# **ELASTIC MEDIA & PHONONS**

#### NOTES BY L. G. MOLINARI

#### 1. The microscopic approach to phonons

Phonons are the quanta of vibrations of ions about their equilibrium positions in crystals, glasses, or molecules. The microscopic theory starts with an Hamiltonian where both electrons and ions are dynamical. The smallness of the mass ratio  $m_e/M_{ion}$  often justifies the resolutive *Adiabatic Approximation* by Born and Oppenheimer, by which the electronic state istantaneously adapts to the slowly changing environment of the ions.

The Schrödinger equation for electrons and ions is then solved in two steps.

First, one solves for the electrons with the ions being fixed at positions  $\mathbf{R}_i$ . The ground state energy  $E_0(\mathbf{R}_1 \dots \mathbf{R}_N)$  defines an *energy landscape*, which can be very complex, with maxima, minima, saddle points and valleys. Since positions are measured in a frame that can be translated or rotated, these least symmetries are present:  $E_0(\mathbf{R}_1 + \mathbf{a}, \dots, \mathbf{R}_N + \mathbf{a}) = E_0(\mathbf{R}_1, \dots, \mathbf{R}_N)$ ,  $E_0(\mathbf{R}\mathbf{R}_1, \dots, \mathbf{R}_N) = E_0(\mathbf{R}_1, \dots, \mathbf{R}_N)$ , where R is a rotation.

Next, the function  $E_0$  is used as a potential for the ions. Minimization in all parameters  $\mathbf{R}_i$  gives the equilibrium configuration  $\{\mathbf{R}_i^0\}$ . The expansion of the energy function around the minimum yields the Hamiltonian for the ions

$$H_{ion} = E_{min} + \sum_{i=1}^{N} \sum_{a=xyz} \frac{P_{ia}^2}{2M_i} + \frac{1}{2} \sum_{ij=1}^{N} \sum_{ab=xyz} H_{ia,jb} \eta_{ia} \eta_{jb}, \qquad \eta_i = \mathbf{R}_i - \mathbf{R}_i^0$$

 $H_{ia,jb}$  is the Hessian matrix, of second derivatives evaluated at the minimum. Terms beyond quadratic are called anharmonic, and are here neglected. The presence of other minima of comparable depth makes the problem very complex, as thermal activation, or tunneling, may drive the system from a configuration to another, or a superposition of them.

The rescaling  $\eta'_i = \eta_i \sqrt{M_i/\mu}$  brings masses to the same value:

(1) 
$$H_{ion} = E_{min} + \sum_{i=1}^{N} \sum_{a=xyz} \frac{P_{ia}^{\prime 2}}{2\mu} + \frac{1}{2} \sum_{ij=1}^{N} \sum_{ab=xyz} \sqrt{\frac{\mu}{M_i}} H_{ia,jb} \sqrt{\frac{\mu}{M_j}} \eta_{ia}^{\prime} \eta_{jb}^{\prime},$$

A rotation in  $\mathbb{R}^{3N}$ ,  $\xi_{ia} = R_{ia,jb}\eta'_{jb}$ , diagonalizes the Hessian. 3N-6 eigenvalues are non-negative, while 6 are zero because of the translation and rotation symmetries, and correspond to barycentric motion. The resulting Hamiltonian is a sum of independent harmonic oscillators (normal modes). In a reference system where the body is at rest:

(2) 
$$H_{ion} = E_{min} + \sum_{a=1}^{3N-6} \frac{p_a^2}{2\mu} + \frac{1}{2}\mu\omega_a^2\xi_a^2$$

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Quantization of each oscillator gives the effective quantum Hamiltonian of the motion of the N ions:

$$H_{ion} = E_{min} + \sum_{a=1}^{3N-6} \hbar \omega_a (c_a^{\dagger} c_a + \frac{1}{2})$$

If the equilibrium configuration of the ions is a lattice, each oscillator is labelled by a vector  $\mathbf{k}$  of the dual lattice. In the long wave-length limit, the dispersion laws  $\omega(\mathbf{k})$ , specific of the lattice, become those of an elastic medium. This is one reason for studying phonons of elastic media.

# 2. Elastic media

In many-body theory, phonons are often introduced by approximating the background of ions as an elastic medium. In the long wavelength limit (i.e. low energy) it gives a simple description of extended systems, the peculiarities of the material being captured by few phenomenological parameters.

As a piece of matter is subjected to an external force, it deforms and develops internal forces that oppose the deformation. Since internal forces are short-ranged, the state of stress depends on how distances of neighboring parts are modified by the deformation. This is encoded in the metric tensor.

Suppose that the medium has been deformed and is in equilibrium with the applied forces. A physical point originally at position  $\mathbf{x}$  is displaced to a position  $\mathbf{x} + \mathbf{u}(\mathbf{x})$ . The field  $\mathbf{u}$  is the displacement of the physical points.

