Skeleton Graph Expansion for Critical Exponents*

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Critical exponents are calculated using conventional many-body perturbation theory by means of a self-consistent skeleton graph expansion in $4-\epsilon$ deminsions, where ϵ is small. The self-consistency is expressed through Ward identities. The results, the same as those of Wilson, are obtained without recourse to renormalization group arguments.

The behavior in the critical region has been discussed recently by Wilson[1] using a Feynman graph technique which exploits an ϵ expansion about four dimensions to give systematic corrections to mean field theory. His method requires the correct choice of coupling constant $u_0(\epsilon)$ in each dimensionality d $(=4-\epsilon)$ to match the critical behavior. The existence of a unique $u_0(\epsilon)$ is deduced from a renormalization group argument.

It is of interest that the same results for critical exponents in powers of ϵ may be obtained by a self-consistent skeleton graph expansion which used renormalized propagators and interaction vertices throughout, does not involve $u_0(\epsilon)$, and requires no appeal to a renormalization group discussion. We give the procedure in this Letter.

Self-consistency is expressed through a set of Ward identities which are evaluated as power series in ϵ. For simplicity we consider only a complex field, e.g., helium. We adopt the Hamiltonian of Ref. 1:

$$H/kT=\int d^dx[r_0|\psi(x)|^2+|\nabla\psi(x)|^2+U_0|\psi(x)|^4],$$

where $\psi(x)$ is the complex order parameter and a large momentum cutoff will be used. The rest of the notation is the same as in Ref. 1. The Feynman rules for statistical averages have been discussed by others[1-3] and correspond to taking all Matsubara frequencies as zero in the usual technique.[4]

The essential point of our method is that the renormalized four-point interaction vertex Γ is of order ϵ. Therefore, the order in ϵ of a skeleton graph is determined by the number of vertices and a systematic ϵ expansion is possible. This fact also enables us to analyze the momentum dependence of Γ, as discussed below.

To find the critical exponents γ and η we consider the renormalized propagator (order parameter correlation function) $g(k;r)$ and four-point vertex $\Gamma(q_1, q_2, q_3; r)$. Here r is the inverse susceptibility which vanishes at the transition point as[1] $(r_0-r_{0c})^\gamma$ and the q_i are the total momenta in the three independent[2] pair channels of Γ (cf. Fig. 1). Thus, $g(0;r)=1/r$, $g(k;0)=k^{\eta-2}$ defines η, and $\Gamma(0,0,0;r)=u_R$, the renormalized coupling constant.[1] We shall make a parquet graph analysis[2,5] of Γ. The relevant Bethe-Salpeter equations are depicted in Fig. 1 where the irreducible kernel I_i is the set of all graphs of Γ which cannot be cut in channel i,[5] whereas the parts Γ_i can be so cut. The totally irreducible part of Γ consists of the bare interaction u_0 plus skeleton graphs R which have at least four vertices and therefore will be at least $O(\epsilon^4)$. We limit ourselves to $O(\epsilon^2)$ in γ so that we need Γ to $O(\epsilon^3)$ and we may neglect the nonparquet graphs. Thus, I_i is given by[5]

$$u_0+\sum_{j\neq 1}\Gamma_j.$$

The parquet graphs have been evaluated with

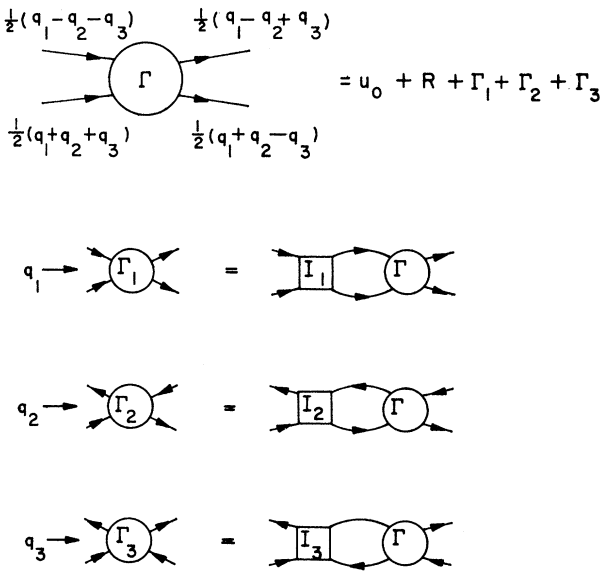

FIG. 1. Decomposition of four-point vertex Γ into its reducible parts.

