Static and dynamic critical behaviour of displacive phase transition at T_c in 1/n expansion

1975 J. Phys. A: Math. Gen. 8 1115

(http://iopscience.iop.org/0305-4470/8/7/014)

J. Phys. A: Math. Gen., Vol. 8, No. 7, 1975. Printed in Great Britain. © 1975

Static and dynamic critical behaviour of displacive phase transition at T_c in $1/n$ expansion†

A Holz‡ and J T N Medeiros

Instituto de Física, Universidade Federal do Rio Grande do Sul, 90000 Porto Alegre, Brazil

Received 6 January 1975, in final form 20 February 1975

Abstract. Quantum effects on the static critical behaviour of an isotropic n-vector model undergoing a displacement-type phase transition are studied at T_c and to $O(1/n)$. For $T_c \neq 0$ there is no quantum effect on η, and for $T_c = 0$ one gets $\eta = 0$ for $d > 3$, and for $2 < d < 3$ η is due to quantum fluctuations, implying that it assumes a different value than in the classical case. The dynamical behaviour of the system violates the dynamic scaling hypothesis.

1. Introduction

In this paper we are essentially interested in static and dynamic critical phenomena in an anharmonic lattice model simulating a displacive-type phase transition (PT). (A brief account of this work has been published elsewhere (Holz and Medeiros 1975).) This model is representative for a structural PT which is mediated by soft phonons (Anderson 1960, Cochran 1960). It has been shown by Cowley and Bruce (1973) and Jouvet and Holz (1974) that the classical critical behaviour of a structural PT mediated by a three-component phonon field can be studied by means of a renormalization group (RG) approach to a Heisenberg-type Hamiltonian. Quantum effects and dynamical properties have not been considered by these authors.

Quantum effects on displacive-type PT were first studied by Barrett (1952) and later by Gillis (1969) in the self-consistent phonon formalism. Both authors obtain deviations from the Curie–Weiss law for the dielectric constant at low temperatures. Rechester (1971) was the first to study low-temperature PT of displacive type within the framework of a self-consistent field theory and in the 'parquet' approximation. In particular he pointed out that as the transition temperature T_c approaches 0 K quantum fluctuations get more and more important. Khmel'nitskii and Shneerson (1971, 1973) extended the work of Rechester by taking anisotropy of the anharmonic interaction and also scattering of critical phonons by impurities into account. These authors, however, did not study the q and ω dependence of the soft-phonon propagators at T_c, ie, the static and dynamic scaling properties of the system which are the objectives of the present work.

Let us briefly point out that the potential experimental background to the present topic is the second-order displacive PT occurring in solid solutions of GeTe and SnTe

† Work supported in part by Conselho Nacional de Pesquisas and Banco Nacional do Desenvolvimento Econômico, Brazil.

‡ Now at Institut für Theoretische Physik, Freie Universität Berlin, 1 Berlin 33, Arnimallee 3, Germany.

with T_c ranging from about 700 K to nearly 0 K respectively (Goldak *et al* 1966, Bierly *et al* 1963), and also $KTaO_3$ (Shirane *et al* 1967) where a PT occurs at about 10 K.

The Hamiltonian we use can be written in the form

$$H = \sum_{\alpha,q} \tfrac{1}{2}(\dot{Q}_{\alpha,q}\dot{Q}_{\alpha,-q} + \omega_q^{02} Q_{\alpha,q}Q_{\alpha,-q}) + \frac{g_0}{4!}\sum_{\substack{\alpha,\beta \\ q}} Q_{\alpha,q_1}Q_{\alpha,q_2}Q_{\beta,q_3}Q_{\beta,-q_1-q_2-q_3}, \tag{1}$$

where the normal coordinates $Q_{\alpha,q}(t)(\dot{Q} = \partial Q/\partial t)$ obey the simple commutation relations

$$[\dot{Q}_{\alpha,q}(t), Q_{\alpha',q'}(t)] = (\hbar/i)\delta_{\alpha\alpha'}\delta_{q,-q'}. \tag{2}$$

Here the Greek letter sums go over the n components of the field, g_0 is the isotropic bare four-phonon vertex and

$$\omega_q^{02} = q^2 + m_0^2,$$

the bare energy of the phonons squared. For further details see eg Kwok (1967). The model described is equivalent to an isotropic n-vector model to which we apply the $1/n$ expansion techniques (see, eg, Ma 1973). Let us point out that Droz (1974) has also studied the problem defined by (1) and (2) in the T-dependent formalism but has not computed dynamical properties. The analysis of Droz is essentially restricted to the case $N \to \infty$. The paper of Sasvári and Szépfalusy (1974) on structural PT will be discussed in § 5.