Two close points  $\mathbf{x}$  and  $\mathbf{x}+d\mathbf{x}$  get displaced to  $\mathbf{x}+\mathbf{u}(\mathbf{x})$  and  $\mathbf{x}+d\mathbf{x}+\mathbf{u}(\mathbf{x}+d\mathbf{x})$ . The squared distance of the two images, to lowest order in  $\mathbf{u}$ , is a quadratic expression that defines the metric tensor:

(3) 
$$ds'^{2} = dx'^{i} dx'_{i} \equiv g_{ij}(\mathbf{x}) dx^{i} dx^{j}$$
$$g_{jk}(\mathbf{x}) = \frac{\partial x'^{i}}{\partial x^{j}} \frac{\partial x'_{i}}{\partial x^{k}} = \delta_{ij} + 2D_{ij}(\mathbf{x})$$

If the Jacobian matrix of the transformation  $\mathbf{x} \to \mathbf{x}'$  is invertible, then the metric tensor is strictly positive. D is the symmetric *strain tensor* (Cauchy):

(4) 
$$D_{ij}(\mathbf{x}) = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

A cube of volume  $d\mathbf{x}$  centred in  $\mathbf{x}$  transforms under the displacement to some shape with volume

$$d\mathbf{x}' = \left|\det\frac{\partial x'^i}{\partial x^j}\right| d\mathbf{x} = \sqrt{g(\mathbf{x})} d\mathbf{x}$$

where  $g = \det g_{ij}$ . For small deformations it is  $\sqrt{g} = \sqrt{\det(I+2D)} \approx \sqrt{1+2\operatorname{tr} D} \approx 1+\operatorname{div} \mathbf{u}(\mathbf{x})$  i.e. the divergence of the displacement field describes the local variation of the volume:

(5) 
$$\frac{\delta V}{V} = \operatorname{div} \mathbf{u}(\mathbf{x})$$

After a deformation, the initially uniform mass-density  $\rho_0$  becomes position dependent, and since the matter content within a closed surface is unchanged, it is  $\rho_0 d\mathbf{x} = (\rho_0 + \delta \rho(\mathbf{x}')) d\mathbf{x}'$  i.e.

(6) 
$$\delta \rho(\mathbf{x}) = -\rho_0 \operatorname{div} \mathbf{u}(\mathbf{x})$$

2.1. The stress tensor. A deformation produces a state of stress, with internal forces that oppose the external forces that produce it. It is clear that only gradients of the displacements are relevant, since a local translation produces no stress (no elementary "springs" are stretched).

The forces in a continuum are described by a symmetric<sup>1</sup> stress tensor field  $\pi_{ij}(\mathbf{x})$ , introduced by Augustine-Louis Cauchy in 1822. He proved that the force acting on a surface element of area da at  $\mathbf{x}$ , with normal vector  $\mathbf{n}$ , is<sup>2</sup>.

$$df^i = \pi^{ij}(\mathbf{x})n_j \, da.$$

In a perfect fluid the stress tensor is isotropic  $\pi_{ij} = -p\delta_{ij}$ , with force orthogonal to the area element, and no tangential components. For a general stress tensor, the pressure is defined as  $p(\mathbf{x}) = -\frac{1}{3}\pi^j_{\ j}(\mathbf{x})$ .

Consider a volume V enclosed by a surface S with outer normal  $\mathbf{n}(\mathbf{x})$ . The force that the exterior exerts on the volume is the resultant of the surface forces:

$$F^{i} = \int_{S} \pi^{ij} n_{j} da = \int_{V} d\mathbf{x} \, \partial_{j} \pi^{ij}$$

by the divergence theorem. Therefore,  $\partial_j \pi^{ij}(\mathbf{x})$  is the force per unit volume.

If  $\rho_0$  is the mass density at equilibrium, the linearized equation of motion for the displacement field is

(7) 
$$\rho_0 \frac{\partial^2}{\partial t^2} u^i(\mathbf{x}, t) = \frac{\partial}{\partial x^j} \pi^{ij}(\mathbf{x}, t)$$

A homogeneous elastic medium is defined by the generalization of Hooke's law<sup>3</sup>:  $\pi_{ij}(\mathbf{x}) = C_{ijkl} D^{kl}(\mathbf{x})$ . If the medium is isotropic it simplifies to

(8) 
$$\pi_{ij}(\mathbf{x}) = \lambda \delta_{ij} D^k{}_k(\mathbf{x}) + 2\mu D_{ij}(\mathbf{x})$$

where  $\lambda > 0$  and  $\mu \ge 0$  are the Lamé constants<sup>4</sup>.