logarithmic accuracy[5] for $d=4$ by Larkin and Khmel'nitskii.[2] Their calculation can be repeated for $d=4-\epsilon$ and it gives directly the first term of the ϵ expansion for $\Gamma(q_i; r)$. To go further, we need to analyze the momentum dependence of Γ. For example, we shall need $\Gamma(q, 0, -q; r)$ (Fig. 2). This is given by a set of parquet graphs which differs from that for u_R by having, in its internal structure, certain pairs of propagators having total momentum q instead of 0. We denote such a pair by $G(q)$ $[G(q)=\int d^d p\, g(p+q)g(p)\cdots]$. If we write $G(q)=G(q)-G(0)+G(0)=\Delta(q)+G(0)$ for every such pair and expand, we get a sum of terms as follows. First, all terms with $G(0)$'s give just u_R. Next, all terms with just one $\Delta(q)$ (inserted in all possible ways but only once) and all the rest $G(0)$ give a contribution $u_R\Delta(q)u_R$, which is $O(\epsilon^2)$. This is shown in Fig. 2 where the wavy line denotes $\Delta(q)$. The next terms have two $\Delta(q)$'s inserted in all possible ways. This gives $u_R\Delta(q)u_R\Delta(q)u_R$, which is $O(\epsilon^3)$, etc. Since we shall need the momentum dependence only to $O(\epsilon^2)$, we may write

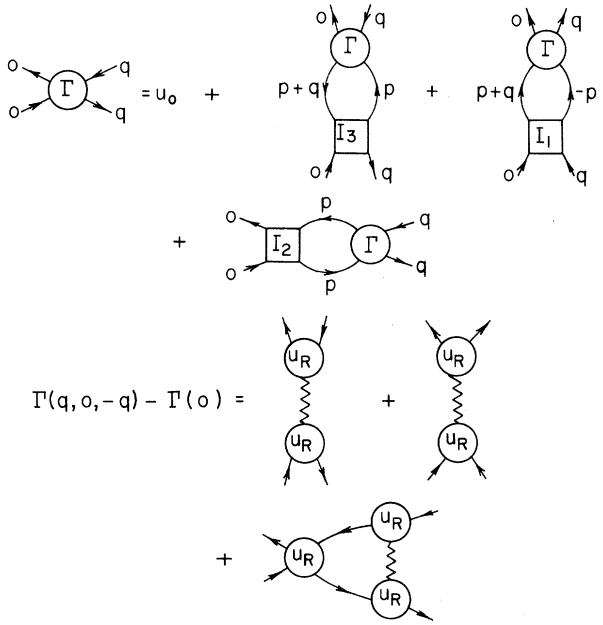

FIG. 2. Skeleton graphs for the momentum dependence of $\Gamma(q, 0, -q; r)$.

$$\Gamma(q, 0, -q; r)=u_R-\tfrac{3}{2}u_R{}^2\Delta(q)=u_R-\tfrac{3}{2}u_R{}^2\int d^d p[g(p+q)g(p)-g^2(p)], \tag{1}$$

where the factor $\frac{3}{2}$ arises because there are two independent channels ($i=1, 3$) in which the pairs $G(q)$ occur.[6] In channel 2, such pairs only occur in the cross bubble of the full Γ in the Bethe-Salpeter equation and give a contribution of $O(\epsilon^3)$ which we neglect (cf. Fig. 2).

