PHYSICAL REVIEW B VOLUME 19, NUMBER 3 1 FEBRUARY 1979

Lee-Yang theory and normal fluctuations

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(Received 2 March 1978; revised manuscript received 2 August 1978)

The convergence of the distribution of block spin variables to a product of independent normal Gaussians is rigorously proved for every ferromagnetic system with nonzero magnetic field. This result extends to more general situations and in fact a simple and general link is exhibited between the absence of a phase transition in the framework of Lee-Yang theory and the convergence to a normal Gaussian fixed point under the action of the renormalization group.

Being given a spin system, on a d-dimensional cubic lattice Z^d, we consider subsets Λ of the lattice, for example cubes, of volume $|\Lambda|$, and we shall denote by $S_\Lambda = \sum_{x\in\Lambda} \sigma_x$ the sum of the spins inside Λ. The fluctuations of σ_x are expected to be normal in various situations away from critical points, and correspondingly the probability distribution of the variable $\overline{S}_\Lambda = (S_\Lambda - \langle S_\Lambda\rangle)/\sqrt{|\Lambda|}$ should tend to the Gaussian measure $(2\pi\chi)^{-1/2}\exp(-k^2/2\chi)\,dk$ when $|\Lambda|$ becomes infinitely large, where $\chi = \lim\langle(\overline{S}_\Lambda)^2\rangle$ is finite and strictly positive. This convergence when it holds is called the central-limit theorem. The block spin variables associated with different blocks Λ_i are expected on the other hand to become independent, in which case there is convergence of the distribution of all block spins variables $\overline{S}_{\Lambda_i}$ to a product of independent Gaussians. This latter convergence property means, when it holds, that there is convergence to a normal Gaussian fixed point under the action of the renormalization group[1] [alternatively, in some approaches,[2] one considers the nonlinear variables $\eta_{\Lambda_i} = \mathrm{sgn}(S_{\Lambda_i} - \langle S_{\Lambda_i}\rangle)$, the distribution of which should then converge to a product of independent variables taking value ±1 with probability $\frac{1}{2}$]. In contrast, the fluctuations are expected to be non-normal at critical points, and convergence to a normal Gaussian fixed point is not expected.

In view of the physical importance of the problem of fluctuations, it is of interest to have a satisfactory theoretical understanding of the conditions under which the central-limit theorem and the convergence to a normal Gaussian fixed point hold.

Several rigorous results have been previously obtained in this domain at large magnetic field,[3] and under various other conditions by means of decay properties of correlations,[4-8] or of correlation inequalities[9] or for one-dimensional systems.[10]

The purpose of the present paper is to present a simple and general proof that the Lee-Yang condition on the absence of phase transitions, i.e., the absence of zeros of the partition function in appropriate regions, implies convergence to a normal Gaussian fixed point. In contrast to previous ones,[11] our method does not depend on conditions on the decrease of the potential or of the correlations, or on the sign of the potential, and thus applies for instance to arbitrary Van der Waals forces. The idea that the Lee-Yang condition might be sufficient to provide a direct and general proof of the central-limit theorem was previously mentioned in Ref. 13, where it was proposed to extend the previous method of Ref. 10 to the multidimensional case. Such an extension presents, however, difficulties.[14] Our method makes a different use of the Lee-Yang condition, which circumvents these difficulties and is also well adapted to the proof of convergence to the normal Gaussian fixed point.

We shall, below, restrict ourselves for simplicity to spin-$\frac{1}{2}$ ferromagnetic systems with two-body potentials and nonzero magnetic field, but the method applies similarly to more general situations, as will be briefly outlined at the end. In the particular case of ferromagnets, our result complements that of Ref. 9 obtained at zero magnetic field above T_c, and those of Refs. 5 and 7 obtained for nonzero magnetic field under certain conditions on the decrease of the potential (see Ref. 11).

