

Elasticity

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May 18, 2023

1 The theoretical framework

1.1 The displacement field

We use \mathbf{r} to refer to the position vector of a position in a continuum, and $\mathbf{r}'(\mathbf{r}, t)$ its corresponding position at time t . The displacement field is therefore

$$\mathbf{u}(\mathbf{r}, t) = \mathbf{r}'(\mathbf{r}, t) - \mathbf{r}. \quad (1)$$

A rough estimation of the number of degrees of freedom implies that all information about the material – the position of each atom – has already been stored in $\mathbf{u}(\mathbf{r}, t)$. To see why, note that we can do Fourier transform to $\mathbf{u}(\mathbf{r}, t)$ in variable \mathbf{r} . Suppose the size of the system is $\sim L^d$, where d is the dimension of the system, and the microscopic length scale of the system is $\sim a$. The wave vector components of $k_{x,y,z}$ therefore are confined to the sequence that starts with 0 and ends with $2\pi/a$ (the microscopic cutoff), with a step of $2\pi/L$; the total length of this sequence is $\simeq L/a$, and thus the total number of possible wave vectors is $(L/a)^d$. Thus the number of real number variables included in the field variable $\mathbf{u}(\mathbf{r}, t)$ at a given time step is $d \cdot (L/a)^d$: the prefactor d comes from the d components of \mathbf{u} . On the other hand, there are $\simeq (L/a)^d$ atoms in the system, and each of them has d directions of motion, and therefore, we find that number of real number variables included in $\mathbf{u}(\mathbf{r}, t)$ is the same as the number of real number variables of the atoms, and thus $\mathbf{u}(\mathbf{r}, t)$ contains all the information contained in the system. This should not be surprising: that we have a wave vector cutoff $\simeq 2\pi/a$ means we have a real space resolution of $\simeq a$, so at each time step t , $\mathbf{u}(\mathbf{r}, t)$ can be completely described by a real space grid with the separation between the sample points being $\simeq a$ – and the points in the grid is just equivalent to the initial positions of the atoms.

There are however some subtleties in the above argument. If the material is not a crystal, when $k \simeq 2\pi/a$, the translational symmetry is already broken, and therefore the wave vector is not well-defined any more; thus the wave vector cutoff should be set to a much lower value. If the system is an insulator, we can take a to be the length scale of the primitive unit cell, and $2\pi/a$ is the magnitude of the width of the first Brillouin zone. If there is only one kind of atom, then indeed $\mathbf{u}(\mathbf{r}, t)$ contains all information in the system; but often we have more than one kind of atoms (two atoms that are not connected by any symmetry operations should be considered to be two kinds of atoms, even when they are of the same species), and then $\mathbf{u}(\mathbf{r}, t)$ only contains the acoustic phonon modes.

So in conclusion, the displacement field $\mathbf{u}(\mathbf{r}, t)$ only contains the acoustic modes, both in crystals and non-crystals; in both cases there may be additional hidden microscopic degrees of freedom.

1.2 The kinetics of deformation

TODO: transport theorem, etc.

1.3 Dynamics of perfect elasticity

We assume u_i and its conjugate momentum are the only dynamic variables; thus, once

TODO: degree of freedom counting: does u_i include optical phonons?

1.4 Dissipation

Dissipation comes from two sources. The first kind of dissipation involves the aforementioned hidden degrees of freedom that we lose track of.

1.5 Finite temperature

The theory of elasticity at $T = 0$ is just the low-energy effective field theory about phonons.
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