Calculation of Dynamic Critical Properties Using Wilson's Expansion Methods

B. I. Halperin and P. C. Hohenberg
Bell Laboratories, Murray Hill, New Jersey 07974

and

Shang-keng Ma*
Department of Physics, University of California, San Diego, La Jolla, California 92037
(Received 10 October 1972)

The dynamic critical behavior of a continuum analog of the kinetic Ising model is studied using a generalization of Wilson's expansion methods. Results are found which disagree with the mode-mode coupling approach and the conventional (Van Hove) theory.

A major advance in our understanding of the properties of a system near its critical point has resulted from the discovery of methods for obtaining static critical exponents as power series expansions in $\epsilon = 4-d$,[1] and in $1/n$.[2] (d is the dimensionality of the system, and n the dimensionality of the order parameter.) We have extended these techniques to calculate the exponent for the time-dependent critical behavior of a simple system—the time-dependent Ginzburg-Landau (TDGL) model. This is a continuum generalization of the kinetic Ising model introduced by Glauber,[3] in which time dependence is introduced via weak coupling to an infinite heat reservoir at each lattice site. In the case where the order parameter is not conserved, we find a characteristic frequency $\omega_k \sim k^{2+c\eta}$, with $c \geq 0$ in all cases. This disagrees with the conventional (Van Hove[4]) prediction ($c=-1$), and results inferred from mode-mode coupling theories.[5] When the order parameter is conserved, on the other hand, we find $\omega_k \sim k^{4-\eta}$, in agreement with these theories.

The TDGL model is described by the equations[6]

$$\frac{\partial s_\alpha}{\partial t} = -\left(\frac{\Gamma}{k_B T}\right)\frac{\delta H}{\delta s_\alpha} + \eta_\alpha, \tag{1}$$

$$\frac{1}{k_B T}\frac{\delta H}{\delta s_\alpha} = (r_0 - \nabla^2 + 4u_0 \sum_{\alpha'} s_{\alpha'}^2) s_\alpha - h. \tag{2}$$

Here $s_\alpha(\vec{x}, t)$ is the α component of the order parameter at position $\vec{x}$ and time t, $\vec{x}$ is a point in a d-dimensional space, and α varies from 1 to n; the Hamiltonian H is the one employed by Wilson,[1] except for the inclusion of an infinitesimal *position-* and *time-dependent* magnetic field $k_B T h(\vec{x}, t)$; and η_α is a Langevin noise source with mean zero, and correlation function

$$\langle \eta_\alpha(\vec{x}, t)\eta_{\alpha'}(\vec{x}', t')\rangle = 2\Gamma\delta(\vec{x}-\vec{x}')\delta(t-t')\delta_{\alpha\alpha'}. \tag{3}$$

It is understood that only fluctuations with wave vectors smaller than a cutoff Λ of order unity are to be included in the above, but frequencies may range from $-\infty$ to ∞. If Γ is proportional to ∇^2, then the integral over space of s_α is *conserved,* and $\partial s_\alpha/\partial t$ is described by a diffusion equation for $T > T_c$. We shall primarily discuss the case where Γ is a constant, so that the value of the $k=0$ component of s_α is *not conserved,* i.e., it relaxes at a finite frequency above T_c. In either case, the static properties are the same, and all thermodynamic properties and equal-time correlation functions are identical to those calculated by Wilson.[1]

We shall study the linear response function $\chi(k, \omega)$, which relates the expectation value of s_α to the time-dependent field h, for small values of the wave vector $\vec{k}$ and frequency ω. For $T = T_c$, according to the dynamic scaling hypothesis,[7] we expect to have

$$\chi^{-1}(k, \omega) = k^{2-\eta} f(\omega/\omega_k), \tag{4}$$

$$\omega_k \equiv \Gamma k^z, \tag{5}$$

where z is an unknown exponent, and f is a dimensionless function. Note that χ is equal to the static correlation function $g(k) \sim k^{\eta-2}$ when $\omega = 0$, so that f must approach a finite constant when its argument approaches zero. The exponent η has been calculated by Wilson[1] to be $\eta = \epsilon^2(n+2)/2(n+8)^2 + O(\epsilon^3)$. For $2 < d < 4$, Ma[2] has found

$$\eta = 4n^{-1}[(4/d)-1]\sin\pi(\tfrac{1}{2}d-1)[\pi(\tfrac{1}{2}d-1)B(\tfrac{1}{2}d-1, \tfrac{1}{2}d-1)]^{-1} + O(n^{-2}),$$

where $B(u, v)$ is the beta function.

