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Convergence of the Variational Cumulant Expansion*

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Abstract *In this article we discuss the convergence of the variational cumulant expansion (VCE) in the Ising model and lattice ϕ^4 model. We find that in critical region VCE results do not converge so quickly as elsewhere and the analyticity of thermo-dynamical functions and the strong correlation in the critical region are responsible for this fact.*

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The variational cumulant expansion (VCE), as an analytic method in the study of the phase transitions, has been used to a number of models in statistical physics and lattice field theory. Some significant results[1] have been obtained using this method.

Because there is no rigorous proof of the convergence of cumulant expansion, the use of this method must be careful. It is known that the phase transitions have very close relation to the non-analytic properties of thermo-dynamical functions of statistical systems. On the other hand, physical systems have large correlation lengths and fluctuate intensively in the critical region. These facts may have an direct effect on the convergence properties of VCE series near the critical point. Lee and Yang[2] have given rigorous discussions on the connection between the zeros of partition function and the existence of phase transition for Ising model. In this article we will study convergence of VCE in Ising model using the existed rigorous results. We will also try to give some qualitative discussion on lattice ϕ^4 case.

VCE has been developed on the basis of the variational method in statistical physics. For a physical system with the action $S(\beta, s)$, where β stands for physical parameters and s is configuration variable, the partition function of the system can be written as

$$Z = \mathrm{e}^{-NF} = \int [\mathrm{d}s]\, \mathrm{e}^{S(s,\beta)}, \tag{1}$$

where N and F are the volume and free energy of the system respectively. The think of variational method is that one can introduce a trial action $S_0(J, s)$ where J is a variational parameter, then equation (1) is modified as

$$Z = \int [\mathrm{d}s]\, \mathrm{e}^{S_0}\, \mathrm{e}^{S-S_0} = Z_0 \langle \mathrm{e}^{S-S_0} \rangle_0 , \tag{2}$$

where

$$Z_0 = \int [\mathrm{d}s]\, \mathrm{e}^{S_0} , \tag{3}$$

$$\langle \cdots \rangle_0 = \frac{1}{Z_0} \int [\mathrm{d}s]\, \mathrm{e}^{S_0} (\cdots) , \tag{4}$$

S_0 must be chosen properly so that equations (3) and (4) can be integrated analytically. From Eqs (1) $\sim$ (4), the free energy can be expressed as

$$F = -\frac{1}{N} \ln Z = -\frac{1}{N} \ln Z_0 - \frac{1}{N} \sum_{n=1}^{\infty} W_n , \tag{5}$$

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where

$$W_n = \langle (S-S_0)^n \rangle_c\,, \quad \langle S-S_0\rangle_c = \langle S-S_0\rangle_0\,, \quad \langle (S-S_0)^2\rangle_c = \langle (S-S_0)^2\rangle_0 - \langle S-S_0\rangle_0^2\,,$$

$$\langle (S-S_0)^3\rangle_c = \langle (S-S_0)^3\rangle_0 - 3\langle (S-S_0)^2\rangle_0 \langle (S-S_0)\rangle_0 + 2\langle S-S_0\rangle_0^3\,.$$

$$\ldots$$

These are the results of cumulant expansion. The variational parameters can be determined by main-value method, full variational method or accumulated point method.[3]

Two-dimensional Ising model is one of the statistical systems which can be rigorously solved. So it can be used to check the efficiency of VCE. The action of Ising ferromagnetic model is expressed as

$$S = K \sum_{\langle ij\rangle} s_i s_j + \beta H \sum_i s_i\,, \tag{6}$$

where $K = \beta J_0$, $J_0 > 0$, H is external magnetic field. In the case of $H = 0$, we introduce a trial action

$$S_0 = J \sum_i s_i\,. \tag{7}$$

We note that at present,

$$\langle (S-S_0)^n\rangle_c = \sum_{m=0}^{n} \frac{n!}{m!(n-m)!} (-J)^m \frac{\partial^m}{\partial J^m} \langle S^{n-m}\rangle_c \tag{8}$$

where $\langle S^0\rangle_c = \ln Z_0$, from Eq. (5), the nth order cumulant expansion series is

$$F_n = -\frac{1}{N}\Big[\sum_{m=0}^{n} \langle S^m\rangle_c + (-J)\frac{\partial}{\partial J}\sum_{m=0}^{n-1}\langle S^m\rangle_c +$$

$$\frac{1}{2}(-J)^2 \frac{\partial^2}{\partial J^2}\sum_{m=0}^{n-2}\langle S^m\rangle_c + \cdots + \frac{1}{n!}(-J)^n \frac{\partial^n}{\partial J^n}\ln Z_0\Big]. \tag{9}$$

Studying Eq. (9), one can find the first term $I_n(J,\beta,H) = \sum_{m=0}^{n}\langle S^m\rangle_c$ is actually the high-temperature moment expansion of the free F at external field $H + J/\beta$.