While initially the pressure is zero, a deformation builds a nonzero pressure  $\delta p(\mathbf{x}) = -\frac{1}{3}\pi^{j}{}_{j} = -\frac{1}{3}(3\lambda + 2\mu) \operatorname{div} \mathbf{u}(\mathbf{x}) = -(\lambda + \frac{2}{3}\mu)\delta V/V$ . This formula links the Lamé constants to the (adiabatic) bulk modulus:

(9) 
$$B = -V \left(\frac{\partial p}{\partial V}\right)_S = \lambda + \frac{2}{3}\mu$$

Other relations link  $\lambda$ ,  $\mu$  to the Poisson and Young parameters.

$$Q_{ir}Q_{js}\pi^{rs}(Q^t\mathbf{x}) = C_{ijkl}Q^{km}Q^{ln}D_{mn}(Q^t\mathbf{x})$$

for any Q and **x**. This means:  $C_{rsmn} = Q_{ri}Q_{sj}C^{ijkl}Q_{km}Q_{ln}$ . In particular,  $C^{r}_{rmn} = C^{r}_{rkl}Q^{k}_{m}Q^{l}_{n}$ , meaning that the matrix  $C^{r}_{rmn}$  commutes with any rotation, i.e.  $C^{r}_{rmn} = Au_{mn}$ . In the same way  $C_{ijm}^{m} = Bu_{ij}$ . Consistency requires A = B. It is also  $C_{rs}^{r}_{n} = Q_{s}^{j}C_{rj}^{r}_{l}Q^{l}_{n}$  meaning that  $C_{rs}^{r}_{n} = Cu_{sn}$ . Putting pieces together, the isotropic tensor is  $C_{ijkl} = \lambda u_{ij}u_{kl} + 2\mu u_{ik}u_{il}$ .

 $\dot{C}_{ijkl} = \lambda u_{ij}u_{kl} + 2\mu u_{ik}u_{jl}.$ <sup>4</sup>For Aluminum:  $\rho_0 = 2.7 \times 10^3 \text{kg/m}^3$ ,  $\lambda = 55$  GPa,  $\mu = 26$  GPa (1 GPa =  $10^9 \text{N/m}^2$ ), sound velocity  $v_s = 6.3$  km/s

 $<sup>^1\</sup>mathrm{symmetry}$  is related to angular momentum conservation.

 $<sup>^{2}\</sup>mathrm{a}$ nice book is: B. Lautrup, Physics of continuous matter, 2nd ed. CRC Press (2011)

<sup>&</sup>lt;sup>3</sup>The most general linear homogeneous relation  $\pi_{ij} = C_{ijkl}D^{kl}$  entails  $3^4 = 81$  coefficients. The simmetry of the stress and the strain tensors reduces the number to  $6^2 = 36$ . Isotropy means that in a rotated frame the coefficients remain unchanged:  $\pi'_{ij}(\mathbf{x}) = C_{ijkl}D'^{kl}(\mathbf{x})$  for all matrices Q and  $\mathbf{x}$ . The stress tensor transforms as  $\pi'_{ij}(\mathbf{x}) = Q_{ir}Q_{js}\pi^{rs}(Q^t\mathbf{x})$  and the same for  $D_{ij}$ . Then we require:

**Proposition 2.1.** If  $C_{ijkl} = C_{klij}$ , there is a conserved elastic energy:

(10) 
$$E = \int d^3x \left[ \frac{1}{2} \rho_0 \dot{u}^2 + \frac{1}{2} C^{ijkl} D_{ij} D_{kl} \right]$$

*Proof.* Contraction of (7) with  $\dot{u}_i$  gives:  $\frac{1}{2}\rho_0\partial_t(\dot{u}^2) = \partial_j(\dot{u}_i\pi^{ij}) - \pi^{ij}\partial_j\dot{u}_i$ . The tensor  $\partial_j\dot{u}_i$ , being contracted with  $\pi^{ij}$  is symmetrized. This gives  $\frac{1}{2}\rho_0\partial_t(\dot{u}^2) + \pi^{ij}\dot{D}_{ij} = \partial_j(\dot{u}_i\pi^{ij})$ . Since  $\pi^{ij} = C^{ij}{}_{kl}D^{kl}$ , a total derivative is obtained:

$$\partial_t \left[ \frac{1}{2} \rho_0 \dot{u}^2 + \frac{1}{2} \pi^{ij} D_{ij} \right] = \partial_j (\dot{u}_i \pi^{ij})$$

The volume integral becomes a surface integral in the right hand side, that vanishes at infinity. The conservation of the energy is obtained.  $\hfill \Box$ 

2.2. Elastic waves. With the stress tensor (8) the equation of motion is

(11) 
$$\rho_0 \partial_t^2 \mathbf{u} = \mu \nabla^2 \mathbf{u} + (\lambda + \mu) \operatorname{grad} \operatorname{div} \mathbf{u}$$

By taking the divergence or the rotor, one obtains two wave equations:

(12) 
$$\begin{bmatrix} \frac{1}{v_L^2} \frac{\partial}{\partial_t^2} - \nabla^2 \end{bmatrix} \operatorname{div} \mathbf{u}(\mathbf{x}, t) = 0 \quad , \quad \begin{bmatrix} \frac{1}{v_T^2} \frac{\partial}{\partial_t^2} - \nabla^2 \end{bmatrix} \operatorname{rot} \mathbf{u}(\mathbf{x}, t) = 0$$

We'll show that the first one describes longitudinal waves, that involve variations of the volume and propagate with velocity  $v_L$ . The second equation describes transversal waves (rot **u** is orthogonal to **u**) with velocity  $v_T$ .

