Comment on "Variational approximations for renormalization-group transformations"

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The variational method proposed by Kadanoff *et al.* is very useful for solving various statistical models. However, there are two major difficulties. Its numerical procedure is tedious and time consuming, and the authors considered that there exists an "internal contradiction." We have resolved both of them by developing a new variational procedure, and examining the physical meaning of the variational parameters.

Kadanoff and co-workers[1,2] proposed a variational method for the renormalization-group transformation. The numerical results are unexpectedly accurate for the two-dimensional Ising model. They computed the free energies both at the fixed point and away from it. This method could be a very powerful statistical technique. Unfortunately, the numerical search in the variational procedure is very involved and the method is then seriously limited. Besides, they also pointed out an "internal contradiction" in this method.

Let us begin with a brief review of their approach. First, they built transformations of an Ising system with spin variable σ to another Ising system with spin variable μ and a lattice constant twice as large. The free energy is unchanged under the transformation. The transformation can be generated by the generating function $T(\sigma, \mu, P)$, where P is assigned to label different transformations. Usually, the new Hamiltonian $H'(\mu)$ transformed from $H(\sigma)$ by $T(\sigma, \mu, P)$ will be in a very complicated form even if $H(\sigma)$ is in a very simple form. Hence Kadanoff *et al.* made an approximation to obtain $H'(\mu)$ in the same simple form at the price that the free energy calculated from

$H'(\mu)$ become somewhat lower than that from $H(\sigma)$ instead of exactly equal. Naturally, the difference in free energy will depend on which transformation $T(\sigma, \mu, P)$ is performed. Among all transformations $T(\sigma, \mu, P)$ there will be one $T(\sigma, \mu, P)$ such that the deviation is the smallest.

The above scheme obviously can be formulated by a variational method. However, the free energy for an arbitrary Hamiltonian is often not easy to obtain. In fact, if the free energy is known, the whole statistical problem has been all solved already. Instead, Kadanoff *et al.* wrote down a lower-bound free-energy formula for a known Hamiltonian. The free energy formula for a known Hamiltonian. The free energy calculated from this formula will be very close to the real one for a Hamiltonian that has been transformed several times from the original Hamiltonian. Thus the variational method can be performed as follows: let n be the number of transformations after which Kadanoff's free-energy formula is close enough to the exact one. A series of parameters $P_1, P_2,$ $\ldots, P_n$ denotes a series of transformations performed successively on $H^{(i)}(\mu)$ to generate $H'^{(i+1)}(\mu)$, i.e.,

$$H(\sigma) \to H^{(1)}(\mu_1) \xrightarrow{T(\mu_1, \mu_2, P_1)} H^{(2)}(\mu_2) \xrightarrow{T(\mu_2, \mu_3, P_2)} H^{(3)}(\mu_3) \cdots \xrightarrow{T(\mu_{n-1}, \mu_n, P_{n-1})} H^{(n)}(\mu_n).$$

Since the free energy for $H^{(n)}(\mu_n)$ can be determined accurately, one can then assign a free energy to a series of P's. Since every transformation makes the free energy decrease despite the impossibility of calculating it at each stage, the free energy estimated from $H^{(n)}(\mu_n)$ is also a lower bound of the exact free energy of $H(\sigma)$. The variational work can then be done by numerical search for a series $P_1, \ldots, P_n$ that maximize the free energy of $H^{(n)}(\mu_n)$.

The procedure is all right except that the numerical search is a very hard task. It corresponds to maximizing a function with n parameters numerically. If the function is a bit more complicated and n is a bit larger than those in Ref. 2, the whole work will become formidable. Hence a simple way to determine the optimal P's is desperately needed.

Since the exact (although uncalculable) free energy decreases each time we make a renormalization-group transformation, the optimal P can be determined at every individual transformation stage in principle. The difficulty is then the correct estimation of the free energy at the state which Kadanoff's lower-bound formula is not accurate enough to judge which P is better. The essence of our approach is as follows: in determining P, the actual free energy is not necessary, only the variation of free energy with respect to P is needed. We now show how to estimate the variation of free energy correctly.

