On free energy of three–dimensional Ising model at criticality

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Higher–order vertices at zero external momenta for the scalar field theory, describing the critical behaviour of the Ising model, are studied within the field–theoretical renormalization group (RG) approach in three dimensions. Dimensionless six–point $g_6$ and eight–point $g_8$ effective coupling constants are calculated in the three–loop approximation. Their numerical values, universal at criticality, are estimated by means of the Pade and Pade–Borel summation of the RG expansions found and by putting the renormalized quartic coupling constant equal to its universal fixed–point value known from six–loop RG calculations. The values of $g_6^*$ obtained are compared with their analogs resulting from the $\epsilon$–expansion, Monte Carlo simulations, the Wegner–Houghton equations and the linked cluster expansion series. The field–theoretical estimates for $g_6^*$ are shown to be in a good agreement with each other, differing considerably from the values given by other methods.
I. INTRODUCTION

The critical thermodynamics of the three-dimensional Ising model is known to be described by Euclidean scalar field theory with the Hamiltonian

\[ H = \int d^3x \left[ \frac{1}{2} (m_0^2 \phi^2 + (\nabla \phi)^2) + \frac{\lambda}{4!} \phi^4 \right], \tag{1} \]

where a bare mass squared \( m_0^2 \) is proportional to \( T - T_c^{(0)} \), \( T_c^{(0)} \) being the phase transition temperature in the absence of the order parameter fluctuations. Taking fluctuations into account leads to renormalization of the mass \( m_0^2 \rightarrow m^2 \), the field \( \phi \rightarrow \phi_R \), and the coupling constant \( \lambda \rightarrow mg_4 \), and also to the appearance of terms of the form \( m^3-n^2_0 \phi_R^2 \) with \( n > 2 \) in the effective action (free energy) of the system. In the critical region, where fluctuations are so strong that they completely screen out the initial (bare) interaction, the behaviour of the system becomes universal and the dimensionless vertices \( g_{2n} \) tend toward their asymptotic limits, i.e. they assume constant values which are also universal.

In this paper, we calculate numerical values of \( g_6 \) and \( g_8 \) at criticality using the field-theoretical renormalization group (RG) approach in three dimensions. Higher-order coupling constants mentioned related to corresponding vertices at zero external momenta will be found as power series in the renormalized dimensionless quartic coupling constant \( g_4 \) up to three-loop order, and the RG series will be resummed by means of the Padé and Padé–Borel techniques. Then \( g_4 \) in resummed RG expansions will be put equal to its universal value \( g_4^* \) known from the canonical six-loop RG calculations resulting in numerical estimates for \( g_6^* \) and \( g_8^* \). The numbers obtained for \( g_6^* \) will be compared with those resulting from the \( \epsilon \)-expansion for \( g_6/g_4^2 \) as well as with the values given by Monte Carlo simulations, by the approximate solution of the Wegner–Houghton equations and by the analysis of the linked cluster expansions.
II. RG EXPANSIONS FOR SEXTIC AND OCTIC EFFECTIVE INTERACTIONS

Since higher–order bare coupling constants are known to be irrelevant at criticality in the RG sense, renormalized perturbative expansions for $g_6$, $g_8$, etc. may be obtained from conventional Feynman–graph expansions of these quantities in terms of the only bare coupling constant – $\lambda$. In its turn, $\lambda$ may be expressed perturbatively as a function of the renormalized dimensionless quartic coupling constant $g_4$. Substituting corresponding power series for $\lambda$ into original Feynman–graph expansions for $g_6$ and $g_8$, we can obtain the RG series for these higher–order effective coupling constants.

Recently, one of the authors has found the sextic coupling constant $g_6$ in the two–loop RG approximation [1]. Thus, what we are interesting in is the three–loop contribution to this quantity. As may be shown, there are 16 graphs contributing to $g_6$ in the three–loop order. In fact, their calculation is neither cumbersome nor lengthy since corresponding contribution may be written down as a sum of a few terms having a form of mass derivatives of some two–point and four–point graphs. So, within the three–loop approximation we get

$$g_6 = \frac{9}{\pi} \left( \frac{g_0 Z^2}{m} \right)^3 \left[ 1 - \frac{33}{2\pi} \frac{g_0 Z^2}{m} + 20.53966666 \left( \frac{g_0 Z^2}{m} \right)^2 \right],$$

where $g_0 = \lambda/4!$ and $Z$ relates the dressed Green function $G$ to the renormalized one $G_R$ in a conventional way:

$$G = Z G_R = \frac{Z}{m^2 + q^2 - \Sigma_R} = \frac{Z}{m^2 + q^2 + O(g_4^3)}.$$

The renormalized perturbative expansion for bare coupling constant $g_0$ may be obtained using the normalizing condition

$$g_0 = m g_4 \frac{Z_4}{Z^2}$$

and the RG expansion for $Z_4$ which has been calculated by many people:

$$Z_4 = 1 + \frac{9}{2\pi} g_4 + \frac{63}{4\pi^2} g_4^2 + O(g_4^3).$$

Combining Eqs. 2, 4 and 5 we obtain
\[ g_6 = \frac{9}{\pi} g_4^3 \left( 1 - \frac{3}{\pi} g_4 + 1.389962952 g_4^2 \right). \]  