The energy of a configuration $\sigma_{\Lambda'}$ of spins σ_x at each point x in a box Λ' is given by

$$U_{\Lambda'}(\sigma_{\Lambda'}) = -\sum_{\substack{x,y\in\Lambda'\\ x\neq y}} J_{x,y}\sigma_x\sigma_y - \sum_{x\in\Lambda'} h_x\sigma_x\,, \qquad (1)$$

where h_x is the magnetic field at the point x and $J_{x,y}$ is the interaction potential between sites x

and y, which is assumed for simplicity to be translation invariant. It satisfies $\sum |J_{0,x}| < \infty$. For a ferromagnet, one has $J_{x,y} \geq 0$ for all points x, y.

The partition function in a box Λ' is defined as

$$Q_{\Lambda'}(\{h_x\}, x \in \Lambda') = \sum_{\substack{\sigma_x = \pm \frac{1}{2} \\ x \in \Lambda'}} \exp[-U_{\Lambda'}(\sigma_{\Lambda'})]. \tag{2}$$

For the infinite system, the one-point and two-point correlations are the average values $\langle \sigma_x \rangle$ and $\langle \sigma_x \sigma_y \rangle$ of one spin or of the product of two spins. The two-point connected correlation is defined by

$$\sigma^T(x, y) = \langle \sigma_x \sigma_y \rangle - \langle \sigma_x \rangle \langle \sigma_y \rangle .$$

These functions can be obtained as limits of the analogous quantities for a system in a box Λ' when Λ' tends to infinity. Finally, when the magnetic field is constant ($h_x = h$ for every x), one can prove[15] that

$$0 < \lim_{\Lambda \to \infty} \left(\frac{1}{|\Lambda|} \sum_{x, y \in \Lambda} \sigma^T(x, y) \right) = \left(\sum_{x \in Z^d} \sigma^T(0, x) \right) < \infty , \tag{3}$$

$$\lim_{|\Lambda| \to \infty} \frac{1}{|\Lambda|} \sum_{x \in \Lambda_1, y \in \Lambda_2} \sigma^T(x, y) = 0 ,$$
$$|\Lambda_1| = |\Lambda_2| = |\Lambda| , \quad \Lambda_1 \cap \Lambda_2 = \emptyset . \tag{4}$$

The two expressions in the large parentheses of (3) will be called, respectively, χ_Λ and χ.

We then state the following.

Theorem: The central-limit theorem holds and the distribution of the block spin variables $\overline{S}_{\Lambda_i}$ converges to a product of independent normal Gaussians for any ferromagnet with nonzero magnetic field. The distribution of the variables η_{Λ_i} converges to a product of independent variables with value ± 1 with probability $\frac{1}{2}$.

Proof: As usual, we introduce for any number $p \geq 1$ of variables $\overline{S}_{\Lambda_j}$ the characteristic function

$$\left\langle \exp\left(i \sum_{j=1}^{p} t_j \overline{S}_{\Lambda_j} \right) \right\rangle .$$

The average value of the variable $\exp(\sum_{j=1}^{p} z_j S_{\Lambda_j})$ for a system in a box Λ' containing Λ can be rewritten, as can be checked from the definitions, as

$$\left\langle \exp\left(\sum_{j=1}^{p} z_j S_{\Lambda_j} \right) \right\rangle_{\Lambda'} = Q_{\Lambda'}\left(h + \sum_{j=1}^{p} z_j \delta_{\Lambda_j} \right) \Big/ Q_{\Lambda'}(h) , \tag{5}$$

where the numerator is the partition function of the system in the box Λ' with magnetic field $h + z_j$ at the points of Λ_j, $j = 1, \ldots, p$, and h at the points of Λ' outside $\cup_{j=1}^{p} \Lambda_j$. The well known Lee-Yang theorem[16] ensures that $Q_{\Lambda'}(h + \sum_{j=1}^{p} z_j \delta_{\Lambda_j}) \neq 0$, whenever $|z_j| < z_0$, $j = 1, \ldots, p$ for some $z_0 > 0$ independent of Λ and Λ'. An expansion to the third order of the analytic function $\ln Q_{\Lambda'}(h + \sum_{j=1}^{p} z_j \delta_{\Lambda_j})$, with respect to $z_1, \ldots, z_p$ then shows, by a direct computation, that

