Scaling function for the critical ultrasonic attenuation in perovskites

Jayanta K. Bhattacharjee
Institut für Festkörperforschung, Kernforschungsanlage Jülich, D-5170 Jülich, West Germany*
and Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
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A scaling function is calculated to the lowest order in n^{-1} expansion for the critical ultrasonic attenuation in perovskites. This yields good agreement with the measurements of Fossheim and Holt.

Ultrasonic investigation has long been a useful tool for probing the critical dynamics of the structural transitions of the perovskites. Since the establishment of the importance of fluctuations in ultrasonic experiments[1] in $SrTiO_3$ several experimental investigations have been performed on the perovskites. Recently the attenuation in $KMnF_3$ has been the subject of a very detailed and careful experimental study by Fossheim and Holt.[2,3] The power law for the temperature dependence in the hydrodynamic regime, as well as the entire scaling function describing the passage from the hydrodynamic to the critical region was accurately determined. The temperature dependence of the attenuation in the low-frequency hydrodynamic region has been studied theoretically by Schwabl[4] and Murata[5] but a calculation of the scaling function has not been attempted before. The purpose of this Communciation is to provide scaling function to the leading order in a n^{-1} expansion.[6] The shape agrees very well with the results of Fossheim and Holt.[2,3]

The Hamiltonian for the structural transition of the perovskites has been studied by several authors.[7,8] It is well established that the strain fields e_{ij} couple quadratically to the order parameter field ϕ_i. The interaction term in the free energy is of the form $e_{ij}Q_{ij}$ where Q_{ij} can have the forms $\sum\phi_i^2$, $\phi_i\phi_j$, and $\phi_i^2-\phi_j^2$ with $i\neq j$. By a fluctuation dissipation theorem, the sound attenuation can then be related to the response functions χ_1, χ_2 , and χ_3 corresponding, respectively, to the correlation functions $\langle\sum\phi_i^2\sum\phi_i^2\rangle$, $\langle\phi_i\phi_j\phi_i\phi_j\rangle$, and $\langle(\phi_i^2-\phi_j^2)(\phi_i^2-\phi_j^2)\rangle$. One can then write the attenuation per wavelength, $\alpha\lambda$, as

$$\alpha\lambda=\sum_i A_i \mathrm{Im}\chi_i(\omega) \quad , \tag{1}$$

where A_i are some constant coefficients. The response functions have the form

$$\chi_i(\omega)=t^{x_i}f_i(\omega/\Gamma) \quad . \tag{2}$$

The critical exponent $x_1=\alpha_0$, the specific-heat exponent, while $x_2=\alpha+2(\phi_2-1)$ and $x_3=\alpha_0+2(\phi_3-1)$, where ϕ_2 and ϕ_3 are the anisotropy crossover exponents. Near the Heisenberg fixed point, $\phi_2=\phi_3$ and consequently $x_2=x_3$. The Γ appearing in Eq. (2) is the relaxation rate for order parameter fluctuations. In this case of a nonconserved order parameter, $\Gamma=\Gamma_0\kappa^z$ with $z\simeq 2$, where $\kappa=\kappa_0 t^\nu$ is the inverse correlation length and t is the reduced temperature. For these systems $\nu\simeq\frac{2}{3}$. In the low-frequency hydrodynamic regime where $\omega<<\Gamma$ the functions f_i, which are really functions of $i\omega/\Gamma$ because of the relaxational process involved, can be expanded in powers of this variable and if the first term is kept yield the answer obtained by Murata[5] in this range:

$$\alpha\propto\omega^2\sum a_i t^{-\rho_i} \quad . \tag{3}$$

$\rho_i=x_i+\nu z$, yields $\rho_1=1.34$ and $\rho_2=\rho_3\approx 1.87$. For certain propagation directions certain particular a_i's are allowed as has been shown by Murata.[5]

At this point we have to decide on the strength of different contributing a_i or equivalently the A_i of Eq. (1). Looking at the experimental results of Fossheim and Holt[2,3] we find that in the region $\omega<<\Gamma$, the temperature dependence is $t^{-1.87}$. This allows us to infer that, at least for $KMnF_3$ in the directions investigated, $a_1<<a_2$ or a_3 and hence $A_1<<A_2$ or A_3. Thus in this case, it is not the energy density correlation function which determines the sound attenuation as is the case for the fluids.[9–13] For the fluid systems it was convenient to calculate $\chi_1(\omega)$ in an ϵ expansion. For this system, where χ_2 and χ_3 need to be computed, we find the use of the n^{-1} expansion were useful.