In the calculation of critical exponents, we shall need the form of $u_R(r)$ and the momentum dependence of Γ for $r=0$. These may be found from an examination of the skeleton graph structure. One sees that the basic building block of skeleton graphs is $\int d^d k\, \Gamma g^2$ which must be constant in the two limits $r=0$ or momentum $=0$. A solution of the coupled skeleton graph equations involving Γ and g is obtained when $g(k; r)$ has the homogeneity form $r^{-1}f(k^{2-\eta}/r)$, where η is to be determined. Then $u_R \propto r^{\epsilon-2\eta/2-\eta}$ and $\Gamma(q; 0)\propto q^{\epsilon-2\eta}$. In particular, the the lowest-order momentum dependence of $\Gamma_i(q; 0)$ is on only the total momentum q_i in the ith channel and occurs in $O(\epsilon^2)$. Thus, $\Gamma_i \simeq A(\epsilon)q_i{}^{\epsilon-2\eta}$ for $r=0$ and small q_i. To $O(\epsilon^2)$, then,

$$\Gamma=A\epsilon+B\epsilon^2+\tfrac{1}{3}A\epsilon^2\ln(q_1q_2q_3) \tag{2}$$

and the coefficients A and B may be determined by methods described below.

Next we show how to find u_K to $O(\epsilon^2)$. In order to express u_R in terms of skeleton graphs, i.e., full Γ's at all vertices, we calculate the derivative

$$u_R{}'=\sum_{i=1}^{3}\partial\Gamma_i(0; r)/\partial r,$$

which, since $u_R \approx \epsilon r^{\epsilon-2\eta/2-\eta}$, we shall need to $O(\epsilon^3)$. For $\partial\Gamma_i/\partial r$, we differentiate in various parts of Fig. 3: First, in all possible $g^2(k)$ between I_i's; this gives a full Γ on each side of $\partial g^2/\partial r$ and so is $O(\epsilon^2)$ at least. Second, in the left-hand-most I_i; this gives $\partial I_i/\partial r$ connected to a full Γ by $g^2(k)$. An equal contribution comes from the right-hand-most I_i. If we differentiate in an internal I_i, we shall have a full Γ on each side of $\partial I_i/\partial r$, a contribution at least of $O(\epsilon^4)$

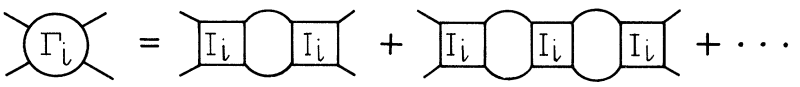

FIG. 3. Ladder graphs in the Bethe-Salpeter equation for Γ_i.

which we drop. Thus we find, for example,

$$\partial\Gamma_2(0;r)/\partial r = -\int d^d k\,\Gamma(0,k)\Gamma(k,0)\partial g^2(k)/\partial r - 2\int d^d k\,\Gamma(0,k)g^2(k)\partial I_2(k,0)/\partial r. \tag{3}$$

We have already treated the momentum dependence of Γ to $O(\epsilon^2)$ in Eq. (1). This is sufficient to give the first integral of Eq. (3) to $O(\epsilon^3)$. In the second integral, we have $\partial I_2/\partial r = \partial(\Gamma_1+\Gamma_3)/\partial r$. In these derivatives it is sufficient to keep only the term corresponding to the first integral of Eq. (3) and to replace all Γ's by u_R's. We find, using Eq. (1),

$$\partial\Gamma_2(0;r)/\partial r = -u_R{}^2\int d^d k\,\partial g^2(k)/\partial r + 3u_R{}^3\int\int d^d p\,d^d k[g(p+k)g(p)-g^2(p)]\partial g^2(k)/\partial r$$
$$+ 3u_R{}^3\int\int d^d p\,d^d k\,g^2(k)\,\partial[g(p+k)g(p)]/\partial r.$$

The result is the same for $\partial\Gamma_3/\partial r$, while for $\partial\Gamma_1/\partial r$ the coefficients of the three terms are $-\frac{1}{2}$, 2, and 2.[6] Summing the three channels, we find

$$u_R'/u_R = (\epsilon - 2\eta/2 - \eta)r^{-1} = -5u_R I'/2 + 4u_R{}^2[2J' - (I^2)'], \tag{4}$$

where

$$I = \int g^2(k)\,d^d k, \quad J = \int\int d^d k\,d^d p\,g(k)g^2(p)g(p+k).$$

At this point, we can extract the leading term in u_R by keeping only the linear terms in ϵ on each side of Eq. (4). In the integral I we may replace g by its zeroth-order value $g^{-1} = r + k^2$ and take $d = 4$. We find $\epsilon/2r = 5u_R/32\pi^2 r$ so that $u_R = (16\pi^2/5)\epsilon + \cdots$. The next term may also be found from Eq. (4) but it is unnecessary for our purpose.

