

Elasticity

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1 The theoretical framework

1.1 The displacement field

For now, 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 . After the discussion below we will need to change the meaning of \mathbf{r} to \mathbf{r}' . 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. These hidden degrees of freedom, like dislocation, can be treated by introducing various discontinuities to $\mathbf{u}(\mathbf{r})$.

Below we often use u_i to represent \mathbf{u} , since we are going to deal with tensors frequently and it's a good idea to keep the notation the same as that of higher order tensors.

1.2 General guidelines of elastic dynamics

Let's now move to the following question of what the dynamics of an elastic solid system looks like. In this section we progressively introduce assumptions on this topic.

1.2.1 Dynamic variables: u_i only

The first assumption we introduce is *the dynamics of the system should be able to be cast into a form that is only about u_i and its conjugate momentum*. Note that even when more dynamic variables are involved, we still can use, say, Mori-Zwanzig formalism to get a theory about u_i only, and thus in order for this approximation to be truly restrictive, we need to impose some implicit constraints on the formalism used when modeling the dynamics. If we constrain the formalism to be Hamiltonian dynamics plus some dissipation terms, then essentially we are assuming that the material is elastic (Section 1.2.2).

This assumption means the system we are investigating into doesn't have typical fluid behavior: in Navier-Stokes equation, the density $\rho(\mathbf{r}, t)$ is also a dynamic variable which can be used to decide p on the RHS of the equation;¹ this isn't necessary in solid mechanics: even when we do have ρ dependence in the EOMs, it should be able to be decided explicitly by, say, $\nabla \cdot \mathbf{u}$.²

In other words, when $T = 0$, the Hamiltonian of the system is basically a Hamiltonian of phonons. The quantum Hamiltonian of fluid, on the other hand, involves ρ and \mathbf{v} (and a strange commutation relation between them) [1].

Sometimes we do need corrections to this assumption: it's possible that long-range electromagnetic fields are created, and in this case \mathbf{E} and \mathbf{B} should also be included into the dynamic variables (or otherwise we have memory effects, retardation effects, etc.). The approximation therefore may be loosened to *no degree of freedom other than u_i that is about the atomic positions in the system is needed in the dynamics*.

1.2.2 Elasticity: statelessness and immediate response

Elasticity is sometimes defined as the follows: *when we stop applying force to the system, it always goes back to one equilibrium shape*. In other words, if we push the system and then stop, the system bounces back.

This definition is too weak: it may be possible that after a loading-unloading process, although the system goes back to its original shape, its inner structure has changed and its reaction to another round of loading and unloading is different from that of the previous round. So we need to impose a stronger formulation of elasticity: *the deformation of the system has nothing to do with its history and is completely decided by the force applied to it*. This formulation implies the weaker version: when no load is present, the system has one and only one configuration.

The above formulation however has some ambiguity. In experiments usually the force applied to the system is changed very slowly, and the system is quasi-static. In dynamics, however, we may be interested in oscillation, where the force applied changes quickly, and now it's possible that the response of the system is retarded;³ if we go to frequency space, we may find that the response of the system has frequency dependence. This is of course possible, and we may still say that the deformation of the system is decided by the force applied to it. Often, we make a even stronger assumption: *the deformation of the system in a particular moment is complete decided by the force applied to it in that very moment*. This means the system has immediate response to the force applied to it.

1.2.3 Dissipation and finite temperature effects

When $T = 0$, we may want to use a Hamiltonian formalism (a quantum many-body theory for phonons, actually) to describe the elastic system; this however is usually not sufficient since we have various dissipations: it's inevitable that some weight flows into the hidden degrees of freedom that we lose track of.⁴ An accurate formalism for dissipation is hard since it involves quantum master equation of the density matrix and dissipative quantum jump channels; but in ordinary elastic theory, usually we don't care about what happens to the quantum many-body

¹When the fluid is incompressible, p needs to be used in place of ρ as a dynamic variable.

²Note that solid-like dynamics is not the logical opposition of fluid-like dynamics: it's possible to have systems with both solid-like and fluid-like behaviors. These materials are studied in rheology.

³Note that as is known in effective field theory, the response of the system to external driving force and internal force should be the same, as long as the external driving force is coupled to the deformation of the system in the same way internal forces are coupled to the deformation system, and since we call external forces "force" this should be true.

⁴It's still possible that even the system does have a dissipation-less Hamiltonian description, there is still damping behavior for a single mode, when the mixing between modes is too severe (as in, say, Landau damping). Since all degrees of freedom are well kept track of, this is "dissipation-less damping".

wave function, and all we want to know is $\langle u_i \rangle$, ignoring its higher order correlations. Thus usually dissipation is just modeled by adding a term like $\partial_t u_i$ to the EOM.

Another issue is finite temperature effects. Here we do *local equilibrium approximation*: we assume that when $T \neq 0$, there can be T gradient in the system, but at each given point, we have local equilibrium with the local temperature, the force and the deformation being thermodynamic coordinates, and the relaxation time is ignored. Local equilibrium approximation is equivalent to the condition that $\omega\tau \ll 1$, where ω is the characteristic frequency scale of the dynamic and τ the relaxation time. This corresponds to the $\omega\tau \ll 1$ limit in Fermi liquid kinetics, where we have ordinary hydrodynamics and ordinary sound mode [2]. Again, the most accurate treatment of finite temperature effects involves quantum kinetic theory, but in the $\omega\tau \ll 1$ limit the quantum kinetic theory is reduced to local thermodynamics.