Dynamical critical properties were studied first using diagram techniques in order to verify microscopically the dynamic scaling hypothesis (Ferrell *et al* 1967, Halperin and Hohenberg 1969) by Halperin *et al* (1972) for the time-dependent Ginzburg–Landau (TDGL) model, ie, a classical model. Recently, however, there have appeared a fair number of papers which treat time-dependent critical phenomena in the T-dependent formalism in particular in connection with Bose–Einstein condensation phenomena (Kondor and Szépfalusy 1974, Abe and Hikami 1974, Suzuki and Igarashi 1974). In these studies the dynamic scaling hypothesis is assumed to hold as a starting point for the $1/n$ expansion. It is found that there is no quantum effect on η to order $1/n$.

The present analysis differs in an essential point from the above-mentioned work in that the unperturbed phonon propagator

$$D^0(q, \omega_n) = (-\omega_n^2 + q^2 + m_0^2)^{-1} \tag{3}$$

has a different frequency dependence from the Bose case, where

$$G^0(q, \omega_n) = (\omega_n - q^2 - m_0^2)^{-1} \tag{4}$$

holds with $\omega_n = 2\pi i n/\hbar\beta$ ($\beta = 1/k_B T$). The difference between (3) and (4) obviously requires a new computation of all relevant graphs.

Let us finally mention some shortcomings of the present model. First the anisotropy of the problem, which is always present, is not taken into account. According to Wallace (1973) and Ketley and Wallace (1973) and Aharony (1973a, b) this may change the second-order PT into a first-order PT or imply a different critical behaviour. For the low-temperature PT the anisotropy has been taken into account by Khmel'nitskii and Shneerson (1973) where a first-order PT is obtained. In a recent study of the general n-vector model by Brézin *et al* (1974) it is shown that to lowest order in ϵ and for $n < 4$ the O(n) symmetry is dynamically generated at the critical point. In view of this result therefore, it does not seem too serious a drawback to neglect the anisotropy. The second more serious point is that (1) does not couple to the acoustic phonon system.

Larkin and Pikin (1969) first noted that this will produce a PT of the first kind. Because in many systems the first-order nature of the PT does not show up within experimental accuracy as far as static properties are concerned, the effect may be neglected. The acoustic phonon interaction is certainly of importance for the dynamics of the system and we will come back to this point in the discussion.

The plan of the paper is as follows. In § 2 we develop the basic formalism of the problem and calculate the elementary phonon bubble for $T_c \neq 0$ and $T_c = 0$. In § 3 we compute η for these two cases. In § 4 the dynamical critical behaviour is studied for $T_c \neq 0$ and in § 5 the results are discussed.

2. Basic formalism

The partition function of the problem in the interaction representation can be written as follows:

$$Z = \operatorname{Tr}\exp\Bigg[-\tfrac{1}{2}\sum_{l,\alpha}\int_{\boldsymbol{q}'}(-\omega_l'^2+q'^2+m_0'^2)Q_\alpha'(\boldsymbol{q}',\omega_l')Q_\alpha'(-\boldsymbol{q}',-\omega_l')$$
$$-\frac{g_0'}{4!}\sum_{\alpha,\beta}\sum_{\omega_1,\omega_2,\omega_3}^{\infty}\int_{\boldsymbol{q}_1'}\int_{\boldsymbol{q}_2'}\int_{\boldsymbol{q}_3'}Q_\alpha'(\boldsymbol{q}_1',\omega_1')Q_\alpha'(\boldsymbol{q}_2',\omega_2')Q_\beta'(\boldsymbol{q}_3',\omega_3')$$
$$\times Q_\beta'\left(-\sum_1^3\boldsymbol{q}_i',-\sum_1^3\omega_i'\right)\Bigg] \tag{5}$$

where we have got rid of all coefficient ballast by going over to dimensionless quantities

$$(\Lambda, m_0, \boldsymbol{q}, \omega_n)\hbar\beta \to (\Lambda', m_0', \boldsymbol{q}', \omega_n'),$$
$$[\beta/(\hbar\beta)^{d+2}]Q^2 \to Q'^2, \tag{6}$$
$$g_0(\hbar\beta)^{4-d}/\beta \to g_0'.$$

With (5) all Feynman rules for graph calculation apply, considering $\hbar$ and $\hbar\beta$ as unity. The symbol $\int_{\boldsymbol{q}} \equiv (2\pi)^{-d}\int d^d\boldsymbol{q}$ will be used throughout. The cut-off Λ is of the order of the inverse interatomic distance.

In order to calculate the static and dynamic $\boldsymbol{q}$ and ω dependence of the propagator at T_c up to $O(1/n)$ it is sufficient to take chain diagrams into account and also to assume $g_0' \sim 1/n$. Imposing the following form on the dressed propagator (for the sake of simplicity all primes are dropped again)

$$D^{-1}(\boldsymbol{q}, \omega_n, m^2) = -\omega_n^2+\boldsymbol{q}^2+m^2-\Sigma(\boldsymbol{q}, \omega_n, m^2), \tag{7}$$