(6)

The RG expansion for the eight–point effective coupling constant \( g_8 \) may be found in an analogous way although it requires more job than in the case of \( g_6 \). Two–loop and three–loop contributions to \( g_8 \) are given by 5 and 36 Feynman graphs respectively. Use of the trick mentioned above, however, considerably simplifies their calculation. The result is as follows

\[ g_8 = -\frac{81}{2\pi} \left( \frac{g_0 Z^2}{m} \right)^4 \left[ 1 - \frac{173}{6\pi} \frac{g_0 Z^2}{m} + 54.81336082 \left( \frac{g_0 Z^2}{m} \right)^2 \right]. \]  

(7)

Expressing \( g_0 \) in terms of \( g_4 \) leads to the RG series for \( g_8 \):

\[ g_8 = -\frac{81}{2\pi} g_4^4 \left( 1 - \frac{65}{6\pi} g_4 + 7.775001310 g_4^2 \right). \]  

(8)

With the RG expansions Eqs. 6, 8 in hand, we can get numerical estimates for universal critical values of \( g_6 \) and \( g_8 \).

### III. RESUMMATION AND NUMERICAL ESTIMATES

Perturbative expansions in a field theory are known to be divergent, at best asymptotic. Moreover, the theory under consideration has no small parameter. That is why direct substitution of the fixed point value \( g_4^* \) to Eqs. 6, 8 can not lead to satisfactory results. These expansions, however, contain important information which may be extracted provided some procedure making them convergent is applied. Here Pade and Pade–Borel methods will play roles of such procedures, i.e. we shall construct Pade approximants \([L/M]\) for the functions given by the series Eqs. 6, 8 as well as for their Borel transforms which are related to the functions to be found (”sum of series”) by the formula

\[ f(x) = \sum_{k=0}^{\infty} c_k x^k = \int_0^{\infty} e^{-t} F(xt) dt, \]  

(9)

\[ F(y) = \sum_{k=0}^{\infty} \frac{c_k}{k!} y^k, \]  

(10)
and then evaluate the integral Eq. 9 where series Eq. 10 possessing nonzero radii of convergence are replaced by corresponding Pade approximants.

Starting from the three–loop expansions available, it is possible to construct Pade approximants of the only reasonable type: [1/1]. On the other hand, one can try several different ways of resummation. Indeed, the Pade–Borel procedure may be applied not only to the series for \( g_6 \) and \( g_8 \) themselves but also to corresponding RG expansions for the ratios \( g_6/g_4^2 \) and \( g_8/g_4^3 \).

Let’s construct first the Pade approximant for the six–point effective coupling constant. From Eq. 6 we readily obtain:

\[
g_6 = \frac{9}{\pi} \frac{g_4^3 (1 + 0.500636g_4^4)}{1 + 1.455566g_4^4}.
\]  

(11)

Substituting into this expression the most accurate numerical estimate \( g_4^* = 0.988 \) for the fixed point value known from six–loop RG calculations in three dimensions [2,3] we find for the universal value of \( g_6^* \):

\[
g_6^* = 1.694.
\]  

(12)

Apply then more sophisticated, Pade–Borel procedure to the series Eq. 6 which is expected to lead to more accurate estimate for \( g_6^* \). After simple algebra we obtain

\[
g_6 = \frac{0.477465g_4^3}{\pi} \int_0^\infty \frac{1 + 0.052382g_4 t^2 e^{-t}}{1 + 0.291114g_4 t^3 e^{-t}} dt.
\]  

(13)

Computation of this integral for \( g_4 = 0.988 \) gives

\[
g_6^* = 1.621.
\]  

(14)

The third way to get numerical estimate for \( g_6^* \) we use here is to construct the Pade–Borel approximant for \( g_6/g_4^2 \) and to estimate the universal value of this ratio at criticality. The corresponding expression is as follows:

\[
\frac{g_6}{g_4^2} = \frac{2.86479g_4}{\pi} \int_0^\infty \frac{1 + 0.0077234g_4 t^2 e^{-t}}{1 + 0.48519g_4 t} dt.
\]  

(15)
For the fixed point value of $g_4$ this formula leads to:

$$g_6^* = 1.577.$$  \hspace{1cm} (16)

To obtain numerical estimates for $g_8^*$ the same procedures are applied to the series Eq. 8. They give

$$g_8^* = 0.68 \quad \text{(Pade)},$$

$$g_8^* = 1.71 \quad \text{(Pade – Borel)},$$

$$g_8^* = 2.71 \quad \text{(Pade – Borel for $g_8/g_4^3$)}.$$ \hspace{1cm} (17)

