LOCAL CONDENSATION AT ELASTIC PHASE TRANSITIONS

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Abstract: We investigate the influence of short-range defects that locally increase the transition temperature on the statics and dynamics of elastic phase transitions. We find local condensation of the order parameter when $T \leq T_c^{loc}$. There are no localized modes in the acoustic phonon spectrum, but there is a resonant vibrational part in each of the scattering states instead which "condenses" at the defect for $T \to T_c^{loc}$. Correspondingly, the relaxation time of a stress-induced cluster diverges as $(T - T_c^{loc})^{-1}$ in the vicinity of T_c^{loc}. The phonon-phonon response function is calculated for a one- and a multi-defect system to first order in the defect concentration, the latter showing the development of a central peak.

1. MODEL EQUATIONS AND STATIC RESULTS

The influence of localized defects on the statics and dynamics of structural phase transitions has been of considerable interest, especially since a narrow central peak was found in the scattering structure function in the vicinity of the transition temperature T_c^0 (for a review see e.g. ref. [1]). The case of distortive structural transitions has been treated in ref. [2]; quite analagously we study the following one-dimensional Ginzburg-Landau free energy functional for a second-order elastic phase transition

$$\mathcal{F}[\epsilon] = \int_L \left[[a'(T - T_c^0) + U_0\,\delta(x)]\,\epsilon(x)^2 + \frac{b}{2}\,\epsilon(x)^4 \;+ d\,\epsilon'(x)^2 \right] dx \quad , \qquad (1)$$

where $a' > 0$, $b > 0$, $d > 0$ and $\epsilon = u' + u'^2/2$ is the strain serving as the order parameter of the transition (u is the displacement); by introducing the term $U_0\delta(x)$ into the harmonic part we describe the influence of a short-range defect (modelling a dislocation or a grain boundary in the three-dimensional case) which locally increases the transition temperature (softens the crystal) for $U_0 < 0$. Following ref. [3], the equation of motion for the soft acoustic phonons is (ρ being the mass density of the elastic medium)

$$\rho\,\ddot{u}(x,t) = -\,\delta\mathcal{F}[u]/\delta u(x,t) \quad . \qquad (2)$$

It is convenient to introduce dimensionless variables [2] $z = \sqrt{\frac{|a|}{d}}\,x$, $\tilde{t} = \sqrt{\frac{2a^2}{\rho\, d}}\,t$, $u(z) = \sqrt{\frac{b}{d}}\,u(x)$, $e(z) = \sqrt{\frac{b}{|a|}}\,\epsilon(x)$, $v_0 = \frac{1}{\sqrt{d|a|}}\,U_0$, $f[e] = \frac{b}{\sqrt{d|a|^3}}\,\mathcal{F}[\epsilon]$, where $a = a'(T - T_c^0)$. Note that the temperature dependence is now mapped onto the effective defect strength v_0 according to $T = T_c^0 + U_0^2/v_0^2 a'd$.

Within the framework of Ginzburg-Landau theory the equilibrium states $\bar{e}(z)$ are found from the stationarity condition $\frac{\delta f[e]}{\delta e(z)}\Big|_{e=\bar{e}} = 0$ with the restriction $f[\bar{e}] < \infty$, leading to the following nonlinear differential equation for $T > T_c^0$: $\bar{e}''(z) = [1 + v(z)]\,\bar{e}(z) + \bar{e}(z)^3$. The homogeneous solution $e_0 = 0$ is stable only when $v_0 > -2$, i.e. $T > T_c^{loc} = U_0^2/4a'd$. Below T_c^{loc} a cluster configuration

$$\bar{e}_C(z) = \pm\sqrt{2}\,[\sinh(|\,z\,| + \rho)]^{-1} \quad , \qquad \rho = \mathrm{arcoth}\,(-v_0/2) \qquad (3)$$

forms around the defect, its width diverging $\propto (T-T_c^0)^{-\frac{1}{2}}$, thereby continuously approaching the low-temperature phase, a phenomenon also termed local condensation [1),2)].

2. PHONON DYNAMICS FOR $T > T_c^{loc}$

Linearizing the fourth order differential equation (2) around the static solution $e_0 = 0$ we obtain an eigenvalue problem for the scattering states

$$\omega_k^2\, u_k(z) = u_k''''(z) - u_k''(z) - v_0\, u_k'(0)\, \delta'(z) \quad , \tag{4}$$

which is solved by $\omega_k^2 = k^2\left(1+k^2\right)$ and

$$u_k^+(z) = \frac{1}{\sqrt{\pi}} \cos kz \tag{5a}$$

$$u_k^-(z) = \frac{\mathrm{sgn}(z)}{\sqrt{\pi}} \left[\cos\varphi_R(k)\, e^{-\sqrt{1+k^2}|z|} - \cos\Big(k \mid z \mid + \varphi_R(k)\Big)\right] \quad . \tag{5b}$$

Here $\tan\varphi_R(k) = \mathrm{Im}\, R(k)/\mathrm{Re}\, R(k)$ and

$$R(k) = \frac{ik\,\frac{v_0}{2}}{\left(\sqrt{1+k^2}+ik\right)\left(\sqrt{1+k^2}-ik+\frac{v_0}{2}\right)} \tag{6}$$

is the reflection coefficient (see Fig.1). The solutions (5) can be shown to form a complete set of orthonormalized eigenfunctions to eq.(4) [4)], which demonstrates that there is no localized mode in the spectrum in contrast to the distortive case [2)]. Note, however, that each of the antisymmetric scattering states (5b) contains a vibrational part $u_k^{loc}(z,t) = \mathrm{sgn}(z)\, R(k)\, e^{-\sqrt{1+k^2}(|z|+ikt)}$ localized at the defect. Both the absolute value and the phase of $R(k)$ reach an extremum at a certain common wavenumber k_0 which is given by $k_0 \approx \sqrt{a'\,(T-T_c^{loc})/3d}$ in the vicinity of T_c^{loc} (in terms of the original variables), i.e. at T_c^{loc} the transmission amplitudes $1-R(k)$ of the long-wavelength phonons vanish and the vibrational part condenses at the defect.

