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Solution to the Φ-derivable approximation for scalar thermodynamics

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We solve the 3-loop Φ-derivable approximation to the thermodynamics of the massless ϕ^4 field theory by reducing it to a 1-parameter variational problem. The thermodynamic potential is expanded in powers of g^2 and m/T, where g is the coupling constant, m is a variational mass parameter, and T is the temperature. There are ultraviolet divergences beginning at 6th order in g that cannot be removed by renormalization. However a finite thermodynamic potential obtained by truncating after terms of 5th order in g and m/T defines a stable approximation to the thermodynamic functions.

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The thermodynamic functions for massless relativistic field theories at high temperature T can be calculated as weak-coupling expansions in the coupling constant g. They have been calculated explicitly through order g^5 for the massless ϕ^4 field theory [1,2], for QED [3,4], and for QCD [5,6]. Unless the coupling constant is tiny, the weak-coupling expansions are poorly convergent and sensitive to the renormalization scale. This makes the weak-coupling expansion essentially useless as a quantitative tool: it seems to be reliable only when the coupling constant is so small that the corrections to ideal gas behavior are negligibly small. The physical origin of the instability seems to be effects associated with screening and quasiparticles.

A possible solution to this instability problem is to reorganize the weak-coupling expansion within a variational framework. A variational approximation can be defined by a *thermodynamic potential* Ω that depends on a set of variational parameters m_i. The free energy and other thermodynamic functions are given by the values of Ω and its derivatives at the variational point where $\partial\Omega/\partial m_i = 0$. A variational approximation is systematically improvable if there is a sequence of successive approximations to Ω that reproduce the weak-coupling expansions of the thermodynamic functions to successively higher orders in g. An example of a systematically improvable variational approximation is *screened perturbation theory*, which involves a single variational mass parameter [7].

A variational approach can be useful only if the correct physics can be captured by appropriate choices of the variational parameters. Information about screening and quasiparticles is contained within the exact propagator of the field theory. The possibility that these effects are responsible for the instability of the weak-coupling expansion suggests the use of the propagator as a variational function. Such a variational formulation was constructed for nonrelativistic fermions by Luttinger and Ward [8] and by Baym [9] long ago, and has been generalized to relativistic theories [10]. In the case of a relativistic scalar field theory, the propagator has the form $[P^2+\Pi(P)]^{-1}$, where $\Pi(P)$ is the self-energy which depends on the momentum P. The thermodynamic potential has the form

$$\Omega_0[\Pi] = \frac{1}{2}\sum\!\!\!\!\!\!\int_P \left[\log(P^2+\Pi) - \frac{\Pi}{P^2+\Pi}\right] + \Phi[\Pi], \quad (1)$$

where the interaction functional $\Phi[\Pi]$ can be expressed as a sum of 2-particle-irreducible diagrams. It is constructed so that the solution to the variational equation $\delta\Omega_0/\delta\Pi = 0$ is the exact self-energy, and the value of Ω_0 at the variational point is the exact free energy. The subscript on Ω_0 emphasizes that this bare thermodynamic potential contains ultraviolet divergences. We can obtain a systematically improvable variational approximation by truncating Φ at nth order in the loop expansion, where $n = 2,3,\ldots$. We refer to such an approximation as the n-loop Φ-*derivable approximation*. The two-loop Φ-derivable approximation for the massless ϕ^4 field theory, which can be solved exactly [11,12], illustrates the basic ideas of the Φ-derivable approximation. The 2-loop Φ-derivable approximation for QCD has recently been used as the basis for quasiparticle models of the thermodynamics of the quark-gluon plasma [12,13]. Since Φ-derivable approximations guarantee consistency with conservation laws, they may be particularly useful for nonequilibrium problems [14].

It is easier to formulate the Φ-derivable approximation than to solve it. If the self-energy Π is independent of P as in the 2-loop Φ-derivable approximation for the massless ϕ^4 field theory [11,12], the problem reduces to a 1-parameter variational problem that can be solved exactly. If Π depends on P, the variational equation is a nontrivial integral equation that is difficult to solve. The main problem is that the thermodynamic potential has severe ultraviolet divergences that vanish at the variational point only if Φ is calculated to all orders. They do not vanish away from the variational point, and they do not vanish at the variational point if the loop expansion for Φ is truncated.