It is convenient to write $\chi(k,\omega)$ in the form

$$\chi(k,\omega)^{-1}=G_0^{-1}(k,\omega)+\Sigma(k,\omega), \tag{6}$$

where G_0^{-1} is the value of χ^{-1} when $u_0=0$, namely

$$G_0^{-1}=-i\omega/\Gamma+r_0+k^2. \tag{7}$$

A perturbation expansion for $\Sigma(k,\omega)$ can be developed, whose general structure is described in Ref. 6 for the TDGL model of a superconductor ($n=2$). A typical diagram of order u_0^2 for the self-energy is shown in Fig. 1(a). The value of this diagram is

$$\Sigma_{(2)}(k,\omega)=24(n+2)(4u_0)^2\int\frac{d^dk_1}{(2\pi)^d}\frac{d^dk_2}{(2\pi)^d}\frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\times G_0(\vec{k}-\vec{k}_1-\vec{k}_2,\omega-\omega_1-\omega_2)\frac{1}{\omega_1}\operatorname{Im}G_0(k_1,\omega_1)\frac{1}{\omega_2}\operatorname{Im}G_0(k_2,\omega_2). \tag{8}$$

Equation (8) in fact gives the entire contribution to Σ of order u_0^2, other than a term independent of k and ω, which contributes to a renormalization of T_c, but does not affect the correlation functions at T_c.

Now let us examine (4) and (8) near four dimensions. In the static case, Wilson[1] has argued that the asymptotic form of $g(k)$ at $T=T_c$ and $k\to 0$ can be obtained directly from the perturbation series for g provided one chooses $u_0=2\pi^2\epsilon/(n+8)$ (correct to lowest order in ϵ), and systematically expands all diagrams in powers of ϵ. We assert that the same procedure will yield the correct form for the dynamic correlation function.[8] To apply the Wilson prescription, we first note that when $r_0=u_0=0$, which is the correct limit for the critical point in four dimensions, χ^{-1} is given by (7), and the exponent z of (5) has the value 2. If we take the limit where $k=0$, while ω/Γ is small but finite, we expect *in general* that χ^{-1} will have a finite value. According to dynamic scaling [Eq. (4)], χ^{-1} will then have the form

$$\chi^{-1}=c_1\omega^{1-\lambda}, \tag{9}$$

where $1-\lambda=(2-\eta)/z$. Furthermore in the limit $\epsilon\to 0$, we should have $\lambda\to 0$, and $c_1\to i\Gamma^{-1}$.

In order to compute $\chi^{-1}(0,\omega)$ to order ϵ^2, we need only evaluate (8) at $d=4$, with $k=0$ and $r_0=0$. The leading term for small ω is proportional to $i\omega\ln\omega$. The coefficient of this term may be evaluated, and we find

$$\chi(0,\omega)^{-1}\sim -i(\omega/\Gamma)[1-u_0^2b_1\ln\omega], \tag{10}$$

where $b_1=3(n+2)\ln(\frac{4}{3})/8\pi^4$. This is compatible with (9) and the expressions for η and u_0 if and only if $\lambda=b_1u_0^2$, or

$$z=2+c\eta, \tag{11}$$

with $c=6\ln(\frac{4}{3})-1$, to order ϵ^2. We note that c is independent of n in this case.

In order to check the dynamic scaling assumption (4) to order ϵ^2, we consider Eq. (8) in the limit $\omega\to 0$, $k\to 0$, with $\omega/\Gamma k^2$ finite. We find

$$\chi^{-1}(k,\omega)=k^2[1-u_0^2b_2\ln k]-i(\omega/\Gamma)[1-u_0^2b_3\ln k]+u_0^2k^2\Phi(\omega/\Gamma k^2), \tag{12}$$

where $b_2=(n+2)/8\pi^4$, $b_3=2b_1$, and Φ is a regular function of its argument, in the sense that all derivatives exist at $\omega/\Gamma k^2\to 0$. Using Wilson's expression for η and Eq. (11), it is now easy to check that Eq. (12) is consistent with the dynamic scaling assumption (4) to order ϵ^2, with the function f identified as

$$f(x)=1-ix+\epsilon^2[2\pi^2/(n+8)]^2\Phi(x). \tag{13}$$

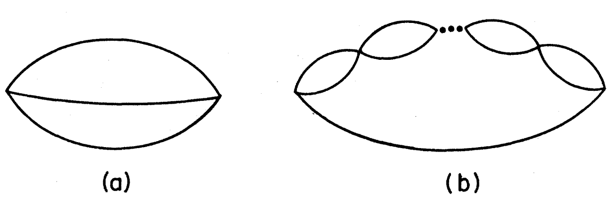

FIG. 1. (a) Diagram contributing to the self-energy to order ϵ^2. (b) General form of the self-energy to order $1/n$.

In the limit $\omega/\Gamma k^2 \to \infty$, of course, $\Phi(\omega/\Gamma k^2)$ diverges as $ib_1(\omega/\Gamma k^2)\ln(\omega/\Gamma k^2)$, in order to make contact with (9) and (10).

