Specific heat amplitude ratio for anisotropic Lifshitz critical behaviors

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Abstract

We determine the specific heat amplitude ratio near a $m$-axial Lifshitz point and show its universal character. Using a recent renormalization group picture along with new field-theoretical $\epsilon_L$-expansion techniques, we established this amplitude ratio at one-loop order. We estimate the numerical value of this amplitude ratio for $m = 1$ and $d = 3$. The result is in very good agreement with its experimental measurement on the magnetic material MnP. It is shown that in the limit $m \rightarrow 0$ it trivially reduces to the Ising-like amplitude ratio.

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I. INTRODUCTION

Among all properties of systems near a second order phase transition, amplitude ratios of certain thermodynamic potentials above and below the critical temperature play a fundamental role together with the critical exponents: they are examples of universal quantities. All universal amounts are characterized by a limited number of parameters defining the universality class and do not depend on the microscopic details of the system under consideration. One particular type of universality class is associated to the Lifshitz critical behavior \cite{1, 2} where the inclusion of competing interactions along one or more spatial directions is the main difference with respect to the ordinary critical behavior.

Recent investigations of the associated critical exponents for the \( m \)-axial Lifshitz universality class have been put forward using numerical Monte Carlo simulations \cite{3} and field-theoretic approaches \cite{4–6}. Within the perturbative \( \epsilon_L \)-expansion, there are two proposals in order to unravel the higher loop structure of this sort of critical behavior. One of them makes use of a semi-analytic \( \epsilon_L \)-expansion for the critical exponents, where some loop integrals are evaluated through numerical integration \cite{4}. Another alternative is the purely analytical treatment of all loop integrals involved, such that new renormalization group as well as \( \epsilon_L \)-expansion ideas have been developed in order to determine those critical indices \cite{5, 6}. We shall focus our attention in the latter throughout this article for convenience.

The Lifshitz multicritical point arises in a variety of real physical systems, but we shall be concerned here only with its manifestation in magnetic systems where it was originally discovered \cite{1}. The uniaxial case \( m = 1 \) can be explained in terms of an Ising model with ferromagnetic interactions among nearest neighbors spins as well as additional antiferromagnetic couplings among the second neighbors along a single axis, known as ANNNI model \cite{7}. The competition originates several modulated phases in addition to the usual paramagnetic and ferromagnetic phases. It is very simple to analyse the situation near the uniaxial Lifshitz point, which arises at the confluence of a modulated and a ferromagnetic phase with the paramagnetic phase. Allowing these competing interactions along \( m \) spatial directions, one obtains the \( m \)-axial Lifshitz critical behavior. The anisotropic Lifshitz universality classes associated to this sort of critical behavior depend upon the number of components of the order parameter \( N \), the space dimension \( d \) and the number of competing axes \( m \) of the system, therefore, extending the Ising-like universality classes characterized solely by \( (N,d) \). An interesting feature of the critical exponents of such systems is the property of universality class reduction: in the limit \( m \to 0 \) the critical indices reduce trivially to those corresponding to the usual Ising-like behavior \cite{5, 6, 8}.

The theoretical determination of the specific heat amplitude ratio is especially worthwhile for two reasons. First, we would like to know whether the universality class reduction also holds for this amplitude ratio. As this property is also obeyed by the susceptibility amplitude ratio \cite{9} one can conjecture that this property might hold for all critical amplitude ratios. Secondly, it would be highly desirable to compare the theoretical value of this amplitude ratio with experiments carried out in some real magnetic material exhibiting the Lifshitz critical behavior. This would yield a test for the convenience (or not) of the theoretical formalism employed in the solution of this problem. From the phenomenological viewpoint, theoretical and experimental studies have proved that manganese phosphide \((MnP)\) presents a pure uniaxial Lifshitz point \((m = 1, d = 3, N = 1)\) \cite{11, 12}. Moreover, the experimental
determination of the specific heat amplitude ratio for \( MnP \) was realized thirteen years ago by means of susceptibility measurements [13]. A theoretical attempt to describe this amplitude ratio was performed using the mean field approximation [14] by neglecting the contribution of the fluctuations, but the agreement with the experiment was not achieved. A proper treatment should include the effect of fluctuations since they play a nontrivial role in the determination of this particular amplitude ratio.