From Lee-Yang's theorem, the free energy $F(\beta,H) = \lim_{N\to\infty}(1/N)\ln Z_N(\beta,H)$ is non-analytic when $\beta > \beta_c$ and $H = 0$, but analytical elsewhere.[4] Taking this into consideration, we study what equation (9) tells us. When $H = 0$,

$$F(\beta,0) = \lim_{H\to 0} F(\beta,H) = \lim_{H\to 0}\lim_{N\to\infty}(1/N)\ln Z_N(\beta,H) = \lim_{H\to 0}\lim_{n\to\infty} F_n(\beta,J,H)\,. \tag{10}$$

i) When $0 < \beta < \beta_c$, $F(\beta,0)$ is analytic. $I_n(J,\beta,H)$ converges uniformly to $F(\beta, H + J/\beta)$, which is analytic too. Assuming that $F_n(\beta,H,J)$ converges uniformly to $F(\beta,H)$ in the full region of J, we get

$$F(\beta,0) = \lim_{H\to\infty}\lim_{n\to\infty} F_n(\beta,H,J) = \lim_{n\to\infty} F_n(\beta,0,J) \tag{11}$$

and we can differentiate $F(\beta,0)$ versus J by the approximation of termwise differentiation of F_n.

ii) When $\beta > \beta_c$, $H = 0$ is the non-analytic point of $F(\beta,0)$, but each term of the right-hand side of Eq. (9) is analytic at $J \neq 0$. There exist two possibilities: a) $F_n(\beta,0,J)$ converges to $F(\beta,0)$ but not uniformly; b) $F_n(\beta,0,J)$ does not converge to $F(\beta,0)$ but something else at some regions of J. Both of these cases restrict the $F_n(\beta,H,J)$ from exchanging the operations of limitation and termwisely differentiation $F_n(\beta,0,J)$ to get $\partial F(\beta,0)/\partial J$. The above facts have direct effects on the determination of variational parameters.

The main-value method, which was derived from the Jensen's inequality, means $\partial F_1/\partial J = 0$, $\partial^2 F_1/\partial J^2 > 0$. The results of this method are in good agreement with rigorous results at high-temperature region and low-temperature region. But the flaw of this method is that it causes a spurious first-order transition at $\beta = 1/2d$ at high-order expansions.[1]

The full variational method, which was generalized by the main-value method, asks for $\partial F_n/\partial J = 0$, $\partial^2 F_n/\partial J^2 > 0$. We used this method to calculate energy E and found that when $\beta < \beta_c^n < \beta_c$, E converges to rigorous result quickly even in the region $1/2d < \beta < \beta_c^n$ where the main-value method cannot work properly, whereas when $\beta > \beta_c$ the curve descends quickly and is not bounded from below. This implies that the full variational method breaks down below the critical temperature.

These facts can be interpreted by the above items i) and ii): When $\beta < \beta_c$, the approximation of $0 = \partial F/\partial J \approx \partial F_n/\partial J$ is right and the parameters meet our need, while when $\beta > \beta_c$, $0 = \partial F/\partial J \neq \partial F_n/\partial J$ and the parameters thus obtained are not the expected ones. One should combine the full variational method with the main-value method to get better results.

Table 1. Critical Temperature of Ising Model.

Order	1	2	3	4	5	Rigorous
β_c^n	0.250	0.333	0.347	0.377	0.384	0.44

We listed the critical temperature in Table 1 and plotted the energy curve in Fig. 1. It was shown that away from the critical region the VCE results are in good agreement with rigorous ones, while in the critical region the VCE results converge to rigorous results order by order but a bit more slowly. This fact may be the result of the strong correlation property of the system in the critical region. The nth-order VCE only takes the correlation of spins in blocks with volume $O(n^d)$ of the system into consideration. When $\beta \gg \beta_c$ and $\beta \ll \beta_c$ the correlation function decays exponentially, but when $\beta \to \beta_c$, the correlation length $L \to \infty$ and $G(r) \to 1/r^{1/4}$ decays much more slowly and results in a larger error of VCE in this region.