Let us now turn to the expansion in $1/n$. As in the static case,[2] in order to evaluate χ^{-1} to first order in $1/n$, we must sum the diagrams shown in Fig. 1(b). This yields, for $T = T_c$,

$$\mathrm{Im}\Sigma(k,\omega) = \left(\frac{2\omega}{\Gamma n}\right)\int_{-\infty}^{\infty}\frac{d\nu}{2\pi\nu}\int\frac{d^dp}{(2\pi)^d}\,\frac{I(p,\nu)}{[\Gamma^{-2}(\omega-\nu)^2 + (\vec{k}-\vec{p})^4]}, \tag{14}$$

$$I(p,\nu) = 2\,\mathrm{Im}\left\{\int\frac{d^dq}{(2\pi)^d}\,q^{-2}(\vec{p}+\vec{q})^{-2}\left[\frac{q^2+(\vec{p}+\vec{q})^2}{q^2+(\vec{p}+\vec{q})^2 - i\nu\Gamma^{-1}}\right]\right\}^{-1}. \tag{15}$$

Taking $k = 0$, and ω small but finite, we again find $\mathrm{Im}\Sigma$ to be proportional to $\omega\ln\omega$; comparing with Eqs. (9), (4), and (5), we find Eq. (11), with

$$c = \left(\frac{4}{4-d}\right)\left\{\frac{dB(\frac{1}{2}d-1,\frac{1}{2}d-1)}{8\int_0^{1/2}dx[x(2-x)]^{d/2-2}} - 1\right\}, \tag{16}$$

where we have used Ma's expression[2] for η, given in the equation preceding (6). It may be shown from Eq. (16) that for $d = 4$, $c = 6\ln(\frac{4}{3}) - 1$, in accordance with our previous result, while for $d = 3$, $c = \frac{1}{2}$, and for $d = 2$, $c = 0$.

The case where the order parameter is *conserved* is similar to that considered above. Equations (1)–(8) are essentially unchanged, except that Γ is everywhere replaced by $\lambda_0 k^2$, where λ_0 is the "unrenormalized transport coefficient" for s. When we evaluate the self-energy in Eq. (8), however, for the case where $\omega \to 0$ and $k \to 0$, with $\omega/\lambda_0 k^2$ small but finite, we find no term of order $(\omega/\lambda_0 k^2)\ln\omega$. Thus there is no correction to the conventional form, $\chi^{-1}(0,\omega) \sim i\omega/\lambda_0 k^2$. We therefore have $\omega_k \sim \lambda_0 k^{4-\eta}$, as predicted by the conventional theory. Similarly, if we consider (8) in the case where $\omega/\lambda_0 k^4$ is a finite constant, we find

$$\Sigma(k,\omega) \sim -\eta k^2\ln k + b_4 k^2\psi(\omega/\lambda_0 k^4), \tag{17}$$

where b_4 is a constant of order ϵ^2, and ψ is a dimensionless regular function of $\omega/\lambda_0 k^4$. Again, this result shows that the conventional theory is correct in this case, and that the dynamic scaling assumption is verified to order ϵ^2.

Let us comment on the relevance of our calculations to other systems. For static properties the universality hypothesis leads one to believe that the exponents of the "Ginzburg-Landau" model[1] will be the same as those for other systems with the same symmetry and dimensionality. For dynamic critical phenomena, we again expect to have a certain degree of universality, but the classes of systems having the same exponents clearly must be smaller than for static properties alone. For example, the two systems considered here (order parameter conserved or not conserved) have identical static properties, but have different dynamic exponents. On the other hand, renormalization-group arguments[8] certainly support the idea that for $n = 1$, our continuum TDGL models should have the same critical exponents as their discrete kinetic Ising model counterparts, independent of the details of the lattice, or of the coupling to the reservoirs, etc.

The TDGL models differ obviously from some of the more commonly considered models, such as the isotropic Heisenberg ferromagnet or antiferromagnet, in that they have no propagating hydrodynamic modes for the order parameter, even for $T < T_c$. The TDGL models are more analogous to anisotropic Heisenberg models, where there are also no propagating hydrodynamic modes. Examples include the uniaxial ferromagnet, where the order parameter is conserved, and models where the order parameter is not conserved, such as the uniaxial *anti*ferromagnet or the anisotropic ferromagnet without a symmetry axis. The TDGL models differ even from these, however, in that the assumption of an infinite heat reservoir at every site eliminates any effects that energy conservation might have on the dynamic critical properties. Within the spirit of mode-mode coupling theory,[5] one might ask whether the absence of a low-frequency thermal diffusion mode in the TDGL models will affect their dynamic critical exponents. In contrast to the TDGL and kinetic Ising models, the isotropic Heisenberg ferromagnet or antiferromagnet does not seem to approach a simple Gaussian fixed point for their dynamic properties as $d \to 4$ or $n \to \infty$, and the methods of the present paper are not directly applicable. For example, by studying the Heisenberg ferromagnet in the limit of long-range forces, or by using dynamic scaling, one finds that the exponent z does not reach its conventional value ($z = 4$) in four dimensions.[9]