In order to evaluate γ we use $r \propto (r_0 - r_{0c})^\gamma$ and obtain r from the set of self-energy (Σ) graphs for zero momentum. Since $r = r_0 - \Sigma(0;r)$, the derivative $\partial r/\partial r_0$ may be constructed graphically by differentiating in turn each internal propagator in each graph of Σ.[7] In this way, one gets the Ward identity for the zero-momentum vertex $\Lambda(0,0;r)$ as depicted in Fig. 4:

$$\Lambda(0,0;r) = \partial r/\partial r_0 = 1 - \int I_2(0,k)g^2(k)\Lambda(k,0;r)\,d^d k.$$

Now, $\partial\Lambda/\partial r$ contains full Γ's only and is constructed in the same manner as $\partial\Gamma_2/\partial r$. The result is (the momentum dependence of Λ enters only in higher order)

$$\Lambda'/\Lambda = (1 - 1/\gamma)r^{-1} = -u_R I' + \tfrac{3}{4}u_R[2J' - (I^2)']. \tag{5}$$

We combine Eqs. (4) and (5) and find

$$[2\epsilon - \tfrac{4}{10}\eta - 5\eta - (1-\gamma^{-1})]r^{-1} = \tfrac{17}{20}u_R{}^2[2J' - (I^2)'].$$

To solve for γ to $O(\epsilon^2)$ we need only the first-order u_R already found and the integrals I, J which may be evaluated in zeroth order. Since η is $O(\epsilon^2)$, we have

$$\gamma = 1 + \tfrac{1}{5}\epsilon + \tfrac{27}{250}\epsilon^2 - \tfrac{2}{5}\eta. \tag{6}$$

We now show how to obtain η to $O(\epsilon^2)$. In this case, we look at the behavior of propagators with $r = 0$ and k finite but small. Then $g^{-1} = k^{2-\eta}$. We consider the Ward identity

$$\nabla_k g^{-1}(k) = (2-\eta)\vec{k}k^{-\eta} = \vec{k}L(k) = -\int d^d p\,I_2(k,p)g^2(p)\vec{p}L(p). \tag{7}$$

We express the right-hand side in terms of skeleton graphs by constructing the derivative

$$\frac{\partial(kL)}{\partial k} = (2-\eta)(1-\eta)k^{-\eta} = -\int d^d p\,\frac{\partial I_2(k,p)}{\partial k}g^2(p)\vec{p}\cdot\hat{k}L(p).$$

The derivative $\partial I_2/\partial k = \partial(\Gamma_1+\Gamma_3)/\partial k$ is found by differentiating in turn each internal propagator in I_2

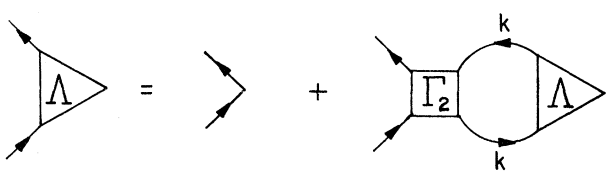

FIG. 4. Bethe-Salpeter equation for the zero-momentum vertex Λ.