$$\begin{aligned} \ln \left\langle \exp\left(\sum_{j=1}^{p} z_j S_{\Lambda_j} \right) \right\rangle_{\Lambda'} &= \sum_{\alpha=1}^{p} z_\alpha \langle S_{\Lambda_\alpha} \rangle_{\Lambda'} + \frac{1}{2} \sum_{\alpha, \beta=1}^{p} z_\alpha z_\beta \sum_{x \in \Lambda_\alpha, y \in \Lambda_\beta} \sigma_{\Lambda'}^T(x, y) \\ &\quad + \sum_{\alpha, \beta, \gamma=1}^{p} z_\alpha z_\beta z_\gamma A_{\alpha, \beta, \gamma}(z_1, \ldots, z_p; \Lambda, \Lambda') , \end{aligned} \tag{6}$$

where $A_{\alpha,\beta,\gamma}$ is an analytic function of $z_1, \ldots, z_p$ in the region $|z_i| < z_0$ and is bounded by

$$\max_{\substack{|z_j'| < |z_j| \\ j=1,\ldots,p}} \left| \frac{\partial^3}{\partial z_\alpha'' \partial z_\beta'' \partial z_\gamma''} \ln Q_{\Lambda'}\left(h + \sum_{j=1}^{p} z_j'' \delta_{\Lambda_j} \right) \right|_{z_j'' = z_j'} .$$

The function $Q_{\Lambda'}$ can be rewritten in view of its definition, as

$$\begin{aligned} Q_{\Lambda'}\left(h + \sum_{j=1}^{p} z_j \delta_{\Lambda_j} \right) &= e^{z_\alpha |\Lambda|} \sum_{0 \leq n \leq 2|\Lambda|} e^{-z_\alpha n} a_n(\Lambda, \Lambda'; h; \overline{z}_\alpha) \\ &= e^{z_\alpha |\Lambda|} a_{2|\Lambda|}(\Lambda, \Lambda', h) \\ &\quad \times \prod_{\rho=1}^{2|\Lambda|} [e^{-z_\alpha} - \xi_\rho(\Lambda, \Lambda'; h; \overline{z}_\alpha)] , \end{aligned} \tag{7}$$

where $\overline{z}_\alpha = (z_1, \ldots, z_{\alpha-1}, z_{\alpha+1}, \ldots, z_p)$ and the quantities ξ_p are the $2|\Lambda|$ zeros of $Q_{\Lambda'}$ in the variable e^{-z_α}. Since $Q_{\Lambda'}$ does not vanish when $|z_j| < z_0$, $j = 1, \ldots, p$ one has $|e^{-z_\alpha} - \xi_\rho(\Lambda, \Lambda'; h; \overline{z}_\alpha)| > \eta$ for $|z_j| < \frac{1}{2} z_0$ and all $\rho = 1, \ldots, 2|\Lambda|$ with some $\eta > 0$ independent of Λ, Λ'. Cauchy formulas for the third derivatives of $\ln Q_{\Lambda'}$ then directly yield

$$|A_{\alpha,\beta,\gamma}(z_1, \ldots, z_p; \Lambda, \Lambda')| < K |\Lambda| \tag{8}$$

when $|z_j| < \frac{1}{2} z_0$ and where K is independent of Λ, Λ' and $z_1, \ldots, z_p$.