where only a mass counter term has been introduced and where we require

$$\Sigma(0, 0, m^2) = 0, \tag{8}$$

we obtain in the chain approximation

$$\Sigma(\boldsymbol{q}, \omega_n, 0) = \frac{n+2}{18}g_0^2\sum_l\int_{\boldsymbol{q}''}\frac{I(\boldsymbol{q}'', \omega_l, 0)}{1+g_0\frac{1}{6}(n+8)I(\boldsymbol{q}'', \omega_l, 0)}$$
$$\times\left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2-(\omega_n-\omega_l)^2}-\frac{1}{q''^2-\omega_l^2}\right), \tag{9}$$

where

$$I(\boldsymbol{q}, \omega_n, m^2) = \sum_l \int_{\boldsymbol{q}'} \frac{1}{[m^2+(\boldsymbol{q}'+\boldsymbol{q})^2-(\omega_n-\omega_l)^2](m^2+\boldsymbol{q}'^2-\omega_l^2)} \tag{10}$$

represents the elementary bubble. The evaluation of (10) is done by means of the Feynman parameter and contour methods where one obtains

$$\begin{aligned} I(\boldsymbol{q}, \omega_n, m^2) = f(d)\left(\frac{-\sin\frac{1}{2}\pi d}{\pi}\right) \int_0^1 \mathrm{d}\alpha \int_B^{(\Lambda^2+B^2)^{1/2}} \frac{\mathrm{d}x(N^0(x+\alpha\omega_n)-N^0(-x+\alpha\omega_n))}{(x^2-B^2)^{2-d/2}} \\ + f(d)\frac{\sin(\frac{1}{2}\pi d)\Lambda^{d-2}}{\pi(2-d)} \int_0^1 \mathrm{d}\alpha \frac{N^0(\alpha\omega_n-(\Lambda^2+B^2)^{1/2})-N^0(\alpha\omega_n+(\Lambda^2+B^2)^{1/2})}{(\Lambda^2+B^2)^{1/2}} \end{aligned} \tag{11}$$

with the abbreviations

$$\begin{aligned} B^2 &= m^2+(1-\alpha)\alpha(\boldsymbol{q}^2-\omega_n^2) \\ f(d) &= 2^{-d}\pi^{-d/2}\Gamma(d/2)^{-1}\frac{(1-d/2)\pi}{\sin\frac{1}{2}\pi d} \end{aligned} \tag{12}$$

and $N^0(x)$ is the Bose–Einstein function.

Expression (11) is already in a form which allows us to make the analytical continuation $\omega_n \to \omega + \mathrm{i}0^+$. Next we study (11) for the two cases $T_c \neq 0$ and $T_c = 0$, and for $m^2 = 0$, ie, at T_c.

2.1. *Classical fluctuation regime* $T_c \neq 0$

The leading contribution to (11) will be that due to the first term and because the most singular behaviour results from $\alpha \to 0$ and $x \to 0$ the Bose–Einstein functions can be expanded in a Taylor series. The integration over x is easily performed and yields for the leading term

$$\begin{aligned} I(\boldsymbol{q}, \omega_n, 0) \sim -\frac{f(d)\sin\frac{1}{2}\pi d}{(d-2)\pi}\frac{4\Lambda^d}{d}\int_0^1 \frac{\mathrm{d}\alpha}{[\frac{1}{2}\alpha(\boldsymbol{q}^2-\omega_n^2)-\frac{1}{4}\alpha^2\boldsymbol{q}^2]^2} \\ \times F(2, d/2; d/2+1; -\Lambda^2/[\tfrac{1}{2}\alpha(\boldsymbol{q}^2-\omega_n^2)-\tfrac{1}{4}\alpha^2 q^2]), \end{aligned} \tag{13}$$

which can be transformed into

$$I(\boldsymbol{q}, \omega_n, 0) \sim -\frac{f(d)\sin\frac{1}{2}\pi d}{(d-2)\pi d}\frac{8\Lambda^2}{q^2}\int_{4\Lambda^2/q^2(2x-1)}^{\infty} \frac{\mathrm{d}zF(2, \frac{1}{2}d; 1+d/2; -z)}{[(-4\Lambda^2/q^2 z)+x^2]^{1/2}} \qquad 2 < d < 4 \tag{14}$$

where $x = (\boldsymbol{q}^2-\omega_n^2)/\boldsymbol{q}^2$. From the property of the hypergeometric function $F(\alpha, \beta; \gamma; x)$ to have a cut along the real axis extending from $x = 1$ to infinity it follows that $I(\boldsymbol{q}, \omega, 0)$ has a cut which extends from $\omega^2 = \boldsymbol{q}^2/2$ to $2\Lambda^2+\frac{1}{2}\boldsymbol{q}^2$. Because the bubble involves two-phonon processes it is clear that in order to transfer momentum $\boldsymbol{q}$ two phonons with momentum $\boldsymbol{q}/2$ have to be created in order to obtain the minimum $\omega^2(=\frac{1}{4}\boldsymbol{q}^2+\frac{1}{4}\boldsymbol{q}^2)$. Because of the momentum cut-off the maximum ω^2 is $\max\omega^2 = 2\Lambda^2$. That the cut extends to $2\Lambda^2+\frac{1}{2}\boldsymbol{q}^2$ is due to translating the origin of the $\boldsymbol{q}'$ integration of the bubble. This is clearly an approximation which is not too important. Because (14) is not easy to handle an approximate form of (13) will be used in the following. A substantial simplification arises once one observes that the $\alpha^2\boldsymbol{q}^2/4$ term in the denominators of the arguments in (13) complicates the situation. Because the main contribution comes from $\alpha \sim 0$, we miss out this term in favour of the term proportional to α and obtain, using the integral representation of the $F(\alpha, \beta; \gamma; x)$ function (Erdélyi 1953) and interchanging integrations,