In this paper the specific heat amplitude ratio near an anisotropic \( m \)-axial Lifshitz point is calculated at one-loop level using a \( \lambda \phi^4 \) field theory combined with new renormalization group and \( \epsilon \)-expansion methods. We shall treat only the especial Ising-like case \( N = 1 \), since for \( N > 1 \) and below the Lifshitz critical temperature the appearance of a massless Goldstone mode leads to infrared problems which require a separate analysis [15]. In the present field-theoretic setting the long-standing difficulty in this calculation is that it requires the knowledge of the coupling constant at the fixed point and the specific heat critical exponent at two-loop level in order to find out this amplitude ratio beyond the mean field approximation. These objects have recently been figured out at two-loop level [6] permitting, therefore, the present analysis. It represents the first theoretical report with the effect of the fluctuations properly included in the specific heat amplitude ratio for the anisotropic Lifshitz critical behavior. We point out that the universality class reduction also holds for this amplitude ratio. This is another step forward towards extending this property to all other critical amplitude ratios. Furthermore, we estimate it for the uniaxial case \( m = 1 \) in three-dimensional systems. The result is in very good agreement with the experimental determination of the specific heat amplitude ratio in the magnetic compound \( MnP \).

II. SPECIFIC HEAT AMPLITUDE RATIO

Since the method of calculation has been described in a previous work [9] and is somewhat standard for ordinary critical systems [10], we will only review briefly the notations and the basic steps. The bare Lagrangian for the \( m \)-axial anisotropic Lifshitz critical behavior reads:

\[
L = \frac{1}{2} |\nabla_m \phi_0|^2 + \frac{1}{2} |\nabla_{(d-m)} \phi_0|^2 + \delta_0 \frac{1}{2} |\nabla_m \phi_0|^2 + \frac{1}{2} t_0 \phi_0^2 + \frac{1}{4!} \lambda_0 \phi_0^4.
\]

The Lifshitz critical region is characterized by \( \delta_0 = 0 \) with the temperature close but not equal to \( T_L \). We are going to restrict our analysis using the condition \( \delta_0 = 0 \) henceforth.

The anisotropic behavior possesses two independent correlation lengths parallel and perpendicular to the competition axes. They allow two independent renormalization group flows in momentum space along directions parallel or perpendicular to the competition axes [5]. Rigorously speaking, we should assign a label to each renormalized vertex part associated to the flow along spatial directions parallel or perpendicular to the competing axes, but we have no need to label the renormalized quantities in this work, since the fixed point is independent of the flow direction used to renormalize the theory [6]. Consequently, the amplitude ratios do not depend on what external momenta scale is varied in order to define the corresponding renormalization group transformation.

The one-loop renormalized Helmholtz free energy density at the fixed point obtained by using a nonvanishing quadratic external momenta scale for the \( m \)-axial Lifshitz critical behavior is given by [16]:

\[
L = \frac{1}{2} |\nabla_m \phi_0|^2 + \frac{1}{2} |\nabla_{(d-m)} \phi_0|^2 + \delta_0 \frac{1}{2} |\nabla_m \phi_0|^2 + \frac{1}{2} t_0 \phi_0^2 + \frac{1}{4!} \lambda_0 \phi_0^4.
\]
\[
F(t, M) = \frac{1}{2} t M^2 + \frac{1}{4!} g^* M^4 + \frac{1}{4} (t^2 + g^* t M^2 + \frac{1}{2} (g^* M^2)^2) I_{SP} \\
+ \int d^{d-m} q d^m k [\ln(1 + \frac{t + \frac{1}{2} g^* M^2}{q^2 + (k^2)^2}) - \frac{g^* M^2}{2(q^2 + k^4)}],
\]