(13) 
$$v_L = \sqrt{\frac{\lambda + 2\mu}{\rho_0}}, \quad v_T = \sqrt{\frac{\mu}{\rho_0}}.$$

Note the inequality  $v_L > \sqrt{2} v_T$ : longitudinal waves are always faster than transversal waves<sup>5</sup> (in general  $v_L \approx \sqrt{3}v_T$ ). The longitudinal velocity coincides with the speed of sound in the medium.

The distinction among longitudinal and transversal refers to the Fourier modes of the waves. In a box of side L:

$$\mathbf{u}(\mathbf{x},t) = \sum_{\mathbf{k}} \mathbf{u}(\mathbf{k},t) \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}},$$

with  $\mathbf{u}(\mathbf{k},t)^* = \mathbf{u}(-\mathbf{k},t)$  for reality. Each Fourier component is then decomposed into a vector parallel to  $\mathbf{k}$  and an orthogonal vector:

$$\mathbf{u}(\mathbf{k},t) = \frac{\mathbf{k}}{|\mathbf{k}|^2} (\mathbf{k} \cdot \mathbf{u}) + \left[ \mathbf{u} - \frac{\mathbf{k}}{|\mathbf{k}|^2} (\mathbf{k} \cdot \mathbf{u}) \right] = \mathbf{u}_L(\mathbf{k},t) + \mathbf{u}_T(\mathbf{k},t)$$

It is  $\mathbf{k} \times \mathbf{u}_L(\mathbf{k}, t) = 0$  and  $\mathbf{k} \cdot \mathbf{u}_T(\mathbf{k}, t) = 0$ . In components:

$$u_i(\mathbf{k}, t) = \frac{k_i k_j}{|\mathbf{k}|^2} u_j + \left[\delta_{ij} - \frac{k_i k_j}{|\mathbf{k}|^2}\right] u_j$$

The matrices are the projectors on the direction parallel to  $\mathbf{k}$  and in the plane orthogonal to  $\mathbf{k}$ .

**Exercise 2.2.** Show that any vector field admits a decomposition into irrotational (longitudinal) and divergence-free (transversal) fields:  $\mathbf{F}(\mathbf{x}) = \mathbf{F}_L(\mathbf{x}) + \mathbf{F}_T(\mathbf{x})$  where rot  $\mathbf{F}_L(\mathbf{x}) = 0$  and div  $\mathbf{F}_T(\mathbf{x}) = 0$ .

<sup>&</sup>lt;sup>5</sup> in seismology they are named P (*prima*) and S (*secunda*)

In  $\mathbf{k}$  space eq.(11) becomes:

$$\frac{d^2}{dt^2}u_i(\mathbf{k},t) = -k^2 v_T^2 \left[\delta_{ij} - \frac{k_i k_j}{k^2}\right] u^j(\mathbf{k},t) - k^2 v_L^2 \left[\frac{k_i k_j}{k^2}\right] u^j(\mathbf{k},t)$$

By acting with the orthogonal projections, one obtains two independent equations:

(14) 
$$\left[\frac{d^2}{dt^2} + v_L^2 k^2\right] \mathbf{u}_L(\mathbf{k}, t) = 0, \qquad \left[\frac{d^2}{dt^2} + v_T^2 k^2\right] \mathbf{u}_T(\mathbf{k}, t) = 0.$$

For each **k**, introduce the orthonormal basis  $\mathbf{e}_{\lambda}(\mathbf{k})$ :  $\mathbf{e}_{3}(\mathbf{k}) = \mathbf{k}/|\mathbf{k}|$  and  $\mathbf{e}_{1,2}(\mathbf{k}) \perp \mathbf{e}_{3}(\mathbf{k})$  (polarization vectors). The general solution of (11) is the real sum of longitudinal and transversal plane waves. A convenient expression is

(15) 
$$\mathbf{u}(\mathbf{x},t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k},\lambda} \mathbf{e}_{\lambda}(\mathbf{k}) \frac{1}{i} \left( d_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{x} - i\omega_{\lambda}(k)t} - d_{\mathbf{k},\lambda}^* e^{-i\mathbf{k}\cdot\mathbf{x} + i\omega_{\lambda}(k)t} \right)$$

with complex amplitudes  $d_{\mathbf{k},\lambda}$  that are determined by the initial conditions, and linear dispersions:

(16) 
$$\omega_{\lambda}(k) = \begin{cases} v_T k & \lambda = 1, 2\\ v_L k & \lambda = 3 \end{cases}$$

**Exercise 2.3.** Show that the polarised fields  $\mathbf{u}_{\lambda}(\mathbf{x}, t)$  with Fourier components  $\mathbf{u}_{\lambda}(\mathbf{k}, t)$  solve the wave equations  $(\partial_t^2 - v_{\lambda}^2 \nabla^2) \mathbf{u}_{\lambda}(\mathbf{x}, t) = 0$  with rot  $\mathbf{u}_L(\mathbf{x}, t) = 0$  and div  $\mathbf{u}_T(\mathbf{x}, t)$  at all times.