$$I_a(\boldsymbol{q}, \omega_n, 0) \sim \frac{-2f(d)\sin\frac{1}{2}\pi d}{(\frac{1}{2}d-1)^2\pi(\boldsymbol{q}^2-\omega_n^2)}\Lambda^{d-2}F(1, \tfrac{1}{2}d-1; \tfrac{1}{2}d; -2\Lambda^2/(\boldsymbol{q}^2-\omega_n^2)). \tag{15}$$

Let us point out that the ratio

$$r = \frac{I(\boldsymbol{q}, 0, 0)}{I_a(\boldsymbol{q}, 0, 0)} = 2^{(d/2)-2}\frac{\Gamma(d/2)\Gamma(\frac{1}{2}d-1)}{\Gamma(d-2)} \tag{16}$$

assumes its maximum value for $d = 3$, $r = \pi/\sqrt{8}$ and is 1 for $d = 2$ and 4. Although the cut of (15) starts now at $\omega^2 = \boldsymbol{q}^2$ it can be considered as a good approximation because the main contribution to the self-energy results from the opposite end of the cut. Due to the fact that the static limits of (14) and (15) almost coincide we think it is justified to study the problem using the approximation (15).

2.2. *Quantum fluctuation regime $T_c = 0$*

In the $T_c = 0$ limit one uses instead of the propagator (3) the propagator

$$D^0(\boldsymbol{q}, \omega) = (-\omega^2 + \boldsymbol{q}^2 + m_0^2 - i\delta)^{-1} \tag{17}$$

and does not perform the normalization (6).

Here the infinitesimal $i\delta$ implies that for $\omega > 0$ the pole is below the real axis whereas for $\omega < 0$ the pole is above the real axis. The propagator is thus the same as the Feynman propagator of the scalar meson theory described by a Klein–Gordon equation. If in addition one substitutes

$$\sum_l \to \frac{\hbar\beta}{2\pi i}\int_{-i\infty}^{i\infty} d\omega \tag{18}$$

all formulae of the T-dependent formalism can be applied. Clearly (18) gives the Wick-rotated contour of the contour for which (17) is specified. The bubble can now be calculated in an analogous way to the earlier calculation and one obtains

$$I(\boldsymbol{q}, \omega_n, 0) = f(d)\left(\frac{-\sin\frac{1}{2}\pi d}{\pi}\right)\frac{\Lambda^{d-3}}{(d-2)(d-1)}\frac{4\Lambda^2}{\boldsymbol{q}^2-\omega^2}F\left(1, \frac{d-1}{2}; \frac{d+1}{2}; \frac{-4\Lambda^2}{\boldsymbol{q}^2-\omega^2}\right). \tag{19}$$

3. Evaluation of η

In order to evaluate η one brings (9) into the form

$$\begin{aligned}\Sigma(\boldsymbol{q}, \omega_n, 0) = {}& \frac{1}{3}\frac{n+2}{n+8}g_0\sum_l\int_{\boldsymbol{q}''}\left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2-(\omega_n-\omega_l)^2} - \frac{1}{\boldsymbol{q}''^2-\omega_l^2}\right)\\ & -\frac{1}{3}\frac{n+2}{n+8}g_0\sum_l\int_{\boldsymbol{q}''}\frac{1}{1+g_0\frac{1}{6}(n+8)I(\boldsymbol{q}'', \omega_l, 0)}\\ & \times\left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2-(\omega_n-\omega_l)^2} - \frac{1}{\boldsymbol{q}''^2-\omega_l^2}\right).\end{aligned} \tag{20}$$

Setting $\omega_n = 0$ one has to find the $q^2 \ln q$ term of this expression. This will be discussed separately for $T_c \neq 0$ and $T_c = 0$.

3.1. *Classical fluctuation regime* $T_c \neq 0$

In order to show that there is no quantum effect on η for $T_c \neq 0$ we follow the demonstration given by Abe (1974) for the boson case. For $\omega_l = 0$, the second term of (20) gives the classical value of η because $I(\boldsymbol{q}, 0, 0)$ coincides with the classical bubble. For $\omega_l \neq 0$ one uses (9) and the fact that the bubble is a positive function along the imaginary axis. This follows from (10) and is the case for (14) and (15). Proceeding in analogous steps to those used by Abe, one concludes that there is no quantum effect on η to $O(1/n)$.