where in the above equation \( t, M \) \((t_0 = Z^{-1}_\phi t, \phi = Z^{-1}_\phi M)\) are the renormalized (bare) reduced temperature and order parameter, respectively, \( Z_\phi^2, Z_\phi \) are normalization functions, \( g^* \) is the renormalized coupling constant at the fixed point, \( \bar{q} \) is a \((d - m)\)-dimensional wave vector perpendicular to the competing axes, whereas \( k \) is a \( m \)-dimensional wave vector whose components are parallel to the competition axes. The integral \( I_{SP} \) is defined by:

\[
I_{SP} = \int \frac{d^{d-m} q d^m k}{[((k + K^*)^2 + (q + P)^2)((k^2)^2 + q^2)}.
\]

We choose to renormalize the theory using normalization conditions where the external momenta scale are zero \((K^* = 0)\) along the competing axes whereas their nonvanishing components are perpendicular to the competition axes. A convenient symmetry point for this integral is chosen at \( P^2 = \kappa^2 \phi = 1 \). As the dimensionful coupling constant is related to that dimensionless by \( g^* = (P^2)^{-\frac{d}{2}} u^* \), where \( \epsilon_L = 4 + \frac{m}{2} - d \), this symmetry point transforms the dimensionful into the dimensionless coupling constant. The typical geometric angular factor for each loop integral characterizing the \( m \)-axial Lifshitz behavior is \( \frac{1}{4} S_{d-m} S_m \Gamma(2 - \frac{m}{d}) \). These factors should be extracted whenever a loop integral is performed and absorbed into a redefinition of the coupling constant \([5, 6, 8]\). At the symmetry point the integral calculated at nonzero external momenta is given by \( I_{SP} = \frac{1}{\epsilon_L^2}(1 + [i_2]_m \epsilon_L) \), where \([i_2]_m = 1 + \frac{1}{2}(\psi(1) - \psi(2 - \frac{m}{d}))\) and \( \psi(z) = \frac{\text{d} \ln \Gamma(z)}{\text{d} z} \) \([8]\).

Since the vertex part \( \Gamma_R^{(0,2)} \) is additively renormalized, the singular part of the specific heat scales with the temperature in the form \([5, 6]\):

\[
C = -A |t|^{-\alpha_L} = -\frac{\nu L^2}{\alpha_L} B(u^*) - \Gamma_R^{(0,2)},
\]

where \( B(u^*) \) is the inhomogeneous term of the renormalization group equation for \( \Gamma_R^{(0,2)} \) and

\[
\Gamma_R^{(0,2)} = \frac{\partial^2 F(t, M)}{\partial t^2},
\]

is the vertex part which is related to the specific heat only at zero external momentum insertion.

Above the Lifshitz temperature, \( M = 0 \) and using Eqs. (2) and (5) we obtain:

\[
\Gamma_R^{(0,2)} = -\frac{1}{2} \int \frac{d^{d-m} q d^m k}{(q^2 + (k^2)^2 + t^2)^2} + \frac{1}{2} I_{SP}.
\]

When \( T < T_L \), we replace the value of \( M \) at the coexistence curve, where \( u^* M^2 = -6t \), to find

\[
\Gamma_R^{(0,2)} = -\frac{3}{u^*} - 2\int \frac{d^{d-m} q d^m k}{(q^2 + (k^2)^2 + 2|t|)^2} - I_{SP}.
\]
The calculation of the one-loop remaining integrals are straightforward. The integration over the quadratic loop momenta is trivial, and when the remaining quartic loop integral is performed we find:

\[ \int \frac{d^{d-m}q d^m k}{(q^2 + (k^2)^2 + t)^2} = \frac{i^{-4}}{\epsilon_L} \left( 1 - \frac{\epsilon_L}{2} \left( \psi(2 - \frac{m}{4}) - \psi(1) \right) \right), \]  

(8)

where we have used the parameter \( \tilde{t} \) in order to unify the language above and below the Lifshitz critical temperature \( T_L \).