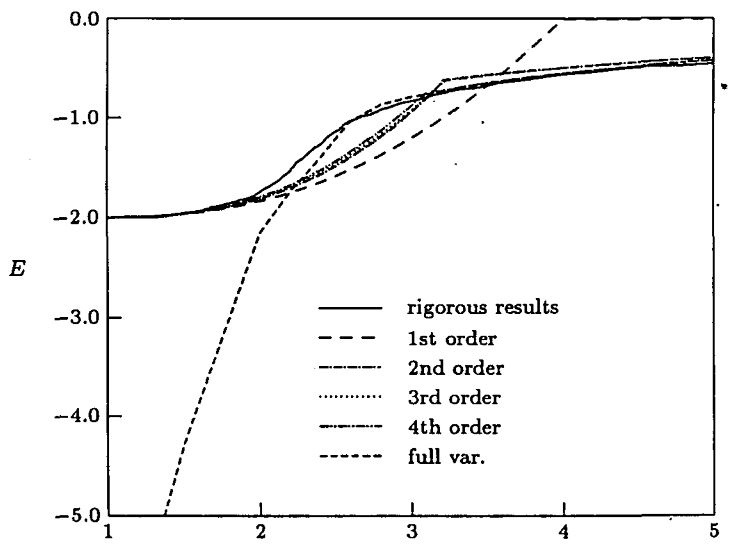

Fig. 1. The internal energy of Ising model.

Now we study 4-d lattice ϕ^4 model. On the super-cubic spacetime lattice with spacing a, the action can be written as[1]

$$S = \sum_{(ij)} \phi_i \phi_j + m_L^2 \sum_i \phi_i^2 - \lambda_L \sum_i \phi_i^4 , \tag{12}$$

where $m_L^2 = d + m_0^2 a^2/2$, $\lambda_L = \lambda_0 a^4/4$. We introduce the trial action

$$S_0 = J \sum_i \phi_i + m_L^2 \sum_i \phi_i^2 - \lambda_L \sum_i \phi_i^4 \tag{13}$$

where J is the variational parameter. Applying VCE to this model and using the full variational method to determine J we find that in the full region of m_L^2 the expansion series take out good convergent behaviors although the transition from symmetry phase to Higgs phase exists at $m_L^2 = m_{Lc}^{(n)2}$ and the results are in good agreement with those of MC[5] (see Table 2).

In fact the lattice ϕ^4 model is equivalent to the S^4 model in statistical physics. We know that in four-dimensional case S^4 model has only one critical point, namely the Gaussian fixed point, where $\lambda_{Lc} = 0$. In other words, the free energy of the system is non-analytical only at this point and analytical elsewhere. In the process of our calculation of VCE, we always deal with the case of $\lambda_L \neq 0$, the difficulty we encountered in the Ising case was out of sight. From Table 2 one can find that the VCE results converge to MC results much more quickly than those of the Ising case. The reason to this may be that for 4-d ϕ^4 theory the critical exponent $\eta = 0$, $G(r) \sim 1/r^2$ at critical point, which decays more quickly than that of Ising model and the limited-order effects was much weaker.

Table 2. The critical point (m_{Lc}^2) of lattice ϕ^4 theory.

λ_L	0.054	0.172	0.443	1.748	3.509	6.036	17.439	30.372	56.733
m_{Lc}^2 (4-th VCE)	3.954	3.854	3.635	2.701	1.606	0.206	−5.037	−10.08	−19.16
m_{Lc}^2 (MC)	3.950	3.843	3.612	2.641	1.580	0.102	−5.210	−10.31	−19.52

We have discussed the convergence of VCE in Ising case and lattice ϕ^4 case respectively in critical region. We found that the convergence properties of VCE have a close relationship to the analyticity of thermodynamical functions, so one must be careful to determine the variational parameters in different temperature regions. On the other hand the order by order corrections of VCE correspond to taking more and more short-range correlation into consideration and some facts show that the asymptotical behavior of the correlation function may have direct effects on the speed of convergence of VCE.

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