3.2. *Quantum fluctuation regime* $T_c = 0$

From (20) one obtains with (18) and with the substitutions (6) in the inverse sense

$$\Sigma(\boldsymbol{q}, \omega, 0) = \frac{1}{3}\frac{n+2}{n+8} g_0 \hbar \frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}z \int_{\boldsymbol{q}''} \left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2 - (\omega - z)^2} - \frac{1}{\boldsymbol{q}''^2 - z^2} \right)$$

$$- \frac{1}{3}\frac{n+2}{n+8} g_0 \hbar \frac{1}{2\pi \mathrm{i}} \int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}z \int_{\boldsymbol{q}''} \frac{1}{1 + \frac{1}{6} g_0 \hbar (n+8) I(\boldsymbol{q}'', z, 0)}$$

$$\times \left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2 - (\omega_n - z)^2} - \frac{1}{\boldsymbol{q}''^2 - z^2} \right) \tag{21}$$

from which the retarded self-energy is obtained by means of the analytical continuation ($\omega \to \omega + \mathrm{i}0^+$). The first term of (21) is proportional to $\boldsymbol{q}^2$. By means of dimensional arguments one finds that for $d \leqslant 3$ there is a term q^{d-1}. However, because the integral is convergent for $\Lambda \to \infty$ and $d < 3$ the origin of the $\boldsymbol{q}''$ integration can be shifted and one finds that the coefficient of q^{d-1} is zero. Accordingly the first term of (21) can be ignored.

It follows from (19) and the properties of the hypergeometric function that $I(\boldsymbol{q}, \omega_n, 0)$ gets large only for $d \leqslant 3$. Accordingly the second term of (21) does not contribute a $q^2 \ln q$ term for $d > 3$ and therefore η $(d > 3) = 0$. For $d \leqslant 3$ the leading contribution to (21) is obtained as usual by expanding the denominator of (21) in a Taylor series to yield

$$\Sigma(\boldsymbol{q}, 0, 0) \sim -\frac{(n+2)}{(n+8)^2} 2^{-d+1} \pi^{-(d+3)/2} \Gamma\left(\frac{d-1}{2}\right)^{-1} \frac{(d-2)(d-1)}{f(d) \tan \frac{1}{2}\pi d} q^2 \int_1^{\Lambda/q} \mathrm{d}x\, x^{d-1}$$

$$\times \int_{-[4\Lambda^2/q^2 - x^2]^{1/2}}^{[4\Lambda^2/q^2 - x^2]^{1/2}} \mathrm{d}z \int_0^{\pi} \mathrm{d}\theta \sin^{d-2}\theta \left(\frac{x^2 + z^2}{4}\right)^{(3-d)/2}$$

$$\times \left(\frac{1}{(1 + x^2 + 2x\cos\theta)^2 + z^2} - \frac{1}{x^2 + z^2} \right). \tag{22}$$

The small x integration contributes a q^2 term and is, therefore, of no interest and for $x \gg 1$ the denominator of the first term in the brackets of (22) can be expanded and eventually one obtains

$$\eta_q = -\frac{n+2}{(n+8)^2} \frac{(d-2)^2(d-1)2^{d-5}\pi^{1/2}}{\tan \frac{1}{2}\pi d \sin \frac{1}{2}\pi d} \frac{\Gamma(d+1/2)}{\Gamma(1+d)} \left(-1 + \frac{(3+2d)(1+2d)}{d(2+d)(1+d)} \right) \qquad 2 < d < 3,$$

$$\eta_q = 0 \qquad d > 3, \tag{23}$$

where the index q is a reminder that we are dealing with a quantum effect. It follows from (23) that $\eta_q \geqslant 0$. For $d = 3$ one gets the extrapolated value $\eta_q = 0$. Accordingly η is continuous at $d = 3$.

The results of this section can be summarized as follows. For $T_c \neq 0$ the static critical behaviour is due to classical critical fluctuations leading to a value of η which is independent of the magnitude of T_c. At $T_c = 0$ quantum fluctuations produce a value of η different from the classical value. This result can be understood as follows. For small T_c the domain in q space $\hbar q < k_B T_c$ showing classical critical behaviour shrinks to zero and the domain $\hbar q > k_B T_c$ of quantum fluctuations with $D^{-1}(q) \sim q^{2-\eta_q}$ approaches zero. Accordingly at $T_c \neq 0$ there is a crossover from η to η_q with increasing momentum but with $q \ll \Lambda$.

4. Dynamical critical behaviour for $T_c \neq 0$

The self-energy of the retarded propagator will be calculated by evaluating first $\mathrm{Im}\,\Sigma(\boldsymbol{q}, \omega + \mathrm{i}0^+, 0)$ and then by use of the dispersion relations which are obeyed by Σ, $\mathrm{Re}\,\Sigma(\boldsymbol{q}, \omega, 0)$ will be calculated.