The exponents \( \nu_{L2}, \alpha_L \) and the fixed point (using normalization conditions) were calculated in Ref. [6] and expressed as:

\[ \alpha_L = \frac{(4 - N)}{2(N + 8)} \epsilon_L - \frac{(N + 2)(N^2 + 30N + 56)}{4(N + 8)^3} \epsilon^2_L, \]  

(9)

\[ \nu_{L2} = \frac{1}{2} + \frac{(N + 2)}{4(N + 8)} \epsilon_L + \frac{1}{8} \frac{(N + 2)(N^2 + 23N + 60)}{(N + 8)^3} \epsilon^2_L, \]  

(10)

\[ u^* = \frac{6}{8 + N} \epsilon_L \left\{ 1 + \epsilon_L \left[ -[i_2]_m + \frac{(9N + 42)}{(8 + N)^2} \right] \right\}. \]  

(11)

Now we take the particular value \( N = 1 \). On the other hand, the additive constant is given by:

\[ B(u^*) = \kappa_1 \left( \frac{\partial \Gamma^{(0,2)}}{\partial \kappa_1} \right)_{\mu^2 = \kappa_1^2 = 1} = -\frac{1}{2} \kappa_1^{-\epsilon_L} \left( 1 + [i_2]_m \epsilon_L \right). \]  

(12)

After taking \( \kappa_1^2 = 1 \) we obtain up to first order in \( \epsilon_L \) the following result:

\[ -\frac{\nu_{L2}}{\alpha_L} B(u^*) = \frac{3}{2} \epsilon_L + \frac{3[i_2]_m}{2} + \frac{1}{4} + \frac{87}{58} = \frac{1}{u^*} + 2. \]  

(13)

Using Eqs.(6), (7) and (8) in conjunction with the value of \( I_{SP} \) we can easily determine \( \Gamma^{(0,2)}_{R} \) above and below \( T_L \). After that, use Eqs.(4) and (12) to derive the specific heat amplitude ratio at one-loop level:

\[ \frac{A_+}{A_-} = \frac{2\alpha_L}{4}(1 + \epsilon_L), \]  

(14)

where in this formula the specific heat critical index is given at \( O(\epsilon_L) \), i.e., \( \alpha_L = \frac{\epsilon_L}{6} \).

### III. DISCUSSION

Firstly, the result displays a universal form, since it only depends on \( m \) and \( d \). Note that this easily reduces to the usual critical behavior in the limit \( m \to 0 \), therefore confirming the reduction of the Lifshitz universality class to the Ising-like universality class. As the susceptibility amplitude ratio presents the same property at one-loop level, this might be a general feature of all critical amplitude ratios, including not only thermodynamic amplitudes but also correlation amplitude ratios as well as mixed (correlation/thermodynamic) amplitude ratios. Future work will be devoted to those issues.
On the other hand, this amplitude ratio was determined experimentally for MnP and found to be $A^{+} = 0.65 \pm 0.05$ [13]. Replacing $m = 1, d = 3$ into the above expression we find $A^{+} = 0.74$. If we neglect the error bar in the experiment, the difference among the two results is about 9%, therefore, in very good agreement with the experimental value obtained for MnP. Nevertheless, it is important to mention that this experimental value of the specific heat amplitude ratio in MnP was obtained using nonlinear least-square fits to adjust it along with the value of the critical exponent $\alpha_L$. The constraint that the value of the critical exponents above and below the Lifshitz critical temperature must be equal ($\alpha^{+}_L = \alpha^{-}_L$ consistent with scaling theory) yielded the experimental result $\alpha_L = 0.46 \pm 0.03$, which in turn led to the value $A^{+} = 0.65 \pm 0.05$ for MnP [13]. Moreover, the different values for the exponents produced by unconstrained fits near $T_L$ were recognized by those authors as a departure from theoretical predictions, but could also be attributed to the closeness of the first-order ferromagnetic-helical(fan) transition, which makes the experimental analysis more difficult. Indeed, the experimental specific heat exponent is in disagreement with different theoretical estimates for the uniaxial three-dimensional case whose specific heat exponent is approximately 0.20 [3–5].