Show that the following expressions are constants of the motion<sup>6</sup>:

(17) 
$$E_L = \frac{1}{2}\rho_0 \int d^3x \left[ (\partial_t \mathbf{u}_L)^2 + v_L^2 (\operatorname{div} \mathbf{u}_L)^2 \right]$$

(18) 
$$E_T = \frac{1}{2}\rho_0 \int d^3x \left[ (\partial_t \mathbf{u}_T)^2 + v_T^2 |\mathrm{rot}\mathbf{u}_T|^2 \right]$$

2.3. The Debye frequency. The number of normal modes  $(\mathbf{k}, \lambda)$  with frequency less than  $\omega$  is

(19) 
$$\mathcal{N}(\omega) = \sum_{\mathbf{k},\lambda} \theta(\omega - v_{\lambda}k) = V \frac{\omega^3}{6\pi^2} \left(\frac{1}{v_L^3} + \frac{2}{v_T^3}\right)$$

If the number of ions in the box of volume V is N, there are 3N independent normal modes of vibration. The relation  $\mathcal{N}(\omega_D) = 3N$  defines the Debye frequency. The Debye frequency is a cut-off  $\omega_{\lambda}(k) \leq \omega_D$  on allowed frequencies, i.e. **k**-vectors<sup>7</sup>.

A rough approximation gives  $\omega_D \approx v_L n^{1/3}$  (the inverse of the Debye frequency is the about the time for sound to travel a lattice spacing).

The Debye temperature is  $k_B T_D = \hbar \omega_D$ . Some values (from Kittel): 428 K (Al), 343 K (Cu), 170 K (Au), 645 K (Si).

<sup>&</sup>lt;sup>6</sup>Note the analogy between  $E_T$  and the e.m. energy density, with field **A**.

 $<sup>^7\</sup>mathrm{For}$  the normal modes of a crystal lattice, the natural cutoff is the restriction of  $\mathbf{k}\text{-vectors}$  to the reciprocal lattice cell.

## 3. Phonons

In Fourier space, the total energy is the sum of single-mode energies, and is quadratic in the amplitudes:  $E = \sum_{\mathbf{k},\lambda} \rho_0 \omega_\lambda^2(k) [d^*_{\mathbf{k},\lambda} d_{\mathbf{k},\lambda} + d_{\mathbf{k},\lambda} d^*_{\mathbf{k},\lambda}].$ With the rescaling  $c_{\mathbf{k},\lambda} = (2\rho_0 \omega_\lambda(k)/\hbar)^{1/2} d_{\mathbf{k},\lambda}$ , it becomes:

$$E = \sum_{\mathbf{k},\lambda} \hbar \omega_{\lambda}(k) \frac{1}{2} [c_{\mathbf{k},\lambda}^* c_{\mathbf{k},\lambda} + c_{\mathbf{k},\lambda} c_{\mathbf{k},\lambda}^*]$$

Quantization is performed by imposing canonical commutation relations

(20) 
$$[\hat{c}_{\mathbf{k},\lambda},\hat{c}_{\mathbf{k}',\lambda'}^{\dagger}] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda\lambda'} \quad [\hat{c}_{\mathbf{k},\lambda},\hat{c}_{\mathbf{k}',\lambda'}] = 0 \quad [\hat{c}_{\mathbf{k},\lambda}^{\dagger},\hat{c}_{\mathbf{k}',\lambda'}^{\dagger}] = 0$$

The total energy becomes the Hamiltonian operator for longitudinal and transverse phonon oscillators:

(21) 
$$\hat{H}_{ph} = \sum_{\mathbf{k},\lambda} \hbar \omega_{\lambda}(k) \left[ \hat{c}^{\dagger}_{\mathbf{k},\lambda} \hat{c}_{\mathbf{k},\lambda} + \frac{1}{2} \right] \theta(\omega_{D} - \omega_{\lambda}(k))$$

whose physical meaning is clear. The vacuum state is characterized by  $\hat{c}_{\mathbf{k},\lambda}|0\rangle = 0$ .

The operators  $\hat{c}_{\mathbf{k},\lambda}^{\dagger}$  and  $\hat{c}_{\mathbf{k},\lambda}$  respectively create and destroy a *phonon* of polarization  $\lambda$ , momentum  $\hbar \mathbf{k}$  and energy  $\hbar \omega_{\lambda}(k)$ .