In this Rapid Communication, we solve the 3-loop Φ-derivable approximation for a massless scalar field theory with a ϕ^4 interaction by reducing it to a 1-parameter variational problem involving a mass parameter m. The resulting thermodynamic functions have ultraviolet divergences beginning at 6th order in the coupling constant g. However a finite thermodynamic potential obtained by truncating after terms of 5th order in g and m/T defines a stable approximation to the thermodynamic functions. In this paper we describe the solution as concisely as possible. The technical details are presented in Ref. [15].

The Lagrangian for the massless scalar field theory with a ϕ^4 interaction with bare coupling constant $\alpha_0 = g_0^2/(4\pi)^2$ is

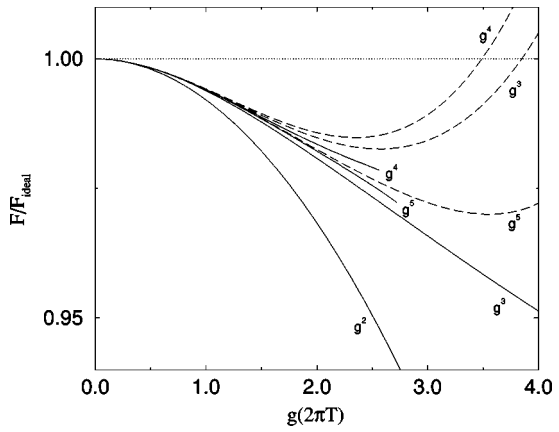

FIG. 1. Free energy divided by that of the ideal gas for the weak-coupling expansion (dashed lines) and the truncated Φ-derivable approximation (solid lines).

$$\mathcal{L}=\frac{1}{2}\partial_\mu\phi\partial^\mu\phi-\frac{1}{24}g_0^2\phi^4. \tag{2}$$

We define the renormalized coupling constant $\alpha=g^2/(4\pi)^2$ using dimensional regularization in $4-2\epsilon$ dimensions and the modified minimal subtraction ($\overline{\rm MS}$) prescription with renormalization scale μ:

$$\alpha_0\mu^{-2\epsilon}=\alpha+\frac{3}{2\epsilon}\alpha^2+\left(\frac{9}{4\epsilon^2}-\frac{17}{12\epsilon}\right)\alpha^3+\cdots. \tag{3}$$

The two-loop beta function for the running coupling constant $\alpha(\mu)$ is $\beta(\alpha)=3\alpha^2-\frac{17}{3}\alpha^3$. The thermodynamic functions for this theory are known to order g^5 [1,2]. The weak-coupling expansion for the free energy density is

$$\frac{\mathcal{F}}{\mathcal{F}_{\rm ideal}}=1+15\Bigg[-\frac{\alpha}{12}+4\left(\frac{\alpha}{6}\right)^{3/2}+9(L+1.097)\left(\frac{\alpha}{6}\right)^2+36[2\log(\alpha/6)-3L+3.665]\left(\frac{\alpha}{6}\right)^{5/2}\Bigg], \tag{4}$$

where $\alpha=\alpha(\mu)$, $L=\log(\mu/4\pi T)$, and $\mathcal{F}_{\rm ideal}$ is the pressure of the ideal gas of a free massless boson: $\mathcal{F}_{\rm ideal}=-(\pi^2/90)T^4$.

The instability of the weak-coupling expansion is illustrated in Fig. 1, which shows the free energy divided by that of the ideal gas as a function of $g(2\pi T)$. The dashed lines are the predictions of the weak coupling expansion (4) with $\mu=2\pi T$ truncated after orders g^n for $n=2,3,4,5$. The dashed line for $n=2$ is hidden under the solid line labeled g^2. The successive approximations show no sign of converging.

