ELASTIC MEDIA & PHONONS

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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 rotated or translated, these least symmetries are present: $E_0(\mathbf{R}_1 + \mathbf{a}, \dots \mathbf{R}_n + \mathbf{a}) = E_0(\mathbf{R}_1, \dots \mathbf{R}_n)$, $E_0(Q\mathbf{R}_1, \dots, Q\mathbf{R}_n) = E_0(\mathbf{R}_1, \dots, \mathbf{R}_n)$, where Q 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 an Hamiltonian for the ions

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

$H_{ia,jb}$ 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 $\boldsymbol{\eta}_i' = \boldsymbol{\eta}_i \sqrt{M_i/\mu}$ brings masses to the same value:

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

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:

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

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Quantization yields phonon oscillators, $H_{ion} = E_{min} + \sum_{a=1}^{3N-6} \hbar\omega_a [c_a^\dagger c_a + \frac{1}{2}]$. For extended lattices, they are labelled by the vectors $\mathbf{k}$ of the dual lattice. In the small k limit, the dispersion relations $\omega(\mathbf{k})$ linearize and coincide with those of an elastic medium. This is a 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 subject 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 being 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:

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

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):

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

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

$$d\mathbf{x}' = |\det[\partial x'^i/\partial x^j]| d\mathbf{x} = \sqrt{g(\mathbf{x})} d\mathbf{x}$$

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

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

After a deformation, the initially uniform mass-density ρ_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.

$$\boxed{\delta\rho(\mathbf{x}) = -\rho_0 \,\mathrm{div}\mathbf{u}(\mathbf{x})} \tag{6}$$

2.1. **The stress tensor.** A deformation produces a state of stress, with internal forces that oppose the external forces that produced 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[1] *stress tensor* field $\pi_{ij}(\mathbf{x})$, introduced by Augustine-Louis Cauchy in 1822. He proved that the force acting on a surface element da at $\mathbf{x}$, with normal vector $\mathbf{n}$, is[2].

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

In a perfect fluid the stress tensor is isotropic $\pi_{ij} = -p u_{ij}$, 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 ρ_0 is the mass density at equilibrium, the linearized equation of motion for the displacement field is

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

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

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

where $\lambda > 0$ and $\mu \geq 0$ are the Lamé constants[4].
While initially the pressure is zero, a deformation builds a nonzero pressure $\delta p(\mathbf{x}) = -\frac{1}{3}\pi^j{}_j = -\frac{1}{3}(3\lambda + 2\mu) \operatorname{div}\mathbf{u}(\mathbf{x}) = -\frac{1}{3}(3\lambda + 2\mu)\delta V/V$. This formula links the Lamé constants to the (adiabatic) bulk modulus:

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

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[1] symmetry is related to angular momentum conservation.

[2] a nice book is: B. Lautrup, Physics of continuous matter, 2nd ed. CRC Press (2011)

[3] 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:

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

for any Q and $\mathbf{x}$. 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. $C^r{}_{rmn} = A u_{mn}$. In the same way $C_{ijm}{}^m = B u_{ij}$. Consistency requires $A = B$. It is also $C_{rs}{}^r{}_n = Q_s{}^j C_{rj}{}^r{}_l Q^l{}_n$ meaning that $C_{rs}{}^r{}_n = C u_{sn}$. Putting pieces together, the isotropic tensor is $C_{ijkl} = \lambda u_{ij} u_{kl} + 2\mu \, u_{ik} u_{jl}$.

[4] For Aluminum: $\rho_0 = 2.7 \times 10^3 \mathrm{kg/m^3}$, $\lambda = 55$ GPa, $\mu = 26$ GPa (1 GPa $= 10^9 \mathrm{N/m^2}$), sound velocity $v_s = 6.3$ km/s

Other relations link λ, μ to the Poisson and Young parameters[5].

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

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

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 π^{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:

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

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

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

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

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

$$\left[\frac{1}{v_L^2}\frac{\partial}{\partial_t^2} - \nabla^2\right] \operatorname{div} \mathbf{u}(\mathbf{x}, t) = 0 \quad , \quad \left[\frac{1}{v_T^2}\frac{\partial}{\partial_t^2} - \nabla^2\right] \operatorname{rot} \mathbf{u}(\mathbf{x}, t) = 0 \tag{12}$$

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 ($\operatorname{rot} \mathbf{u}$ is orthogonal to $\mathbf{u}$) with velocity v_T.

