Symmetry of Elastic Tensor: Hydrodynamics versus Lattice Dynamics

In an interesting recent Letter Nelson[1] has suggested that there are, in general, 45 independent elastic constants, if a long-wavelength lattice-dynamical calculation is used. He obtained this nonclassical result (45 instead of 21 elastic constants) by coupling optical phonons to the acoustic phonons. The assumption of small frequencies is not being made in this type of description. Here we investigate how this situation can be analyzed in a hydrodynamic approach. We find that of the 45 elastic constants 9 are surface and only 36 are bulk elastic constants. We also discuss that this nonclassical result is relevant for intermediate frequencies only.

By hydrodynamics we mean the macroscopic description of condensed systems (c.f., e.g., Forster and coworkers[2] and Martin, Parodi, and Pershan[3] for an overview) which is applicable to excitations relaxing with vanishing frequencies in the limit of very large wavelengths. One obtains in this regime—considering only truly hydrodynamic variables, i.e., only those without a gap in the excitation spectrum—the classical value of 21 different elastic constants in the general case.[3,4] More constants can thus only arise if nonhydrodynamic variables, e.g., those connected with optical phonons, are considered.

In the last few years it has turned out that under certain conditions one has to generalize hydrodynamics by incorporating dynamic degrees of freedom into the long-wavelength description, which relax in a very large, but finite time. This approach has been called macroscopic dynamics and it has proven to be a fruitful one for a large class of systems including incommensurate systems,[5] liquid crystals close to a phase transitions,[6] the superfluid phases of ^{3}He,[7] tilted hexatic liquid crystals,[8] and even propagating incommensurate structures in nonequilibrium systems[9]; further examples are discussed elsewhere.[10]

If we take into account (in addition to the displacement $\mathbf{u}$) nonhydrodynamic variables, like $\mathbf{w}$, the relative displacement of atoms of different sorts, the elastic energy takes the form

$$2f = C_{ijkl}(\nabla_j u_i)(\nabla_l u_k) + A_{ij} w_i w_j + 2B_{ijk} w_k \nabla_j u_i + D_{ijkl}(\nabla_j w_i)(\nabla_l w_k) + E_{ijkl}(\nabla_j u_i)(\nabla_l w_k), \quad (1)$$

where the coefficients A_{ij} reflect the gap of the optical mode $\mathbf{w}$. Far away from any phase transition $\mathbf{w}$ is averaged out on sound or ultrasound time scales and Eq. (1) reduces to the ordinary elastic energy. Somewhat closer to a phase transition, where $\mathbf{w}$ becomes soft, but is still fast enough so that $\mathbf{w}$ is faster than $\mathbf{u}$, one obtains after elimination of $\mathbf{w}$ an effective elastic energy

$$2f = \tilde{C}_{ijkl}(\nabla_j u_i)(\nabla_l u_k), \quad (2)$$

where $\tilde{C}$ does not have the symmetry $C_{ijkl} = C_{jikl} = C_{ijlk}$ of the true elastic tensor. That part of $\tilde{C}$ that has a $\tilde{C}_{ijkl} = \tilde{C}_{ilkj}$ symmetry gives rise to (36) bulk effective coefficients and the other part to (9) surface effective coefficients.

Very close to the phase transition, where A (and B) vanishes, one has to keep both $\mathbf{u}$ and $\mathbf{w}$ in Eq. (1) and the number of effective elastic coefficients is the sum of the C, D, and E coefficients, which exceeds by far the number 36 found in the intermediate-frequency regime. Similar considerations are possible for the piezoelectric coefficients, where we find for the intermediate regime 18 bulk and 9 surface terms (compared with the 10 bulk and 8 surface terms in the hydrodynamic regime); the latter are surface terms, if curl $\mathbf{E}$ is zero.

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