To illustrate our method in the simplest possible context, we first consider the 2-loop Φ-derivable approximation. The self-energy is independent of P, so we denote it by $\Pi=m^2$. The interaction functional in Eq. (1) is

$$\Phi(m)=\frac{1}{8}g_0^2\mu^{-4\epsilon}\mathcal{I}_{\rm tad}^2, \tag{5}$$

$$\mathcal{I}_{\rm tad}=\sum\!\!\!\!\!\!\int_Q\frac{1}{Q^2+m^2}.$$

The measure for the dimensionally regularized sum-integrals in Eqs. (1) and (5) includes a factor of $(e^\gamma\mu^2/4\pi)^\epsilon$, where γ is Euler's constant. We insert a factor of $\mu^{-2\epsilon}$ into the sum-integral in Eq. (1), so Ω_0 is independent of the renormalization scale. The variational equation $\partial\Omega_0/\partial m=0$ reduces to the simple gap equation

$$m^2=\frac{1}{2}g_0^2\mu^{-2\epsilon}\mathcal{I}_{\rm tad}. \tag{6}$$

The sum integrals in Eqs. (1) and (5) contain ultraviolet divergences. Some of the divergences vanish at the variational point. They can be removed by adding a term proportional to the square of the gap equation:

$$\Omega=\Omega_0-(m^2-G)^2/(32\pi^2\alpha_0), \tag{7}$$

where G is the expression on the right-hand side of Eq. (6). The additional term gives no contribution to those thermodynamic functions that are determined by the value of Ω and its first derivatives at the variational point. The remaining divergences can be absorbed into a renormalized coupling constant $\overline{\alpha}(\mu)$ defined by $\alpha_0\mu^{-2\epsilon}=\overline{\alpha}(1-\overline{\alpha}/2\epsilon)^{-1}$. Expanding in powers of m/T, the resulting thermodynamic potential Ω is

$$\Omega/\mathcal{F}_{\rm ideal}=1+15[3\hat{m}^4/\overline{\alpha}-\hat{m}^2+4\hat{m}^3+3(L+\gamma)\hat{m}^4+\cdots], \tag{8}$$

where $\hat{m}=m/(2\pi T)$. The coupling constant $\overline{\alpha}$ runs with the beta function $\beta(\overline{\alpha})=\overline{\alpha}^2$, whose first coefficient is too small by a factor of 3 compared to that of the true coupling constant. Thus $\overline{\alpha}$ can be identified with the true coupling constant α only at a single scale μ_0. If one expresses the thermodynamic potential in terms of the true coupling constant α defined by Eq. (3), the ultraviolet divergences cannot be eliminated. The closest one can come to defining a finite thermodynamic potential is to truncate Eq. (8) after the term of order m^3:

$$\Omega/\mathcal{F}_{\rm ideal}=1+15[3\hat{m}^4/\alpha-\hat{m}^2+4\hat{m}^3]. \tag{9}$$

The truncation eliminates the ultraviolet divergences, which are of order g^4. In Eq. (8), those divergences are hidden in the coupling constant $\overline{\alpha}$ that runs with the wrong beta function. The gap equation obtained by varying Eq. (9) with respect to m with α fixed is

$$\hat{m}^2=\alpha\left(\frac{1}{6}-\hat{m}\right). \tag{10}$$

Solving this quadratic equation and substituting the solution into Eq. (9), the free energy is

$$\mathcal{F}/\mathcal{F}_{\rm ideal}=1-5\alpha/4[1+6\alpha+6\alpha^2-4(2+3\alpha)\sqrt{\alpha/6+\alpha^2/4}], \tag{11}$$

where $\alpha=\alpha(\mu)$. When expanded in powers of g, this agrees with the weak-coupling expansion (4) through order g^3. It depends on the renormalization scale μ through the dependence of $\alpha(\mu)$ on μ. However, it is much less sensitive to variations in μ than the truncated weak-coupling expansion. The reason is that the truncated weak-coupling expansion grows like a power of α in the strong-coupling limit, while the expression (11) approaches the limiting value $\frac{31}{36}$.

We now proceed to consider the three-loop Φ-derivable approximation. The interaction term in Eq. (1) is

$$\Phi[\Pi]=\frac{1}{8}g_0^2\mu^{-4\epsilon}\mathfrak{I}_{\rm tad}^2-\frac{1}{48}g_0^4\mu^{-6\epsilon}\mathfrak{I}_{\rm ball}, \tag{12}$$

$$\mathfrak{I}_{\rm tad}=\sum\!\!\!\!\!\!\int_Q \frac{1}{Q^2+\Pi(Q)},$$

$$\mathfrak{I}_{\rm ball}=\sum\!\!\!\!\!\!\int_{Q_1Q_2Q_3}\prod_{i=1}^{4}\frac{1}{Q_i^2+\Pi(Q_i)},$$