To illustrate this fact we study the relaxation of a stress-induced cluster $u^0(z) = \mathrm{sgn}(z)\ e^{-\kappa|z|}$ $(\kappa > 0)$ by expanding the corresponding wavepacket in terms of the functions (5b). Its center of mass motion can then be found by the method of stationary phase yielding $z_m(\tilde{t}) = \pm(\tilde{t}-\tilde{t}_0)$ for $z \gtrless 0$, where near T_c^{loc} the relaxation time t_0 is given by

$$t_0 \approx \sqrt{2\rho d/a'^2}\,(T-T_c^{loc})^{-1} \tag{7}$$

(in the original variables) reflecting the fact that the corresponding displacement becomes stable at the local transition point.

3. RESPONSE FUNCTION AND CENTRAL PEAK

Introducing a heuristic damping coefficient $\gamma_k = D\,k^2\,(1+k^2)$ we proceed to discuss the phonon-phonon response function

$$\chi(z,z';\omega) = \frac{1}{2\pi}\int^{+\infty} \frac{u_k^+(z)\,u_k^+(z') + u_k^-(z)\,u_k^-(z')}{\omega^2 - \omega^2 - i\,\gamma\;\;\omega}\,dk \quad . \tag{8}$$

The integration can be performed analytically in the complex k-plane [4], the result being of the form $\chi(z,z';\omega) = \chi_0(z-z';\omega) + v_0\,\chi_D(z,z';\omega)$. As has been shown in ref. [5] by the means of a cumulant expansion we can calculate the corresponding response function for a *random multi-defect system* to first order in the defect concentration n using the formula

$$\chi(z-z';\omega) = \chi_0(z-z';\omega) + n\,v_0 \int_{-\infty}^{+\infty} \chi_D(z-z_D, z'-z_D;\omega)\,dz_D \quad . \tag{9}$$

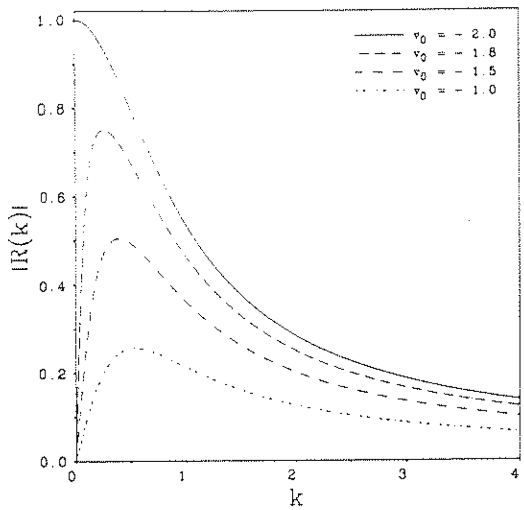

Fig.1: Reflection coefficient for different values of v_0

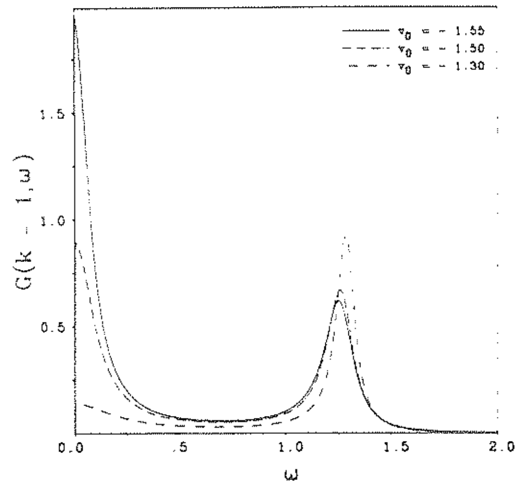

Fig.2: Correlation function $G(1,\omega)$ near $T_c^{loc}(n)$ (n=0.1, D=0.01)

Using the abbreviation $2\nu^2 = \sqrt{1+4\omega^2/(1-iD\omega)} - 1$ we finally obtain the Fourier-transformed response function

$$\chi(k,\omega) = \frac{1}{2\pi\left((1-iD\omega)\,k^2\left[(1+k^2) + n\,v_0\,\frac{\sqrt{1+\nu^2}-i\nu}{\sqrt{1+\nu^2}-i\nu+\frac{v_0}{2}}\right] - \omega^2\right)} \quad , \tag{10}$$

where the term $\propto nv_0$ has been written in the form of a self-energy correction. The corresponding correlation function $G(k,\omega) = \mathrm{Im}\,\chi(k,\omega)/\omega$ is shown in fig.2 for $k=1$, $n=0.1$ and $D=0.01$. There is a marked development of a *central peak* when the temperature approaches the shifted local transition temperature $T_c^{loc}(n) = T_c^{loc}(0) + n\,(1+n)\,U_0^2/a'd$. The width of the central peak turns out to be independent of the phonon-damping D and behaves as $T - T_c^{loc}(n)$. Note that in fig.2 the soft phonon peak position is fixed due to the use of scaled variables.

We remark that the results of sections 2. and 3. also apply to the case of a first-order transition (e.g. described by a ϕ^6-model [6]) because the nonlinear terms disappear when eq.(2) is linearized around $\epsilon_0 = 0$.

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