The Heisenberg evolution of the canonical operators is

(22) 
$$\hat{c}_{\mathbf{k},\lambda}(t) = e^{-i\omega_{\lambda}(k)t}\hat{c}_{\mathbf{k},\lambda}, \quad \hat{c}^{\dagger}_{\mathbf{k},\lambda}(t) = e^{i\omega_{\lambda}(k)t}\hat{c}^{\dagger}_{\mathbf{k},\lambda}$$

The displacement operator is

$$\hat{\mathbf{u}}(\mathbf{x}) = \sqrt{\frac{\hbar}{2\rho_0 V}} \sum_{\mathbf{k},\lambda} \frac{1}{i\sqrt{v_\lambda k}} \mathbf{e}_\lambda(\mathbf{k}) \left[ \hat{c}_{\mathbf{k},\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} - \hat{c}_{\mathbf{k},\lambda}^{\dagger} e^{-i\mathbf{k}\cdot\mathbf{x}} \right] \theta(\omega_D - kv_\lambda)$$

In particular, if  $n_I$  is the number of ions per unit volume, the ionic density fluctuation operator  $\delta \hat{n}_I(\mathbf{x}) = -n_I \operatorname{div} \hat{\mathbf{u}}(\mathbf{x})$  is

(23) 
$$\delta \hat{n}_{I}(\mathbf{x}) = -\frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sqrt{\frac{\hbar n_{I} k}{2v_{L} M}} \left[ \hat{c}_{\mathbf{k},L} + \hat{c}_{-\mathbf{k},L}^{\dagger} \right] e^{i\mathbf{k}\cdot\mathbf{x}} \theta(\omega_{D} - kv_{L})$$

where M is the ionic mass,  $\rho_0 = n_I M$ .

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**Exercise 3.1.** Define the correlator  $id(x, x') = \langle 0 | \mathsf{T} \delta n_I(x) \delta n_I(x') | 0 \rangle$ . Show that, in Fourier space:

(24) 
$$d(k,\omega) = \frac{\hbar n_I}{M} \frac{k^2}{\omega^2 - (v_L k - i\eta)^2} \theta(\omega_D - v_L k)$$

**Exercise 3.2.** (Debye theory) Evaluate the partition function of the phonon gas  $Z = \text{tr} \exp(-\beta H_{ph})$  and the thermodynamic potential. Then study the specific heat, with the limits  $T \ll T_D$  and  $T \gg T_D$  (Dulong-Petit law).

#### 4. Electron-Phonon Interaction

In the theory of the homogeneous electron gas (HEG) the charged background is now described as an elastic medium, with charge density  $Ze(n_I + \delta n_I(\mathbf{x}))$ , where  $Zen_I$  is the uniform charge density that makes the system neutral  $(Zn_Ie - N_ee = 0)$ and  $\delta n_I(\mathbf{x}) = -n_I \operatorname{div} \mathbf{u}(\mathbf{x})$ . Neutrality requires  $\int d\mathbf{x} \delta n_I(\mathbf{x}) = 0$ . The Hamiltonian of the electron gas with phonons is:  $H = H_{el}^0 + H_{ph}^0 + H_{int}$ , where  $H_{el}^0$  is the kinetic Hamiltonian of the electrons,  $H_{ph}^0$  is (21), and the interaction is the sum of the Coulomb term and the electron-phonon term

$$H_{int} = \iint d\mathbf{x} d\mathbf{y} \frac{e^2}{2} \sum_{\mu\nu} \frac{\psi_{\mu}^{\dagger}(\mathbf{x})\psi_{\nu}^{\dagger}(\mathbf{y})\psi_{\nu}(\mathbf{y})\psi_{\mu}(\mathbf{x})}{|\mathbf{x} - \mathbf{y}|} - Ze^2 \sum_{\mu} \frac{\psi_{\mu}^{\dagger}(\mathbf{x})\psi_{\mu}(\mathbf{x})\delta n_{I}(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}$$

In the interaction picture, the expression of the scattering operator is<sup>8</sup>:

(25) 
$$S = \mathsf{T} \exp \frac{1}{i\hbar} \iint dx \, dy \left[ \frac{e^2}{2} n(x)n(y) - Ze^2 n(x)\delta n_I(y) \right] \frac{\delta(t_x - t_y)}{|\mathbf{x} - \mathbf{y}|}$$

where Ze is the charge of an ion and the operators evolve according to  $H_{el}^0$  and  $H_{ph}^0$ . Since the operators of electrons and phonons in the integral commute<sup>9</sup>, the scattering operator factors:  $S = S_{ee}S_{ep}$ .

Consider the electron propagator (or any correlator of electronic field operators) in interaction picture with ground state  $|F, 0\rangle$  (Fermi sphere and state with zero phonons).

$$iG(x,y) = \frac{\langle F, 0 | \mathsf{T}S_{ee}S_{ep}\psi(x)\psi^{\dagger}(y)|F, 0 \rangle}{\langle F, 0 | \mathsf{T}S_{ee}S_{ep}|F, 0 \rangle}$$

In the numerator, expand in power series the phonon scattering operator

$$S_{ep} = \mathsf{T} \exp \frac{-Ze^2}{i\hbar} \int dx \, dy \; n(x) U_c^0(x, y) \delta n_I(y)$$

where  $U_c^0(x, x') = \delta(t - t')/|\mathbf{x} - \mathbf{x}'|$ , and use the fact that T-ordering and Wick's theorem apply to fermion and phonon operators independently. Then, the matrix element factors:

$$iG(x,y) = \sum_{k=0}^{\infty} \frac{(-Ze^2)^k}{k!(i\hbar)^k} \int \prod_{j=1}^k dx_j dy_j \ U_c^0(x_1,y_1) \dots U_c^0(x_k,y_k)$$
$$\times \langle F | \mathsf{T}S_{ee}n(x_1) \dots n(x_k) \psi(x) \psi^{\dagger}(y) | F \rangle \ \langle 0 | \mathsf{T}\delta n_I(y_1) \dots \delta n_I(y_k) | 0 \rangle$$