By choosing $z_j = i t_j / \sqrt{|\Lambda|}$ and letting Λ' first tend to infinity (thermodynamic limit) for any given box Λ, one then sees in view of Eqs. (3), (4), and (8) that $\langle \exp(i \sum_{j=1}^{p} t_j \overline{S}_{\Lambda_j}) \rangle$ tends to $\prod_{j=1}^{p} \exp(-\chi \frac{1}{2} t_j^2)$ for any $t_1, \ldots, t_p$ when $|\Lambda|$ tends to infinity. This convergence of the characteristic function ensures, through general results of probability, (weak) convergence to the normal Gaussian fixed point. Finally weak convergence of probability measure implies also convergence in a well-defined integral sense; in particular the joint probability that $\overline{S}_{\Lambda_j}$ be positive or negative, $j = 1, \ldots, p$ converges to the integral of the product of the Gaussians in corresponding regions, from which the result for the variables η_{Λ_j} follows. Q.E.D.

Under the condition of our theorem and a further slight condition on the decay of the potential,

$$|J(x)| < C(1+|x|)^{-d-\epsilon} \text{ for some } \epsilon > 0 \ ,$$

we have also obtained the local version of the central-limit theorem, which strengthens the integral one and asserts that for any $\epsilon > 0$, there exists Λ_0 sufficiently large such that for any Λ containing Λ_0:

$$\sup_k |\sqrt{|\Lambda|}\, \Pr(\bar{S}_\Lambda = k) - (2\pi\chi)^{-1/2}\exp(-k^2/2\chi)| < \epsilon \,. \quad (9)$$

The interest of the local-limit theorem has been pointed out by Dobrushin and Tirozzi,[13] who proved that the local theorem can be derived from the integral theorem in the case of finite-range potentials. Our proof of the local theorem, outlined below, applies to more general potentials. One considers the formula

$$\sqrt{|\Lambda|}\,\Pr(\bar{S}_\Lambda = k) = \frac{1}{2\pi}\int_{-\pi\sqrt{|\Lambda|}}^{\pi\sqrt{|\Lambda|}} \langle \exp(it\bar{S}_\Lambda)\rangle \exp(-itk)\, dt \,, \qquad (10)$$

which follows from the definition of the characteristic function by inverse Fourier transformation.

Equations (8) and (6) in the case $p=1$ allow one here to check that, for some $\delta > 0$, the contribution to the right-hand side of (10) coming from the integration domain $|t| < \delta\sqrt{|\Lambda|}$ tends to the analogous contribution of the Gaussian. On the other hand, the contribution of the domain $\delta < t/\sqrt{|\Lambda|} < \pi$ can be shown to tend uniformly to zero when $|\Lambda| \to \infty$, by an extension of a related calculation made in Ref. 13 for finite-range potentials. This extension can be found in Ref. 8 and is therefore omitted here.

As a conclusion, we mention that our theorem has been stated in the simplest case, but in fact it holds in more general situations: the interactions are not necessarily ferromagnetic, and the only condition needed to show the results for some magnetic field h_0, is that the partition function $Q_{\Lambda'}(\{h_x\}, x \in \Lambda')$ should not vanish when all h_x belong to some complex neighborhood of h_0 independent of Λ'. This is the condition of absence of phase transition at h_0 in the Lee-Yang theory. As a matter of fact, the original Lee-Yang condition required only that $Q_{\Lambda'}(h)$ should not vanish when all h_x are equal to h. However, the counterexample of low-temperature antiferromagnets[17] shows that this weaker condition does not prevent symmetry breaking. In the framework of Lee-Yang theory, the condition for the absence of phase transition has therefore to be stated in the stronger form mentioned above. Besides ferromagnetic systems, this condition has been proved for example for systems with arbitrary interactions and arbitrary magnetic field, at high temperature.[18]

Our proof of convergence to a Gaussian fixed point can be extended to more general spins than spins $\frac{1}{2}$. It extends also to other observables, for instance we can obtain that the fluctuations of the energy are normal, by using conditions of absence of zeros of the partition function in appropriate domains of the potential, such as those proved in Ref. 19.