IV. DISCUSSION

Although the RG expansions found in Sec.2 are, in fact, rather short, numerical estimates for $g_6$ obtained from Eq. 6 by several resummation techniques are seen to be close to each other. That is why we believe that the numbers (12) and, in particular, (14) and (16) are also close to the exact value of $g_6^*$. Moreover, taking into account of the three–loop RG contribution to $g_6^*$ turns out to change corresponding estimate by less than 10 per cent (Pade–Borel resummation of the two–loop RG expansion have lead to $g_6^* = 1.50 \text{ [1]}$) what may be considered as an extra argument in favour of fair numerical accuracy of the results presented above.

Let’s compare our estimates for $g_6^*$ with their counterparts obtained by different methods. The solution of the Wegner–Houghton equations within the local potential approximation presented by C.Bagnuls and C.Bervillier has yielded $(g_6/g_4^2) = 3.59$, $g_6 = 2.40$ at the non–trivial fixed point \text{[3]}. Determining by Monte Carlo simulations probability distributions for averaged magnetization of the 3D Ising model in an external magnetic field, M.M. Tsypin has found from his data that $g_6^* = 2.05 \text{ [4]}$. The analysis of the linked cluster expansion series performed by T.Reisz has lead to $g_6^* = 1.92 \text{ [6]}$. 
All these estimates are seen to be significantly larger than ours obtained by means of perturbative RG calculations for the field–theoretical model. In such a situation, it is interesting to evaluate $g_{6}^{*}$ using some alternative field–theoretical perturbative approach. The $\epsilon$–expansion for the ratio $g_{6}/g_{4}^{2}$ which results from the equation of state may be used for this purpose. Up to the $\epsilon^3$ order, it is as follows [7]:

$$\frac{g_{6}}{g_{4}^{2}} = 2\epsilon - \frac{20}{27}\epsilon^2 + 1.2759\epsilon^3.$$  

(18)

Resumming this expansion by Pade and Pade–Borel methods we find for $\epsilon = 1$ and $g_{4} = 0.988$:

$$g_{6}^{*} = 1.687 \quad \text{(Pade)},$$

$$g_{6}^{*} = 1.653 \quad \text{(Pade – Borel)}.$$  

(19)

The Pade–Borel estimate for $g_{6}^{*}$ thus obtained is remarkably close to those given by RG calculations in three dimensions (Eqs. 14 and 16). So, the field–theoretical RG approach in three and $(4 - \epsilon)$ dimensions provides, within the three–loop approximation, the values of $g_{6}^{*}$ which agree well to each other but differ considerably from the Monte Carlo and some other estimates mentioned above.

Let’s discuss further the predictions concerning the eight–point effective coupling constant. The estimates following from the three–loop RG expansions in 3D are clearly seen to be strongly scattered being therefore numerically unreliable. It is not surprising since coefficients in the RG expansion for $g_{8}$ grow much faster than those in the RG series for $g_{6}$ making the former series less suitable for resummation than the latter. Correspondingly, much less reliable numerical estimates for $g_{8}$ at the critical point are obtained. On the other hand, all three numbers Eqs. 17 are i) positive, i.e. have a sign opposite to that of the lowest–order (one–loop) RG estimate $g_{8}^{*} = -12.28$, and ii) much smaller than the absolute value of this one–loop estimate. It means that higher–order RG contributions to $g_{8}$ being extremely important tend to strongly diminish its universal value at the critical point with respect to the number given by the lowest–order RG approximation. This conclusion seems
to be in accord with the fact that the recent analysis of relevant Monte Carlo data failed to reveal some appreciable (non–zero) value of $g^*_8$.

V. CONCLUSION

In the paper, the RG series for coefficients before $M^6$ and $M^8$ in the expansion of the free energy of the three–dimensional Ising model in powers of the order parameter $M$ have been calculated in the three–loop approximation. Numerical estimates for universal values of $g_6$ and $g_8$ at the critical point have been found by Pade and Pade–Borel resummations of the series obtained and by putting the quartic coupling constant equal to its fixed point value 0.988. Pade–Borel procedure applied to the expansions for $g_6$ and $g_6/g_4^2$ has given $g^*_6 = 1.621$ and $g^*_6 = 1.577$, respectively, while analogous treatment of the $\epsilon$–expansion for $g_6/g_4^2$ has been shown to result in $g^*_6 = 1.653$. Being in a good agreement to each other, these field–theoretical estimates are considerably smaller than those obtained by other methods. The RG expansion for $g_8$ has turned out to be less suitable for resummation than that for $g_6$ since it possesses rapidly growing coefficients. As a result, strongly scattered numerical estimates for $g^*_8$ lying between 0.68 and 2.71 have been found.

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