Turning first to the statics, we note that for both $\langle\phi_i\phi_j\phi_i\phi_j\rangle$ and $\langle(\phi_i^2-\phi_j^2)(\phi_i^2-\phi_j^2)\rangle$ the leading order graph in a n^{-1} expansion consists of the single bubble of Fig. 1. It is obvious that at $D=3$ the bubble scales as κ^{-1} and hence

$$x_2\nu^{-1}=x_3\nu^{-1}=1+O(1/n) \quad . \tag{4}$$

The two-loop ϵ expansion gives 0.8 for this number and hence we find that the lowest-order $O(1/n)$ expansion is a good approximation in this case. This is in contrast to the specific-heat exponent α_0, which can be obtained to the leading order in n^{-1} expansion only by summing over all bubbles, and which turns

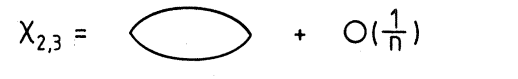

FIG. 1. The lowest-order diagram in n^{-1} expansion for χ_2 and χ_3.

out to be given by $\alpha_0\nu^{-1} = -1 + O(1/n)$. The accepted result for $n=3$ is $\alpha_0/\nu \approx -0.18$, in strong disagreement with the leading term in n^{-1} expansion. However, as argued above, we will not be interested in this response function in the present work, but instead with χ_2 and χ_3, which can be well approximated by the leading term in the n^{-1} expansion and which in this case corresponds to the decoupling approximation. This also implies $\chi_2 = \chi_3$ in the present scheme.

To determine the dynamics associated with the graph of Fig. 1, we note that at a given value of κ, a fluctuation of wave number p relaxes according to the relaxation rate $\gamma(p\kappa) = \Gamma_0(p^2+\kappa^2)$. The time-dependent correlation function corresponding to the bubble graph is then given by

$$C(t_{12}) = \frac{1}{4\pi}\int \frac{d^3p}{(p^2+\kappa^2)^2}\exp[-2\gamma(p,\kappa)t_{12}] \quad . \tag{5}$$

The corresponding frequency-dependent response function is

$$\chi(\omega) = \frac{\Gamma_0}{2\pi}\int \frac{d^3p}{p^2+\kappa^2}\frac{1}{-i\omega+2\Gamma_0(p^2+\kappa^2)} \quad . \tag{6}$$

Defining the reduced frequency $\Omega = \omega/\Gamma_0\kappa^2$ and evaluating the elementary integral[14] in Eq. (6) gives

$$\chi(\omega) = \frac{i\pi}{\kappa\Omega}\left[\left(1+\frac{i\Omega}{2}\right)^{1/2} - 1\right] \quad . \tag{7}$$

Thus the attenuation α, which is proportional to $\omega \mathrm{Im}\chi^{-1}(\omega)$, is given by

$$\alpha = A\frac{\omega}{\kappa}\frac{1}{\Omega}\left[\left(1+\frac{\Omega^2}{4}\right)^{1/4}\cos\left(\frac{1}{2}\tan^{-1}\frac{\Omega}{2}\right) - 1\right] \quad , \tag{8}$$

where A is some undetermined constant. The scaling function $G(\Omega)$ for α has been defined by Fossheim and Holt[2,3] so that it is normalized to unity in the hydrodynamic region. Choosing the same convention we then find

$$G(\Omega) = \frac{32}{\Omega^2}\left[\left(1+\frac{\Omega^2}{4}\right)^{1/4}\cos\left(\frac{1}{2}\tan^{-1}\frac{\Omega}{2}\right) - 1\right] \quad . \tag{9}$$