The first term of (20) does not have an ω dependence and can therefore be ignored in the following. The l summation in (20) will be substituted by an integration along the contour C′ which encloses the cuts and poles of (20) in the ω plane. One obtains

$$\Sigma(\boldsymbol{q}, \omega_n, 0) = -\frac{1}{3}\frac{n+2}{n+8} g_0 \frac{1}{2\pi \mathrm{i}} \int_{C'} \mathrm{d}z \int_{\boldsymbol{q}''} \frac{N^0(z)}{1 + \frac{1}{6} g_0 (n+8) I(\boldsymbol{q}'', z, 0)} \times \left(\frac{1}{(\boldsymbol{q}+\boldsymbol{q}'')^2 - (\omega_n - z)^2} - \frac{1}{\boldsymbol{q}''^2 - z^2} \right). \tag{24}$$

Because the methods of evaluating (24) are well known they will not be dwelt on further. Only one point has to be established: that the first term of (24) can be approximated as in the static case

$$[1 + \tfrac{1}{6} g_0 (n+8) I(\boldsymbol{q}'', z, 0)]^{-1} \sim [\tfrac{1}{6} g_0 (n+8) I(\boldsymbol{q}'', z, 0)]^{-1}, \tag{25}$$

for $z^2 < 2\Lambda^2 + \boldsymbol{q}''^2$. This approximation is clearly justified for $z^2 \sim \boldsymbol{q}''^2$ as follows from (15) for $2 < d < 4$ and it can also be assumed that it is the region $z^2 \sim \boldsymbol{q}''^2$ which will give the main contribution to (24).

The evaluation of the imaginary part is now straightforward. One obtains, after some calculation, for the leading part of the imaginary part of the self-energy:

$$\begin{aligned} &\mathrm{Im}\,\Sigma(\boldsymbol{q}, \omega + \mathrm{i}0^+, 0) \\ &\sim +\mathrm{i}\,\mathrm{sgn}\,\omega\,\mathrm{coeff}/q \int_0^{\Lambda} \mathrm{d}\boldsymbol{q}''\, \boldsymbol{q}''^{d-2} \Bigg(\int_0^{\infty} \mathrm{d}z [(z+\omega)^2 - \boldsymbol{q}''^2]^{2-d/2} (1 - f^{-2}(z))^{d/2-\frac{3}{2}} \\ &\quad \times \theta((z+\omega)^2 - \boldsymbol{q}''^2) \theta(2\Lambda^2 + \boldsymbol{q}''^2 - (z+\omega)^2) \theta(f^2(z) - 1) [N^0(z+\omega) - N^0(z)] \\ &\quad + \int_0^{\infty} \mathrm{d}z [(z-\omega)^2 - \boldsymbol{q}''^2]^{2-d/2} (1 - f^{-2}(z))^{d/2-\frac{3}{2}} \theta((z-\omega)^2 - \boldsymbol{q}''^2) \\ &\quad \times \theta(2\Lambda^2 + \boldsymbol{q}''^2 - (z-\omega)^2) \theta(f^2(z) - 1)(1 - 2\theta(\omega - z)) \\ &\quad \times [N^0(-z+\omega) - N^0(-z)] \Bigg), \end{aligned} \tag{26}$$

where

$$\text{coeff} = 2^{d/2-1}\frac{n+2}{(n+8)^2}\pi^{-1/2}\frac{\sin(\frac{1}{2}\pi d)(\frac{1}{2}d-1)}{\Gamma((d-1)/2)\Gamma(2-d/2)}$$

$$\theta(x) = \begin{cases} 0 & x<0, \\ 1 & x>0, \end{cases}$$

$$f(x) = 2\boldsymbol{q}\boldsymbol{q}''/(\boldsymbol{q}''^2+\boldsymbol{q}^2-z^2)$$

and all ω's inside brackets are understood as $|\omega|$. The asymmetrical form of (26) is due to the latter convention. The leading contribution to (26) can now be obtained by expanding the Bose–Einstein function, normalizing all variables with $\boldsymbol{q}$ and convincing oneself that the leading contribution to (26) is obtained from the large $\boldsymbol{q}''/\boldsymbol{q}$ integration interval. Eventually one obtains for $\omega \ll \Lambda$ and $q \ll \Lambda$ the two limiting cases

$$\operatorname{Im}\Sigma(\boldsymbol{q}, \omega+\mathrm{i}0^+, 0) \sim \begin{cases} \mathrm{i}\operatorname{sgn}\omega|\omega|^{3-d/2}\Lambda^{d/2-1}, & \varkappa \gg 1 \\ \mathrm{i}\operatorname{sgn}\omega\,\omega^2(\Lambda/q)^{d/2-1}, & \varkappa \ll 1, \end{cases} \tag{27}$$

where $\varkappa = |\omega|/q$. In order to calculate the real part of the self-energy for $q = 0$ it is considerably more simple to start from (24) and set $q = 0$. The real part is obtained via the dispersion relation with a subtraction at $\omega = 0$. Expanding the Bose–Einstein function as usual one obtains after a number of intermediate steps

$$\operatorname{Re}\Sigma(0,\omega,0) \sim 2^{d/2}\frac{n+2}{(n+8)^2}\frac{\sin^2\frac{1}{2}\pi d}{\pi^2}\omega^2\int_0^\Lambda \mathrm{d}q\,q^{d-3}\,\mathrm{P}\int_0^{2\Lambda^2}\frac{\mathrm{d}x}{x+q^2}x^{2-d/2}$$
$$\times\frac{(x+2q^2-\omega^2)}{(x-\omega^2-2\omega q)(x-\omega^2+2\omega q)}. \tag{28}$$