where $Q_4=-(Q_1+Q_2+Q_3)$ in the definition of the basketball sum-integral. The variational equation obtained by varying with respect to $\Pi(P)$ is

$$\Pi(P)=\frac{1}{2}g_0^2\mu^{-2\epsilon}\mathfrak{I}_{\rm tad}-\frac{1}{6}g_0^4\mu^{-4\epsilon}\mathfrak{I}_{\rm sun}(P), \tag{13}$$

$$\mathfrak{I}_{\rm sun}(P)=\sum\!\!\!\!\!\!\int_{Q_1Q_2}\prod_{i=1}^{3}\frac{1}{Q_i^2+\Pi(Q_i)},$$

where $Q_3=-(P+Q_1+Q_2)$ in the definition of the sunset sum-integral. The variational equation (13) is a nontrivial integral equation for $\Pi(P)$ whose solution is complicated by the presence of severe ultraviolet divergences in the sum-integrals.

Our strategy is to introduce a variational mass parameter m that is of order gT in the weak-coupling limit and calculate the sum-integrals as double expansions in g and m/T. The variational equation (13) is then solved for $\Pi(P)$ as a function of P and m. Inserting the solution into Eqs. (1) and (12) and expanding in powers of g and m/T, the thermodynamic potential Ω reduces to an algebraic function of m. The final step is to minimize Ω with respect to the variational parameter m.

There is some freedom in the choice of the mass parameter m. We define m implicitly by the equation

$$m^2=\frac{1}{2}g_0^2\mu^{-2\epsilon}\mathfrak{I}_{\rm tad}-\frac{1}{6}g_0^4\mu^{-4\epsilon}\mathfrak{I}_{\rm sun}(0,\mathbf{p})\big|_{p=im}. \tag{14}$$

The solution to this gap equation for m can be interpreted as the screening mass. This choice is motivated by the fact that the screening mass is a physical quantity, so it should be ultraviolet finite up to perturbative truncation errors. There are two important momentum scales: the *hard* scale $2\pi T$ and the *soft* scale m. The hard region for the momentum $P=(2\pi nT,\mathbf{p})$ includes $n\neq 0$ for all $\mathbf{p}$ and also $n=0$ with $\mathbf{p}$ of order T. The soft region is $n=0$ and $\mathbf{p}$ of order m. We will solve the variational equation in the two momentum regions separately. We expand $\Pi(P)$ in powers of g_0 and m/T. For hard momentum P, the expansion has the form

$$\Pi(P)=m^2+g_0^4\mu^{-4\epsilon}[\Pi_{4,0}(P)+\Pi_{4,1}(P)+\cdots]+g_0^8\mu^{-8\epsilon}[\Pi_{8,-2}(P)+\cdots]+\cdots, \tag{15}$$

where $\Pi_{n,k}(P)$ is of order $T^2(m/T)^k$ when P is of order T. For soft momentum $P=(0,\mathbf{p})$, the function $\sigma(p)$ in the self-energy $\Pi(0,\mathbf{p})=m^2+\sigma(p)$ has the form

$$\sigma(p)=g_0^4\mu^{-4\epsilon}[\sigma_{4,-2}(p)+\sigma_{4,0}(p)+\cdots]+g_0^8\mu^{-8\epsilon}[\sigma_{8,-4}(p)+\cdots]+\cdots, \tag{16}$$

where $\sigma_{n,k}(p)$ is of order $m^2(m/T)^k$ when p is of order m. We insert the expansions (15) and (16) into the variational equation (13) and expand in powers of g_0^4 and m/T. Matching the coefficients at each order in g_0^4 and m/T, we find a recursive structure in which the functions $\Pi_{n,k}(P)$ and $\sigma_{n,k}(p)$ are either completely determined or expressed in terms of lower order functions. For example, the solutions to the first few self-energy functions at hard momentum P are

$$\Pi_{4,0}(P)=-\frac{1}{6}\sum\!\!\!\!\!\!\int_{Q_1Q_2}\frac{1}{Q_1^2Q_2^2Q_3^2}+\frac{1}{6}T^2I_{\rm sun}(im), \tag{17}$$

$$\Pi_{4,1}(P)=-\frac{1}{2}TI_1\sum\!\!\!\!\!\!\int_Q\left(\frac{1}{Q^2(P+Q)^2}-\frac{1}{(Q^2)^2}\right), \tag{18}$$

where $Q_3=-(P+Q_1+Q_2)$. The solutions to the first few self-energy functions at soft momentum $(0,\mathbf{p})$ are

$$\sigma_{4,-2}(p)=-\frac{1}{6}T^2[I_{\rm sun}(p)-I_{\rm sun}(im)], \tag{19}$$

$$\sigma_{4,0}(p)=\frac{1}{6}(p^2+m^2)\sum\!\!\!\!\!\!\int_{QR}\frac{Q^2-(4/d)\mathbf{q}^2}{(Q^2)^3R^2(Q+R)^2}.$$