Since the experimental specific heat amplitude ratio depends upon the specific heat exponent, the best fit which produced the $\alpha_L$ exponent nearly two times larger than that from theoretical calculations should affect the value of that amplitude ratio due to error propagation. Of course, a different fit resulting in another experimental value of $\alpha_L$ does modify the above amplitude ratio due to crossover effects which take place when the temperature is varied [17]. For instance, when the value of $\alpha_L$ is close to 0.270 in a certain fit, the value of the corresponding experimental amplitude ratio (fixed by this value of the specific heat exponent) is given by $A^{+} = 0.435$, but the system is at $T = 132.4K$ [17] which is away of the Lifshitz temperature $T_L = (121 \pm 1)K$ for MnP and is affected by the crossover to the Ising universality class. The funny surprise is that very close to the Lifshitz critical temperature this error is rather small when theoretical and experimental estimates for this amplitude ratio are compared as discussed in the present work, in spite of the large deviation between the measured specific heat critical exponent for MnP and calculated values using theoretical tools as discussed above.

A comparison of theoretical and experimental results of this critical amplitude ratio with the one associated to the Ising-like universality class is illuminating. For $N = 1, d = 3$ the $\epsilon$-expansion ($\epsilon = 4 - d$) result of this amplitude ratio at one-loop level yielded $A^{+} = 0.56$ [15]. By neglecting the error bars, specific heat measures in different materials belonging to the same universality class resulted in critical amplitude ratios varying from 0.53 to 0.58 [18]. On the other hand, series expansion studies of this ratio produced values in the range 0.62 - 0.70 [19]. The $\epsilon$-expansion estimate furnishes better values than those coming from series expansion even though the $\epsilon$ parameter is not a small number in this case ($\epsilon = 1$).

For three-dimensional uniaxial systems $\epsilon_L = 1.5$ is even bigger than in the situation for the Ising-like case analysed above. This might be the main consequence for a greater difference between the experimental and theoretical results of this amplitude ratio when compared to the ordinary critical behavior. In order to see whether this is a good argument, we suggest the measurement of this specific heat amplitude ratio in other uniaxial magnetic materials like CoNb$_2$O$_6$ [20]. For Ising-like magnets the deviation of these specific heat amplitude ratios for different materials is rather small among themselves as well as when
they are compared with results derived from the $\epsilon$-expansion. Hence, from our $\epsilon_L$-expansion results we would expect a larger deviation of this amplitude ratio for different materials presenting a uniaxial critical behavior. Nevertheless, our results are rather encouraging in comparison with experiments in $MnP$, indicating the reliability of the $\epsilon_L$-expansion approach to this sort of behavior. Since further numerical works have not been pursued for critical amplitude ratios pertaining to the anisotropic Lifshitz universality classes, we hope our endeavor can stimulate other numerical estimates like series expansions or Monte Carlo simulations, in order to improve the comprehension of as many critical amplitude ratios as possible for competing systems.

In summary, we have derived the specific heat critical amplitude ratio above and below the Lifshitz critical temperature for a general anisotropic behavior $1 < d < m - 1$. The anisotropic universality class reduces easily to the Ising-like one in the limit $m \to 0$. Needless to say, the result is independent of the choice of the symmetry point employed: had we started with a symmetry point characterized by zero external momenta perpendicular to the competing axes and nonvanishing external momenta components parallel to the competition axes, we would have arrived at the same result. The uniaxial value of this ratio is in very good agreement to that measured for $MnP$. Hence, the analytical approach presented here in order to treat this amplitude ratio is convenient to describe phenomenological aspects of real physical systems presenting competing interactions. A thorough study of all critical amplitude ratios as well as a nonperturbative proof of their universal character based solely on renormalization group arguments for both anisotropic and isotropic cases will be an interesting topic for future investigation.

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