A. D. Bruce, T. Schneider, and E. Stoll, Phys. Rev. Lett. 43, 1284 (1979); A. D. Bruce, in *Nonlinear Phenomena at Phase Transitions and Instabilities,* edited by T. Riste (Plenum, New York, 1981).
[7]K. Binder, Z. Phys. B 43, 119 (1981).