By Wick's theorem, the phonon average is the sum of total contractions, where a contraction is a factor  $id(y, y') = \langle 0 | T \delta n_I(y) \delta n_I(y') | 0 \rangle$ . Terms with odd k vanish. Since phonon variables are integrated, each total contraction yields the same result. There are  $(2k-1)(2k-3)\cdots 1 = \frac{(2k)!}{2^k k!}$  identical terms:

$$\begin{split} &= \sum_{k=0}^{\infty} \frac{(Ze^2)^{2k}}{(2k)!(i\hbar)^{2k}} \frac{(2k)!}{2^k k!} \, i^k \int \prod_{j=1}^{2k} dx_j \, dy_j \, U_c^0(x_1, y_1) d(y_1, y_2) U_c^0(x_2, y_2) \cdots \\ & \times \cdots d(y_{2k-1}, y_{2k}) U_c^0(x_{2k}, y_{2k}) \, \langle F | \mathsf{T} S_{ee} n(x_1) \dots n(x_{2k}) \psi(x) \psi^{\dagger}(y) | F \rangle \\ &= \sum_{k=0}^{\infty} \frac{1}{(i\hbar)^k k!} \frac{1}{2^k} \, \int \prod_{j=1}^{2k} dx_j \, V_{ph}^0(x_1, x_2) \cdots V_{ph}^0(x_{2k-1}, x_{2k}) \\ & \times \langle F | \mathsf{T} S_{ee} n(x_1) \dots n(x_{2k}) \psi(x) \psi^{\dagger}(y) | F \rangle \end{split}$$

<sup>&</sup>lt;sup>8</sup>note that within T-ordering the Coulomb interaction can be written with density operators. <sup>9</sup>Show that  $[\psi^{\dagger}(\mathbf{1})\psi^{\dagger}(\mathbf{2})\psi(\mathbf{2})\psi(\mathbf{1}),\psi^{\dagger}(\mathbf{3})\psi(\mathbf{3})] = 0$ 

where  $V_{ph}^{0}(x, x') = \frac{1}{\hbar} (Ze^{2})^{2} \int dy dy' U_{c}^{0}(x, y) d(y, y') U_{c}^{0}(x', y')$ . Then

$$= \langle F | \mathsf{T}S_{ee} \exp \frac{1}{i\hbar} \left[ \frac{1}{2} \iint dx' dy' n(x') V_{ph}^0(x', y') n(y') \right] \psi(x) \psi^{\dagger}(y) | F \rangle$$
$$= \langle F | \mathsf{T}S_{eff} \psi(x) \psi^{\dagger}(y) | F \rangle$$

 $S_{eff}$  is built only with electronic operators and a two-body e-e interaction that is the sum of the Coulomb interaction and a Coulomb-phonon-Coulomb interaction:

(26) 
$$S_{eff} = \mathsf{T} \exp \frac{1}{2i\hbar} \sum_{mm'} \int dx \, dx' \psi_m^{\dagger}(x) \psi_{m'}^{\dagger}(x') U_{tot}^0(x, x') \psi_{m'}(x') \psi_m(x)$$

(27) 
$$U_{tot}^{0}(x,x') = e^{2}U_{c}^{0}(x,x') + \frac{Z^{2}e^{4}}{\hbar} \int dy dy' U_{c}^{0}(x,y) d(y,y') U_{c}^{0}(x',y')$$

As a consequence, one obtains the same diagrams of the model with Coulomb interaction, with  $e^2 U_c^0$  being replaced by  $U_{tot}^0$ . With this replacement, the diagrams with vacuum factors exactly cancel the denominator in the reduction formula:

$$G(1,2) = \langle F | \mathsf{T}S_{eff}\psi(1)\psi^{\dagger}(2) | F \rangle_{\star}$$

In momentum space the total e-e bare interaction is:

(28) 
$$U_{tot}^{0}(k,\omega) = \frac{4\pi e^2}{k^2} + \left(\frac{4\pi Z e^2}{k^2 v}\right)^2 \frac{n_I}{M} \frac{(vk)^2}{\omega^2 - (vk - i\eta)^2} \theta(\omega_D - vk)$$

where v is the velocity of sound (hereafter we neglect to specify L =longitudinal).