Finally, the stronger convergence obtained for the block spin distribution (local-limit theorem) is not only a mathematical refinement, but is linked, through an extension of the results to appropriate conditional probabilities, to the equivalence of ensembles (see Ref. 13). In this connection, we can prove for general potentials the equivalence of the grand canonical and canonical ensembles in the absence of phase transitions. Note, however, that a different approach to the problem of equivalence of ensembles has been given in Ref. 20.

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[11]The results of Ref. 5 for finite-range ferromagnetic potentials are also based on the Lee-Yang condition, but the Lee-Yang results are used there in an indirect

way, namely, through the exponential decay properties of correlations that follow from them. The method can be easily extended to exponentially or rapidly decreasing potentials, in view of the corresponding results of Ref. 12 on the decay of correlations. The extension of the method to potentials that do not decrease rapidly presents, however, difficulties. It is known that the correlations cannot decrease rapidly if the potential does not decrease rapidly: see Ref. 7. Sufficient decrease properties of correlations, and the central-limit theorem, are still derived in Ref. 7 at any nonzero magnetic field, but only for potentials that decrease faster than r^{-3d}. Moreover, the proof is much more complicated and the Lee-Yang condition is insufficient: results on the zeros of the partition function with respect to the potential are required in that approach.

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[14]The method of Ref. 10 consists of two steps. In the first one [theorem (8)], the convergence to a Gaussian, in the $|\Lambda|\to\infty$ limit, of the probability distribution of the variable $\overline{S}_\Lambda$ is proved *for a system in the same box* Λ. The central-limit theorem of physical interest in connection with renormalization-group theory (convergence to a Gaussian of the distribution of $\overline{S}_\Lambda$ *for an infinite system*) is then a consequence of the previous theorem (7). The extension of the first step to the multidimensional case is straightforward on the basis of the Lee-Yang condition, but the extension of the second one seems difficult in view of problems with boundary conditions.

[15]The quantities

$$|\Lambda|^{-1}\sum_{x,y\in\Lambda}\sigma_{\Lambda'}(x,y)\,,\quad |\Lambda|^{-1}\sum_{\substack{x\in\Lambda_1\\ y\in\Lambda_2}}\sigma^T_{\Lambda'}(x,y)$$

and

$$\sum_{x\in\Lambda''}\sigma_{\Lambda'}(0,x)$$

are directly related, by elementary calculations, to derivatives of $\ln Q_{\Lambda'}$ with respect to additional magnetic fields at the points of Λ, of Λ_1 and Λ_2, and of Λ'' and the origin, respectively. They can thus be bounded independently of Λ, Λ', or Λ_1, Λ_2, Λ', or Λ'', Λ'. The arguments are similar to those used in the proof of the theorem and are in fact more simple. We thus omit them. For ferromagnets, $\sigma^T(x,y)$ is known to be always positive. Hence, χ is well defined, as the limit of an increasing bounded sequence. The fact that $\lim_{|\Lambda|\to\infty}\chi_\Lambda=\chi$ is obtained easily by writing, for instance, $\chi=|\Lambda|^{-1}\sum_{x\in\Lambda}\sum_{y\in Z^d}\sigma^T(x,y)$ and by dividing Λ into a part $\Lambda^{(1)}$, whose distance to the boundary of Λ tends to infinity in the $|\Lambda|\to\infty$ limit and chosen such that $|\Lambda^{(1)}|/|\Lambda|\to 1$, and its complement. The proof of (4) is obtained similarly by considering an analogous decomposition of Λ_1, or Λ_2. (These arguments can be extended to nonferromagnetic systems by using known absolute convergence properties of σ^T_Λ, at large magnetic field, together with analyticity properties with respect to the magnetic field and Vitali's theorem.) Finally, χ is known to be strictly positive for ferromagnets since $\sigma^T(x,y)$ is always positive and since $\sigma^T(0,0)=1-[\sigma(0)]^2$ is strictly positive.

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