Let us begin with the equation

$$F = -\ln Z = -\ln \sum_{\{\mu\}} e^{-H'(\mu)} . \tag{1}$$

A variation of P results in different $H'(\mu)$, and what we want to know is the free-energy difference of different $H'(\mu)$'s. Hence the interesting quantity is

$$\Delta F = F(H' + \Delta H) - F(H') . \tag{2}$$

Up to first order in ΔH,

$$\Delta F \simeq \sum_{\{\mu\}} \Delta H e^{-H'} \Big/ \sum_{\{\mu\}} e^{-H'} . \tag{3}$$

To calculate ΔF exactly would involve solving the model even though the interactions are within the unit cell. But since the purpose of this calculation is to judge the optimal P, we can take a reasonable estimation. It seems natural to approximate the probabilities of various configurations by their Boltzmann factors within the unit cell. The optimal P turns out to be insensitive to this approximation. We have tried the equally probable configurations and found little difference.

The whole program then becomes the following: a transformation denoted by $T(\mu_1, \mu_2, P_1)$ with a parameter P_1 transform a system with interaction $v^{(1)}(\mu_1)$ in a unit cell to a system with interaction $v^{(2)}(\mu_2, P_1)$ in a larger unit cell. A small variation in P_1 will result a difference in $v^{(2)}$ by

$$\Delta v^{(2)} = v^{(2)}(\mu_2, P_1 + \Delta P) - v^{(2)}(\mu_2, P_1)$$

$$= \frac{\partial v(2)(\mu_2, P_1)}{\partial P_1} \Delta P \Delta v^{(2)}$$

is configuration dependent and the free energy variation is then

$$F[v^{(2)}(\mu_2, P_1 + \Delta P_1)] - F[v^{(2)}(\mu_2, P_1)]$$

$$\propto \sum_{\{\mu\}} \frac{\partial v^{(2)}(\mu_2, P_1)}{\partial P_1}$$

$$\times \left(e^{-v^{(2)}(\mu_2, P_1)} \Big/ \sum_{\{\mu\}} e^{-v^{(2)}} \right) \Delta P_1 , \tag{4}$$

where $\sum_{\{\mu\}}$ denotes the sum of all possible congurations for a unit cell. Hence the optimal P_1 is determined by requiring

$$\sum_{\{\mu\}} \frac{\partial v^{(2)}(\mu_2, P_1)}{\partial P_1} e^{-v^{(2)}(\mu_2, P_1)} = 0 . \tag{5}$$

It is now a matter of solving this equation for P_1, which is done very easily numerically.

In order to show the effectiveness of our approach, we calculated the $K_{nn} = 0.4$ and $K_{nn} = 0.5$ cases for the two-dimensional Ising model. The reason we take these two K_{nn}'s is to compare our numerical values to Kadanoff's results. Tables I(a) and II(a) list the numerical values of our optimal p's and free energy. We also list Kadanoff's results in Tables I(b) and II(b) for comparison. They are almost identical. However, for the case $K_{nn} = 0.5$ the optimal p's have a noticeable discrepancy for larger iteration stages although the final free energies are the same. This is because the final value of free energy is not very sensitive to K_2 and K_4 as a result of the 4^n factor in Kanadoff's free-energy equation when n is large. We can also see that the variation of P, K_2, and K_4 are smoother in our calculation. We do believe that our p's are more reasonable physically. The reason that Kadanoff's calculation shows some abnormal variation in P, K_2 and K_4 is probably their numerical difficulty. The final free energy changes very little with respect to a variation of P at stages with larger n.

It is not surprising that Kadanoff's free energies are identical to our's since they exhausted all possible series of p's. If there is no numerical error limitation they should get the best result. However, we do show that our determination of P is very accurate. The major practical difference between our approach and that of Kadanoff *et al*.