A resummation of diagrams replaces the Coulomb factors  $U_c^0$  in the phonon integrals (27) with factors  $U_c$  dressed by polarization insertions. In Fourier space and in the Thomas Fermi approximation, we replace  $4\pi/k^2$  with  $4\pi/(k^2 + k_{TF}^2)$ . Next, because of the Debye cutoff, we further simplify to  $4\pi/k_{TF}^2$ . In this approximation, the interaction mediated by phonons has a new coupling constant at each vertex, that accounts for the Thomas-Fermi momentum:

(29) 
$$U_{ep}^{0}(k,\omega) = \gamma^{2} \frac{(vk)^{2}}{\omega^{2} - (vk - i\eta)^{2}} \theta(\omega_{D} - vk) \qquad \gamma = \frac{4\pi Z e^{2}}{k_{TF}^{2} v} \sqrt{\frac{n_{I}}{M}}$$

In direct space, the replacement of the Coulomb interaction  $4\pi e^2/k^2$  with the number  $4\pi e^2/k_{TF}^2$  simplifies the term in the Hamiltonian that couples electrons to phonons:

(30) 
$$H_{ep} = \gamma \int d\mathbf{x} \, \hat{n}(\mathbf{x}) \hat{\varphi}(\mathbf{x})$$

(31) 
$$\hat{\varphi}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sqrt{\frac{vk}{2}} (\hat{c}_{\mathbf{k}} + \hat{c}_{-\mathbf{k}}^{\dagger}) e^{i\mathbf{k}\cdot\mathbf{x}} \theta(\omega_D - kv)$$

A list of important properties of the e-e potential mediated by phonons:

1) For  $\mathbf{k} = 0$  the potential is zero. Therefore, in a translation invariant model, there are no tadpoles.

2) For  $|\omega| < vk$  the potential is negative (attractive): this is significant for the Cooper pairing in superconductivity.

3) In the static limit ( $\omega = 0$ ) the potential is constant in **k**-space, i.e. a quartic interaction in **x**-space (this will be the interaction in the B.C.S. model).

4) Because of the Debye cut-off, an electron with momentum  $|\mathbf{k}| < k_F$  may be

excited above the Fermi energy by absorption of a phonon of momentum  $\mathbf{q}$  (i.e.  $|\mathbf{k} + \mathbf{q}| > k_F$ ) only if the electron is in the energy shell

$$E_F - \hbar\omega_D \le \frac{\hbar^2 k^2}{2m} \le E_F$$

# 5. Dressed e - e interaction

The total bare interaction  $U_{tot}^0 = U_c^0 + U_{ep}^0$  becomes dressed by the polarization insertions. In a translation-invariant system it can be given an interesting expression:

$$U_{tot}(\mathbf{q},\omega) \approx \frac{4\pi e^2}{q^2 \epsilon(\mathbf{q},\omega)} + \frac{\gamma^2}{\epsilon^2(\mathbf{q},0)} \frac{\omega_q^2}{\omega^2 - \Omega_{\mathbf{q}}^2}$$

where the Coulomb term is screened by the dielectric function  $\epsilon(\mathbf{q}, \omega) = 1 - (4\pi e^2/q^2)\Pi^*(\mathbf{q}, \omega)$ , and the phonon term is modified in the coupling and in the pole:

$$\Omega_{\mathbf{q}}^2 = \omega_q^2 [1 + \frac{\gamma^2}{\epsilon(\mathbf{q}, 0)} \Pi^{\star}(\mathbf{q}, 0)]$$

The phonon bare dispersion  $\omega_q = vq$ , is now  $\omega_q = \Omega(q)$ . *Proof*: Write  $U = (v_c/\epsilon) + U_{ep}$ , where  $v_c$  is the bare Coulomb potential. Then:

$$U_{ep} = \frac{U_{tot}^0}{1 - U_{tot}^0 \Pi^\star} - \frac{U_c^0}{\epsilon} = \frac{U_{tot}^0}{\epsilon - U_{ep}^0 \Pi^\star} - \frac{v_c}{\epsilon} = \frac{U_{ep}^0}{\epsilon(\epsilon - U_{ep}^0 \Pi^\star)}$$

because  $\epsilon - v_c \Pi^* = 1$ . Now insert  $U_{ep}^0$  to obtain the result for the dressed interaction mediated by phonons.  $\Box$ 

In the RPA the static expression for  $\Pi^{(0)}$  has singular derivative in  $q = 2k_F$ , which reflects in the singular derivative  $\partial\Omega/\partial q$  at  $q = 2k_F$ . This is Kohn's anomaly<sup>10</sup>.

The Kohn anomaly is known as an abrupt change in the slope of the phonon dispersion curves and is considered to be induced by the logarithmic singularity of the dielectric function, which is a reflection of the special shape of the Fermi surfaces. Until now, the Kohn anomaly has been reported for various metallic elements, such as lead, palladium, aluminum, chromium and niobium<sup>11</sup>.

 $<sup>^{10}\</sup>mathrm{W.}$  Kohn, Image of the Fermi surface in the vibration spectrum of a metal, Phys. Rev. Lett.  $\mathbf{2}$  (1959) 393

<sup>&</sup>lt;sup>11</sup>Platinum is also an element in which the Kohn anomaly was observed in the early age of inelastic neutron scattering (from Y. Tsunoda, T. Kodama, and M. Nishia, *Question on the Kohn Anomaly and Screening Effects in Pt and Pt Alloys*, J. Phys. Soc. Japan **80** (2011) 054603).