From (28) it is a simple matter to extract the $\ln\omega$ term and one obtains

$$\operatorname{Re}\Sigma(0,\omega,0) \sim 2^{d/2}\frac{n+2}{(n+8)^2}\frac{\sin\frac{1}{2}\pi d}{\pi}\omega^2\ln\Lambda/\omega. \tag{29}$$

One anticipates that the real part depending simultaneously on ω and q is less important being probably of the form $|\omega|q\ln|\omega|q$.

The dressed retarded propagator to $O(1/n)$ is now obtained as follows:

$$D^{-1}(\boldsymbol{q},\omega+\mathrm{i}0^+,0) \sim q^{2-\eta_a}\left[1-(\omega/q^z)^{2+\lambda_a}-\frac{\mathrm{i}\omega}{q^{1-\eta_a}}\left(\frac{\Lambda}{q}\right)^{\frac{1}{2}d-1}g(|\omega|/q)\right], \tag{30}$$

where

$$\lambda_a = \eta_a\frac{\mathrm{d}}{4-d}, \qquad z = (2-\eta_a)/(2+\lambda_a) \tag{31}$$

and the two limiting values of $g(x)$ can be obtained from (27). Because all calculations have been done with (15) instead of with (11) all exponents carry an index a. From (16) follows

$$\eta_a = r\eta \tag{32}$$

which is a good approximation as discussed below (16).

It follows from (31) that the dynamic scaling hypothesis (Ferrell *et al* 1967) which requires the propagator to have the form

$$G^{-1}(q, \omega, 0) \sim q^{2-\eta} g(\omega/\omega_q), \qquad \omega_q \propto q^z \tag{33}$$

is violated due to the Λ/q factor of the dissipative term. This implies that the dissipative processes resolve the atomic length of the system. Let us point out that except for that factor the dynamic scaling hypothesis is satisfied to order $1/n$ with

$$z = 1 - \eta_a \frac{2}{4-d}. \tag{34}$$

5. Discussion

We have studied the critical properties of an isotropic n-vector model for a displacement type PT at T_c. It is found that at $T_c \neq 0$ there is no quantum effect on the critical coefficient η, a result which was also found by Abe and Hikami (1974) for Bose systems. However, as $T_c \to 0$ the domain in q space which shows classical critical behaviour $\hbar q < k_B T_c$ shrinks to zero and η assumes discontinuously new values as a function of d which are produced by quantum critical fluctuations. This means simply that the domain of quantum fluctuations $\hbar q > k_B T_c$ approaches zero. The result (23) is qualitatively easy to understand. The quantum critical fluctuations correspond always to a problem in $d+1$ dimensions. Accordingly for $d > 3$ mean-field behaviour should be expected, ie, $\eta = 0$. For $d \leqslant 3$ the theory has infrared singularities and an anomalous dimension can be anticipated. However, the time dimension does not necessarily correspond to an additional dimension of the classical problem, ie, $\eta_q(d) \neq \eta(d+1)$ for $2 < d < 3$. It is also important to notice that for $T_c \neq 0$ no matter how small it is the singular behaviour of the Bose–Einstein function for small arguments produces classical critical behaviour.

Let us point out that $\eta_q(d = 3)$ has not been calculated separately, but vanishes when extrapolated from (23). It appears, therefore, that the problem shows mean-field behaviour for $d = 3$ and $T_c = 0$. A second-order PT at $T_c = 0$ has been studied by Rechester (1971) where it is also pointed out that this problem for $d = 3$ is formally equivalent as far as static properties are concerned to the classical treatment of a ferroelectric PT with long-range dipole interaction studied by Larkin and Khmel'nitskii (1969). The propagator at T_c, however, is not computed by these authors. Let us point out that it would be an interesting problem to evaluate the critical coefficient γ in a $1/n$ expansion for $T_c = 0$.