The sunset integral appearing in Eqs. (17) and (19) is

$$I_{\rm sun}(p)=\int_{\mathbf{q}_1\mathbf{q}_2}\prod_{i=1}^{3}\frac{1}{q_i^2+m^2},$$

where $\mathbf{q}_3=-(\mathbf{p}+\mathbf{q}_1+\mathbf{q}_2)$, while the integral I_1 in Eq. (18) is

$$I_1=\int_{\mathbf{p}}\frac{1}{p^2+m^2}.$$

Having solved the gap equation, we can reduce the bare thermodynamic potential Ω_0 to a function of the single variational parameter m by inserting the expansions (15) and (16) into Eqs. (1) and (12) and expanding in powers of α_0 and m/T. The function Ω_0 contains ultraviolet divergences in the form of poles in ϵ. Some of them are eliminated when Ω_0 is evaluated at the solution of the gap equation. We can

cancel them through 5th order in g and m/T by adding a term proportional to $(m^2-G)^2$, where G is the expression on the right side of the gap equation (14):

$$\Omega=\Omega_0-\left[\frac{1}{\alpha_0}+\frac{\Lambda^{-2\epsilon}}{\epsilon}\right]\frac{(m^2-G)^2}{32\pi^2}. \tag{20}$$

We have introduced an arbitrary momentum scale Λ in order that all terms have the correct dimension $4-2\epsilon$ when $\epsilon\neq 0$. Other ultraviolet divergences in Ω_0 can be removed by using Eq. (3) to renormalize the coupling constant. The remaining ultraviolet divergences are 6th and higher order in g and m/T. The most severe divergences at 6th order are double poles in ϵ proportional to αm^4, $\alpha^2 m^2$, and α^3. These divergences are unavoidable consequences of the truncation of the loop expansion. If we used the 4-loop Φ-derivable approximation, the truncation error would be reduced to order g^8. Expanding Eq. (20) in powers of g and m/T and then truncating after terms of 5th order, we obtain a finite thermodynamic potential:

$$\begin{aligned}\frac{1}{15}(\Omega/\mathcal{F}_{\rm ideal}-1)&=3\hat{m}^4/\alpha\\&+[-\hat{m}^2+4\hat{m}^3+3(3L-2l+\gamma)\hat{m}^4]\\&+\alpha[2(l-2\log\hat{m}-2.757642)\hat{m}^2\\&-12(l+\gamma)\hat{m}^3]+\alpha^2\left[-\frac{1}{6}(l-4\log\hat{m}\right.\\&\left.-9.873296)+2(l-2\log 2+\gamma)\hat{m}\right],\end{aligned} \tag{21}$$

where $\alpha=\alpha(\mu)$, $\hat{m}=m/(2\pi T)$, $L=\log(\mu/4\pi T)$, and $l=\log(\Lambda/4\pi T)$.

The gap equation obtained by varying the finite thermodynamic potential (21) with respect to m^2 with μ and Λ fixed is

$$\begin{aligned}\hat{m}^2&=\alpha\left[\frac{1}{6}-\hat{m}-(3L-2l+\gamma)\hat{m}^2\right]\\&+\alpha^2\left[-\frac{1}{3}(l-2\log\hat{m}-3.75764)+3(l+\gamma)\hat{m}\right]\\&+\alpha^3\left[-\frac{1}{18}-\frac{1}{6}(l-2\log 2+\gamma)\hat{m}\right]\Big/\,\hat{m}^2.\end{aligned} \tag{22}$$

If we solve this gap equation iteratively in powers of g and insert the solution into Eq. (21), we recover the weak-coupling expansion (4) for the free energy. Solving the gap equation numerically, we find a solution only below a critical value of g that depends on μ and Λ. For $\mu=\lambda=2\pi T$, the critical value is $g=2.61$. For larger values of g, the thermodynamic potential (21) has a run-away minimum at $m=0$. A similar behavior was observed in screened perturbation theory at 3 loops [16]. When the screening mass is used as the mass parameter, the solution to the gap equation terminates at nearly the same critical value of g.