1.2.4 The form of EOM

The variables u_i and the internal force density f_i are not thermalized; as [2] says, they are subject to conservation laws, and from momentum conservation we get Newton's second and third laws, so the EOM of the system looks like

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\delta F[\mathbf{u}]}{\delta u_i} + f_i^{\text{dissipation}}(\partial_t \mathbf{u}, \partial_t^2 \mathbf{u}, \dots), \quad (2)$$

where F is the free energy, and the functional derivative is taken by keeping the temperature variable constant. But this formalism works even when the temperature changes: the change of the temperature is reflected by the temperature dependence of $\delta F[\mathbf{u}]/\delta u_i$ after we take the derivative. When $T \rightarrow 0$, F becomes the total energy of the system and we go back to Hamiltonian dynamics.

It's kind of silly to spend so much time to get (2), but we have seen that for many frequently seen materials, we need to go beyond (2): when the system has strong fluid-like behavior, when we have plastic deformation, and when there is retardation.

1.3 Stress

1.3.1 There are only surface forces

For real elastic systems, the form of the EOM often can be further constrained. First, $F[\mathbf{u}]$ is *usually local*, and thus we have

$$\frac{\delta F[\mathbf{u}]}{\delta u_i} = \frac{\partial f}{\partial u_i}, \quad F = \int d^d \mathbf{r} f, \quad (3)$$

where f is the volume density of free energy; in the rest of this note we simply use F to refer to the volume density of free energy, because f may be confused with “force”. Moreover, we can assume that the length scale of the interaction between atoms is very small – if we have an interaction channel with a large length scale then we just introduce the relevant part of electromagnetic field into dynamic variables – and since the spatial resolution of \mathbf{u} is taken to be much larger than a , effectively we can assume that *the internal forces are all surface forces*, and therefore

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \partial_j \sigma_{ji} + f_i^{\text{dissipation}}, \quad (4)$$

that's to say, the total force on a volume is

$$\int_V d^d \mathbf{r} \partial_j \sigma_{ji} = \int_{\partial V} d^{d-1} s_j \sigma_{ji}. \quad (5)$$

We can alternatively get σ_{ji} by writing down the conservation equation of the momentum. We call σ_{ij} the **stress tensor**.

From (5) we immediately get the boundary condition about force passing: if the force acting on a surface element $d^{d-1} s_i$ is $p_i d^{d-1} s_i$, then at the position of the surface element, we have

$$p_i = n_j \sigma_{ji}, \quad (6)$$

where n_j is the j th component of the normal vector \mathbf{n} of the surface element $d^{d-1} s_i$, and we have

$$d^{d-1} s_i = n_i ds. \quad (7)$$

1.3.2 Is the stress tensor symmetric?

An additional constraint on σ_{ij} that is not necessary but works for most elastic bodies is that σ_{ij} is *symmetric*. This constraint is equivalent to the condition that *there is no body torsion*: the torsion on a volume is

$$\begin{aligned} M_{ij} &= \int d^d \mathbf{r} (r_i \partial_k \sigma_{kj} - \partial_k \sigma_{ki} r_j) \\ &= \int d^d \mathbf{r} (\partial_k (r_i \sigma_{kj}) - \sigma_{kj} \delta_{ik} - \partial_k (r_j \sigma_{ki}) + \sigma_{ki} \delta_{jk}) \\ &= \int d^{d-1} s_k (r_i \sigma_{kj} - r_j \sigma_{ki}) - \int d^d \mathbf{r} (\sigma_{ij} - \sigma_{ji}), \end{aligned} \quad (8)$$

and it can be seen that the first term is just the torsion caused by the forces applied to the surface of this volume; if we assume that there is no body torsion, then the second term should always be zero regardless of the exact shape and position of the volume, and this condition is equivalent to

$$\sigma_{ij} = \sigma_{ji}. \quad (9)$$

Of course, we don't have body torsion in an equilibrium system, since if we have, then a part of the system will begin to rotate. However we do have body torsion sometimes: in a liquid crystal system, for example, if a group of rod-like molecules get an angle difference from the rods near them, they will be pulled back, and in this *transient* process a torsion is created.

Since this note is about quasi-static behaviors of ordinary elastic materials, we will just adopt the assumption (9).

1.3.3 Stress and free energy

1.4 Strain

1.4.1 The kinematics of deformation

Laws governing the time evolution of $\mathbf{u}(\mathbf{r}, t)$ are to be written in terms of $\partial_{\mathbf{r}} \mathbf{u}$, $\partial_t \mathbf{u}$, etc. But there is a problem:

TODO: transport theorem, etc.

TODO: from microscopic theory to this

1.4.2

TODO: in \mathbf{r} or \mathbf{r}'

References

- [1] Alexander G. Abanov and Paul B. Wiegmann. "Quantum Hydrodynamics, the Quantum Benjamin-Ono Equation, and the Calogero Model". In: *Physical Review Letters* 95.7 (2005). ISSN: 1079-7114. DOI: [10.1103/physrevlett.95.076402](https://doi.org/10.1103/physrevlett.95.076402). URL: <http://dx.doi.org/10.1103/PhysRevLett.95.076402>.
- [2] D Belitz and TR Kirkpatrick. "Soft modes in Fermi liquids at arbitrary temperatures". In: *Physical Review B* 105.24 (2022), p. 245146.