With respect to the dynamical critical behaviour at $T_c \neq 0$ we have found that the dynamic scaling hypothesis is not observed by the system but that the atomic length enters the dissipative part of the propagator. Let us mention that Sasvári and Szépfalusy (1974) have treated structural PT using the same model but using a variable potential range σ. The dynamical critical exponent z is calculated in the limit $n \to \infty$ where dynamical scaling is obtained. In particular they obtain $z = 1$ for $\sigma = 2$ which agrees with our result. The present result may be related to the difficulties of the RG approach to this problem mentioned in the literature (Halperin *et al* 1972, 1974). As a consequence of energy conservation in this problem the renormalized four-phonon vertex will not be regular in frequency for small momentum transfer. For $q = 0$ one obtains for the bubble which determines also the renormalized vertex

$$I(0, \omega + \mathrm{i}0^+, 0) \sim (2\Lambda^2/\omega^2)^{2-d/2} \exp(\mathrm{i}\, \mathrm{sgn}\, \omega \pi d/2). \tag{35}$$

In the Bose problem where dynamic scaling is observed (Kondor and Szépfalusy 1974) the quantity (35) vanishes. It has been mentioned by Halperin *et al* (1974) that once the long-wavelength modes get overdamped, the propagator of the critical phonons goes over into

$$D^{-1}(\boldsymbol{q}, \omega+\mathrm{i}0^+, 0) \sim q^2 - \mathrm{i}\omega/\Gamma, \tag{36}$$

which allows standard RG methods to be applied. Because it follows from (30) that the excitation spectrum of the phonons may approximately be represented by

$$\omega_q \sim -\mathrm{i}q^{2-d/2}\Lambda^{-1+d/2} \tag{37}$$

(36) is perhaps a good approximation especially when damping is taken into account. However, from a principal point of view it does not solve the problem. Further research on this problem is presently in progress. Dynamical properties at $T_c = 0$ have not been considered so far.

Because the $1/n$ approximation gives rather poor results and should be extended to $1/n^2$ (Abe 1973) comparison with experiment is not easily possible. On the other hand there exist no data on η for low-temperature displacive PT. With respect to the dynamic critical behaviour it is known that there occur rather strong acoustic anomalies (Fleury 1971). It is therefore doubtful if the present idealized model can be tested experimentally.

References

Abe R 1973 *Prog. Theor. Phys.* **49** 1877–88

—— 1974 *Prog. Theor. Phys.* to be published

Abe R and Hikami S 1974 *Phys. Lett.* **47A** 341–2

Aharony A 1973a *Phys. Rev.* B **8** 3349–57, 4270–3

—— 1973b *Phys. Rev. Lett.* **31** 1494–7

Anderson P W 1960 *Fizika Dielektrikov* ed G I Shansvi (Moskow: USSR Academy of Science)

Barrett J H 1952 *Phys. Rev.* **86** 118–20

Bierly J N, Muldawer L and Beckman O 1963 *Acta Metallurg.* **11** 447–54

Brézin E, Le Guillou J C and Zinn-Justin J 1974 *Phys. Rev.* B **10** 892–900

Cochran W 1960 *Adv. Phys.* **9** 387–423

Cowley R A and Bruce L D 1973 *J. Phys. C: Solid St. Phys.* **6** L191–6

Droz M 1974 *J. Phys. C: Solid St. Phys.* **7** 2953–60

Erdélyi A 1953 *Higher Transcendental Functions*, vol 1 (New York, Toronto, London: McGraw-Hill) pp 56–119

Ferrell R A, Menyhárd N, Schmidt H, Schwabl F and Szépfalusy P 1967 *Phys. Rev. Lett.* **18** 891–4

Fleury P A 1971 *J. Acoust. Soc. Am.* **49** 1041–51

Gillis N S 1969 *Phys. Rev. Lett.* **22** 1251–4

Goldak J, Barrett C S, Innes D and Youdelis W 1966 *J. Chem. Phys.* **44** 3323–5

Halperin B I and Hohenberg P C 1969 *Phys. Rev.* **177** 952–71

Halperin B I, Hohenberg P C and Ma S 1972 *Phys. Rev. Lett.* **29** 1548–51

—— 1974 *Phys. Rev.* B **10** 139–53

Holz A and Medeiros J T N 1975 *Phys. Lett.* **51A** 93–4

Jouvet B and Holz A 1974 *J. Phys. C: Solid St. Phys.* **7** 1449–61

Ketley I J and Wallace D J 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1667–78

Khmel'nitskii D E and Shneerson V L 1971 *Sov. Phys.–Solid St.* **13** 687–94

—— 1973 *Sov. Phys.–JETP* **37** 164–70

Kondor I and Szépfalusy P 1974 *Phys. Lett.* **47A** 393–4

Kwok P C K 1967 *Solid St. Phys.* **20** 213–303

Larkin A I and Pikin S A 1969 *Sov. Phys.–JETP* **29** 891–6

Ma S 1973 *Phys. Rev.* A **7** 2172–87

Rechester A B 1971 *Sov. Phys.–JETP* **33** 423–30

Sasvári L and Szépfalusy P 1974 *J. Phys. C: Solid St. Phys.* **7** 1061–8

Shirane G, Nathans R and Minkiewicz V I 1967 *Phys. Rev.* **157** 396–9

Suzuki M and Igarashi G 1974 *Phys. Lett.* **47A** 361–2

Wallace D J 1973 *J. Phys. C: Solid St. Phys.* **6** 1390–404