which contains k. To $O(\epsilon^2)$ only those appearing in the intermediate pairs of total momentum k contribute. The sum of such contributions gives a full Γ on each side of the derivative of the propagators. The result is

$$\partial\Gamma_2/\partial_k = -A^2\partial[\int d^4q\, g(q+k)g(p+q)]/\partial k,$$

$$\partial\Gamma_1/\partial k = -\tfrac{1}{2}A^2\partial[\int d^4q\, g(q+k)g(p-q)]/\partial k,$$

where A is the value of $\Gamma(r=0)$ to $O(\epsilon)$ and is thus independent of momentum [cf. Eq. (2)]. The value $A = 16\pi^2/5$ may be found by just these same techniques. However, it is the same as u_K to $O(\epsilon)$ since the lowest (logarithmic) approximation for the parquet graphs gives the same result for $r=0$, $k\neq 0$ as for $k=0$, $r\neq 0$.[2] Combining these results and taking another k derivative to isolate the most singular term, we find

$$\frac{d^2(kL)}{dk^2} = \frac{2\eta}{k} = \frac{-A^2L_0(4\pi)^{-4}}{k}, \quad \eta = \tfrac{1}{50}\epsilon^2, \tag{8}$$

where, from Eq. (7), $L_0 = 2$ is the zeroth-order value of L. In summary then, from Eqs. (6) and (8) we have, as in Ref. 1,

$$\gamma = 1 + \tfrac{1}{5}\epsilon + \tfrac{1}{10}\epsilon^2, \quad \eta = \tfrac{1}{50}\epsilon^2.$$

It is not difficult to carry out the evaluation of η to $O(\epsilon^3)$. The calculation requires the evaluation of the second-order coefficients in Eq. (2) by means of an ϵ expansion of $\partial\Gamma_i/\partial q_i$ using the methods already discussed.

All of the foregoing development can be done for the general case of a field with n real components, although some care must be taken in the construction of a Ward-like identity to replace Eq. (7). The results are again the same as those of Wilson.[1]

The calculation of correlation functions may be done using our methods. We can, for example, find the specific heat exponent α to $O(\epsilon^2)$ by calculating $\partial^2 S/\partial r^2$, where $S = \int d^dk\, g^2(k;r)\Lambda(k;r)$ is the "density-density" correlation function for $q = 0$. The dependence of S on r gives α since $S \propto (r_0 - r_{0c})^{-\alpha}$.[2] Derivatives are taken as before in the singular intermediate pair states and the momentum dependence of the $r\neq 0$ density vertex $\Lambda(k;r)$ is treated in the same way as in the discussion leading to Eq. (1). Our results agree with those obtained with Wilson's method by Ma.[8]

We are extending these perturbation-theoretic methods to include the nonequilibrium case in order to discuss dynamical critical effects.

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[1]K. G. Wilson, Phys. Rev. Lett. 28, 548 (1972).

[2]A. I. Larkin and D. E. Khmel'nitskii, Zh. Eksp. Teor. Fiz. 56, 2087 (1969) [Sov. Phys. JETP 29, 1123 (1969)].

[3]E. Brezin, D. J. Wallace, and K. G. Wilson, to be published.

[4]A. Z. Patashinskii and V. L. Pokrovskii, Zh. Eksp. Teor. Fiz. 46, 994 (1964) [Sov. Phys. JETP 19, 677 (1964)].

[5]B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. 178, 1072 (1969).

[6]The Feynman rules give, for channel 1 graphs, a factor of 1/2 which arises from the two equivalent lines.

[7]P. Nozières, *Interacting Fermi Systems* (Benjamin, New York, 1964), Chap. 6.

[8]S.-K. Ma, Phys. Rev. Lett. 29, 1311 (1972).

Macroscopic Model of Formation of Vacancies in Semiconductors

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We treat the vacancy as a bubble of one atomic volume. We use empirical values of the surface tension measured for the metallic liquid phase to estimate the free energy of formation of this bubble. A small additive correction is made to account for covalent bonding in the semiconducting phase. The model is reasonable for cases where the Wigner-Seitz atomic radius is large compared with the dielectric screening length. Good agreement with experiment is found for available data for Si, Ge, and Sn.

The electronic structure and energy of formation ΔF_v of vacancies in crystals have been discussed theoretically using a variety of wave-mechanical methods. Pseudopotential calculations have been reported for alkali[1,2] and noble[3] metals, Al,[4] Si,[5,6] and Ge.[6] Molecular-orbital calculations have been made for diamond,[7] Si,[8] and Ge.[9] In general this work has shown that for