TABLE I. Results of our method and Kadanoff's method for $K_{nn} = 0.4$.[a]

Iteration number	Parameter value p	Coupling constants	
		V_2	V_4
(a) Our results			
0	0.655	0.1180	-0.0270
1	0.557	0.0947	-0.0096
2	0.408	0.0603	-0.0018
3	0.222	0.0218	-8.5×10^{-5}
4	0.068	0.0022	-5.0×10^{-6}
5	0.004	2.08×10^{-5}	-1.3×10^{-8}
(b) Kadanoff's results			
0	0.655	0.118	-0.027
1	0.557	0.094	-0.010
2	0.408	0.060	-0.002
3	0.221	0.022	-8.7×10^{-5}
4	0.067	0.002	-7.7×10^{-8}
5	0.033	2.07×10^{-5}	1.4×10^{-9}

[a] Final free energy: -0.88393.

TABLE II. Results of our method and Kadanoff's method for $K_{nn} = 0.5$.[a]

Iteration number	Parameter value p	Coupling constants	
		V_2	V_4
(a) Our results			
0	0.860	0.165	-0.0510
1	0.942	0.181	-0.0375
2	1.127	0.218	-0.0380
3	1.536	0.298	-0.0550
4	2.392	0.457	-0.0732
5	3.810	0.708	-0.0790
6	5.465	1.015	+0.7210
7	7.821	1.414	+1.2240
(b) Kadanoff's results			
0	0.871	0.165	-0.051
1	0.967	0.181	-0.036
2	1.179	0.216	-0.029
3	1.610	0.287	-0.014
4	2.252	0.401	+0.107
5	2.465	0.561	+0.451
6	2,466	1.034	-0.638
7	2.437	1.146	-0.973

[a] Final free energy: -1.0268.

is in computing time. For example, if it needs 10 P's, then for n stages calculation they would need 10^n free-energy calculations to find the optimal series of p's. On the other hand, we would need $n \times 10$ calculations only. Our procedure of variation is so simple that a usual calculator will do the job. Hence our procedure can be a very powerful technique to solve various models.

We now turn to the problem of the internal contradiction mentioned in Ref. 1. In our opinion, the fact that P varies with stages of transformation is not only plausible but also necessary. Let us take a simplified version of the renormalization transformation to examine this situation. Let K denote the strength of the interaction. K^* is defined as the strength at the fixed point. If K is transformed to $K'(K)$ then $\epsilon \equiv K - K^*$ transforms to $\epsilon' \equiv K' - K^*$. Near the fixed point ϵ and ϵ' are very small and $\epsilon' \approx C\epsilon$. Here $C = (\partial K'/\partial K)_{K=K^*}$, which depends on K^* and the particular transformation only. The critical behavior then depends on the constant C. What we want to point out here is that no matter how close the temperature is to the critical temperature, the strength ϵ' will become large after enough times of transformation. Since $|C| > 1$ there will be some n such that C^n is quite large. At that stage, K should be quite different from K^*, and the transformation operator $C = \partial K'/\partial K_{K=K^*}$ is no longer the correct one to transform ϵ. However, this deviation has nothing to do with the critical exponents.

In the present method, C is determined by the fixed point interactions K_2^* and K_4^* and the parameter P^*. The departure of parameter P from P^* shows the deviation of transformation from C. This deviation leads to the limitation of the range of critical temperature but not the critical behavior. It is then not surprising that critical exponents are determined by $P = P^*$ only, and p's are varied stage by stage in obtaining free energies. A detailed examination of the relation of the deviation from fixed point transformation to the limitations on critical behavior will be discussed elsewhere.[3]

In conclusion, a consistent and efficient procedure to calculate the free energy of a spin system has been presented here. The method is demonstrated for the two-dimensional Ising system. The formulation is quite general and the applications to other unsolved spin systems would be straightforward.

[1]L. P. Kadanoff, A. Houghton, and M. C. Yalahik, J. Stat. Phys. **14**, 171 (1976).

[2]L. P. Kadanoff, Phys. Rev. Lett. **34**, 1005 (1975).

[3]Yu Ming Shih, Dong Chuang Jou, C. K. Pan, W. S. Lee, Wen Den Chen, H. M. Huang, Chin-Kun Hu, Kuo Gen Chen, and Hsein Che Tseng (unpublished).