By truncating the thermodynamic potential (21) and the gap equation (22) after terms of nth order in g and m/T, where $n=2,3,4,5$, we obtain a series of successive approximations to the free energy. The stability of these successive approximations is exhibited in Fig. 1, which shows the free energy divided by that of the ideal gas as a function of $g(2\pi T)$ for $\mu=\Lambda=2\pi T$. For the g^4 and g^5 truncations, the solutions to the gap equation terminate at critical values of g. In contrast to the weak-coupling expansion, the predictions of the truncated Φ-derivable approximation seem to be converging for values of g below these critical values. The truncated Φ-derivable approximations depend on the renormalization scale μ and also for $n=4,5$ on the momentum scale Λ introduced in Eq. (20). However the changes in the predictions from varying the arbitrary scales is significantly smaller than in the weak-coupling expansion.

An important application of our method would be to solve the Φ-derivable approximation for QCD. One should be able to reduce the 2-loop and 3-loop Φ-derivable approximations to single-parameter variational problems by expanding systematically in powers of g^2 and m/T, where m is some appropriate electric screening mass of order gT. The Debye screening mass might not be an appropriate choice for m, because the perturbative Debye screening mass is infrared divergent at next-to-leading order in g [17]. The solution to the 2-loop Φ-derivable approximation should give an entropy consistent with the ''HTL approximation'' of Blaizot, Iancu and Rebhan [12], which has an error of order g^3. Their ''NLO HTL approximation,'' which has an error of g^4, reduces essentially to the *ad hoc* substitution $g^2\to g^2/(1+g/\pi)$ in their ''HTL approximation. In their ''NLA HTL approximation,'' their mass parameter is the solution to a simple polynomial gap equation analogous to Eq. (10). Our approach would give an entropy with error of order g^4 that is part of a systematically improvable sequence of approximations. It would also allow the calculation of the pressure and other thermodynamic variables for which the ultraviolet divergences of the 2-loop Φ-derivable approximation cannot be avoided. A serious obstacle for using our method to solve the 3-loop Φ-derivable approximation for QCD would be evaluating the resulting sum-integrals and integrals. At 4-loops, our strategy for reducing the Φ-derivable approximation to a single-parameter variational problem would necessarily break down, because the thermodynamic variables become sensitive to the scale g^2T associated with magnetic screening. Another complication of the Φ-derivable approximation for QCD is that the thermodynamic potential is gauge-dependent, simply because it is a functional of the gluon propagator, which is gauge-dependent. The expansion of the thermodynamic potential in powers of g^2 and m/T is therefore likely to depend on a gauge parameter ξ. At the variational minimum, the dependence on ξ must of course cancel up to the order in g set by the truncation error. This complication of a gauge-dependent thermodynamic potential could perhaps be avoided by using a more general variational approach in which the thermodynamic potential is expressed

as a functional of exact vertices as well as exact propagators [18].

We have solved the 3-loop Φ-derivable approximation for the thermodynamics of the ϕ^4 field theory by reducing it to a problem with a single variational parameter m. We constructed a finite thermodynamic potential by adding a term proportional to the square of the gap equation and truncating after terms of 5th order in g and m/T. This thermodynamic potential has a minimum as a function of m only for g below some critical value. Below this critical value of g, the successive approximations obtained by truncating the thermodynamic potential at orders $n=2,3,4,5$ give predictions for the pressure that are stable with respect to both the order of truncation and variations in μ and Λ. The resulting predictions for the pressure are numerically close to those of screened perturbation theory [16]. The advantage of the Φ-derivable approximation is that it is an infinite-parameter variational approximation. Our solution to the Φ-derivable approximation can in principle be extended to higher orders in the loop expansion. The primary obstacle to extending it to 4-loop order would be evaluating the same sum-integrals that would be required to extend the weak-coupling expansion to order g^6. Thus our approach provides a systematically improvable approximation to the thermodynamic functions that seems to have very good convergence properties.

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