To compare with the experimental data of Fossheim and Holt, we note that the scale has to be fixed. Unlike the case of fluids where the scale is uniquely fixed from the measurement of some other property, here there is a freedom. Fossheim and Holt[2,3] have determined a value for the amplitude of the relaxation rate that sets the scale by determining the temperature at which deviation from hydrodynamic behavior sets in and requiring this to occur at $\omega/\Gamma = 1$. $\Gamma = \tau^{-1}$ in Fossheim and Holt notation. We decided to compare our frequency scale with that of Fossheim and Holt by requiring that the frequency Ω_0 at which $G(\Omega_0) = 0.5$ be identical to the frequency Ω_0' at which the experimental scaling function reaches the value 0.5. This leads to $\Omega_0 = \Omega_0'$. Comparison of the rest of the scaling function is shown in Fig. 2. The agreement is excellent.

We note that Eq. (9) predicts that $G(\Omega) \sim \Omega^{-3/2}$ when $\Omega \gg 1$. This implies that $\alpha_c(\omega)$, i.e., the critical point value of the attenuation as a function of frequency, will increase as $\omega^{1/2}$. This exponent is inaccurate because of the approximations used in calculating the scaling function. A more accurate value will now be obtained by the dynamic scaling procedure shown in Refs. 9 and 11. The critical part of the sound velocity in the hydrodynamic range is shown to be given by an expression of the form

$$\frac{\Delta U}{U} = \sum C_i t^{-x_i} \quad , \tag{10}$$

where x_i are the indices introduced earlier and C_i are constants. In terms of the relaxation rate $\Gamma = \Gamma_0 t^{2\nu}$, Eq. (10) can be written as

$$\frac{\Delta U}{U} = \sum C_i' \Gamma^{-x_c/2\nu} \quad . \tag{11}$$

Now as we pass into the critical region where $\omega \gg \Gamma$, dynamic scaling requires the replacement of Γ by ω; more correctly by $-i\omega$ as a relaxation process is involved. Thus the complex frequency-

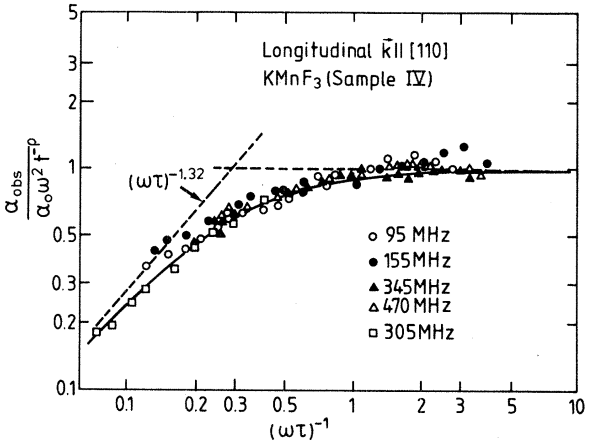

FIG. 2. Comparison of the theoretical scaling function (solid curve) with the data of Fossheim and Holt (Refs. 2 and 3).

dependent velocity at T_c is given by

$$\frac{\Delta U}{U}(\omega) = \sum c_i' \left(\frac{-i\omega}{a} \right)^{-x_i/2\nu} . \quad (12)$$

Here a is a number of order unity that can be determined from the scaling function given in Eq. (9) and is found to be 6.4. The real and imaginary parts of Eq. (12) now give the dispersion and attenuation per wavelength at $T = T_c$. It is then easy to see that $\alpha_c \propto \omega^{1-x_i/2\nu}$. For the experiment of Fossheim and Holt[1,2] where $x_i \approx 0.5$, $\alpha_c \propto \omega^{0.63}$ instead of the $\omega^{0.5}$ obtained on the basis of the large-Ω limit of Eq. (9). It should be noted that once the c_i is known from the hydrodynamic data and Γ_0 is fixed, the dispersion and the magnitude of the attenuation at the critical point are fixed unambiguously. This can be checked by future experiments.

Note added in proof. After this work was submitted for publication it was pointed out by F. Schwabl and H. Ivo that they have attempted to obtain a scaling function by the ϵ expansion. This has appeared in Ferroelectrics 35, 215 (1981).

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*Present address.

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