The frequencies ω_k found in the present paper are always equal to or smaller than those predicted by the conventional theory. This is consistent with a rigorous theorem that has been proved[10] for purely dissipative models of the present type, and may be contrasted with cases such as the Heisenberg ferromagnet or antiferromagnet where the characteristic frequencies, according to dynamic scaling[7] or the mode-mode theories,[5] are always larger than the conventional predictions. A characteristic frequency slower than the conventional theory has previously been obtained for the two-dimensional kinetic Ising model by Yahata and Suzuki,[11] based on high-temperature series expansions. Specifically, these authors found a relaxation frequency $\omega \sim \kappa^2$ for the $k=0$ component of the magnetization above T_c(i.e., $z=2$), whereas the conventional theory predicts $z=\frac{7}{4}$ for this case. We note that the result $z=2$ ($c=0$) for two dimensions is precisely the one obtained in Eq. (16) to leading order in $1/n$. Recently, however, Schneider, Stoll, and Binder[12] have studied the same model using a Monte Carlo molecular-dynamics approach, and find results which agree with the conventional theory for the relaxation of the uniform mode.

*Alfred P. Sloan Foundation Fellow.

[1]K. G. Wilson and M. E. Fisher, Phys. Rev. Lett. 28, 240 (1972); K. G. Wilson, Phys. Rev. Lett. 28, 548 (1972).

[2]R. Abe, Progr. Theor. Phys. (to be published); M. Suzuki, to be published; K. G. Wilson, private communication; S. Ma, Phys. Rev. Lett. 29, 1311 (1972), and to be published; R. A. Ferrell and D. J. Scalapino, Phys. Rev. Lett. 29, 413 (1972).

[3]R. Glauber, J. Math. Phys. (N. Y.) 4, 294 (1963).

[4]L. Van Hove, Phys. Rev. 93, 1374 (1954).

[5]K. Kawasaki, Progr. Theor. Phys. 40, 706 (1968); G. E. Laramore and L. P. Kadanoff, Phys. Rev. 187, 619 (1969); E. Riedel and F. Wegner, Phys. Lett. 32A, 273 (1970).

[6]See, for instance, J. R. Tucker and B. I. Halperin, Phys. Rev. B 3, 3768 (1971), and references therein.

[7]R. A. Ferrell *et al.*, Phys. Rev. Lett. 18, 891 (1967); B. I. Halperin and P. C. Hohenberg, Phys. Rev. 177, 952 (1969).

[8]The justification for this procedure in terms of Wilson's renormalization group ideas is similar to one that can be given for the static case. In particular, we have studied the infinitesimal generator of the renormalization group for the dynamic system in the vicinity of the Gaussian fixed point [$u_0=r_0=0$ in Eq. (2)], and we find that in four dimensions there is only one nontrivial zero eigenvalue, just as in the static case. The corresponding low-lying eigenvalue can be prevented from "contaminating" the ϵ expansion of the exponents by properly choosing a single parameter in the Hamiltonian, specifically by choosing u_0 according to Wilson's prescription. Details will be published elsewhere.

[9]P. C. Hohenberg, M. De Leener, and P. Résibois, to be published.

[10]K. Kawasaki, Phys. Rev. 148, 375 (1966).

[11]H. Yahata and M. Suzuki, J. Phys. Soc. Jap. 27, 1421 (1969).

[12]T. Schneider, E. Stoll, and K. Binder, Phys. Rev. Lett. 29, 1080 (1972).

Superconductivity Mechanisms and Covalent Instabilities

J. C. Phillips
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 28 September 1972)

Quantitative estimates are made of the maximum value of the superconductive transition temperature T_c attainable through combining electron-exciton interactions with electron-phonon interactions in metal-semiconductor sandwiches. Because of covalent instabilities, it is argued that no enhancement of T_c can be expected if the initial value of T_c in the pure metal was greater than 5°K.

Some fifteen years ago the discovery by Bardeen, Cooper, and Schfieffer[1] (BCS) of a microscopic theory of superconductivity raised hopes of achieving higher superconducting transition temperatures T_c through careful choice of coupling parameters and sample configurations. However, as Matthias has often emphasized,[2] these hopes have yet to be realized. One reason for this is that the mechanism utilized in the BCS theory, the electron-phonon interaction, is well understood in the normal state only for structurally stable metals like Al (with low values of T_c) and not for structurally unstable metals like Pb, NbN, and Nb_3Sn with high values of T_c. After more