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

Note the inequality $v_L > \sqrt{2}\, v_T$: longitudinal waves are always faster than transversal waves[6] (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 a transversal 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 $\mathbf{k}$.

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[5] This is a nice book: B. Lautrup, *Physics of continuous matter*, 2nd ed, CRC Press, Taylor & Francis, 2011.

[6] in seismology they are named P (*prima*) and S (*secunda*)

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 $\operatorname{rot} \mathbf{F}_L(\mathbf{x}) = 0$ and $\operatorname{div} \mathbf{F}_T(\mathbf{x}) = 0$.

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 equations:

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

For each $\mathbf{k}$, 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 transversal and longitudinal plane waves. A convenient expression is

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

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

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

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 $\operatorname{rot}\, \mathbf{u}_L(\mathbf{x}, t) = 0$ and $\operatorname{div}\, \mathbf{u}_T(\mathbf{x}, t)$ at all times. Show that the following expressions are constants of the motion[7]:

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

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

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

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

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 $\omega_\lambda(k) \le \omega_D$ on allowed frequencies, i.e. $\mathbf{k}$-vectors[8].

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).

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[7] Note the analogy between E_T and the e.m. energy density, with field $\mathbf{A}$.

[8] For the normal modes of a crystal lattice, the natural cutoff is the restriction of $\mathbf{k}$-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:

$$E = \sum\nolimits_{\mathbf{k},\lambda} \hbar\omega_\lambda(k) \tfrac{1}{2} [c^*_{\mathbf{k},\lambda} c_{\mathbf{k},\lambda} + c_{\mathbf{k},\lambda} c^*_{\mathbf{k},\lambda}]$$

Quantization is performed by imposing canonical commutation relations

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

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

$$\boxed{\hat{H}_{ph} = \sum\nolimits_{\mathbf{k},\lambda} \hbar\omega_\lambda(k) \left[\hat{c}^\dagger_{\mathbf{k},\lambda} \hat{c}_{\mathbf{k},\lambda} + \tfrac{1}{2} \right] \theta(\omega_D - \omega_\lambda(k))} \tag{21}$$

whose physical meaning is clear.
The vacuum state is characterized by $\hat{c}_{\mathbf{k},\lambda}|0\rangle = 0$. The operators $\hat{c}^\dagger_{\mathbf{k},\lambda}$ and $\hat{c}_{\mathbf{k},\lambda}$ respectively create and destroy a *phonon* of polarization λ, momentum $\hbar\mathbf{k}$ and energy $\hbar\omega_\lambda(k)$.
The Heisenberg evolution of the canonical operators is

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

The displacement operator is

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

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

$$\delta\hat{n}_I(\mathbf{x}) = -\frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \sqrt{\frac{\hbar n_I k}{2 v_L M}} \left[\hat{c}_{\mathbf{k},L} + \hat{c}^\dagger_{-\mathbf{k},L} \right] e^{i\mathbf{k}\cdot\mathbf{x}} \theta(\omega_D - k v_L) \tag{23}$$

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

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:

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

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

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4. Electron-Phonon interaction

In the theory of the electron gas 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 $\delta n_I(\mathbf{x}) = -n_I \mathrm{div}\mathbf{u}(\mathbf{x})$. Neutrality requires $\int d\mathbf{x}\delta n_I(\mathbf{x}) = 0$.
The Hamiltonian of the electron gas with phonons is: $H = H^0_{el} + H^0_{ph} + H_{int}$,

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

In the interaction picture, the expression of the scattering operator is[9]:

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

where Ze is the charge of an ion and the operators evolve according to H^0_{el} and H^0_{ph}. Since the operators in the integral commute[10], 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

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

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

$$\begin{aligned} iG(x,y) = \sum_{k=0}^{\infty}\frac{(-Ze^2)^k}{k!(i\hbar)^k}\int\prod_{j=1}^{k}dx_jdy_j\; U^0_c(x_1,y_1)\ldots U^0_c(x_k,y_k) \\ \times\langle F|\mathsf{T}S_{ee}n(x_1)\ldots n(x_k)\psi(x)\psi^\dagger(y)|F\rangle\;\langle 0|\mathsf{T}\delta n_I(y_1)\ldots\delta n_I(y_k)|0\rangle \end{aligned}$$

By Wick's theorem, the phonon average is the sum of total contractions, where a contraction is a factor $id(y,y') = \langle 0|\mathsf{T}\delta n_I(y)\delta n_I(y')|0\rangle$. Terms with odd k vanish. Since phonon variables are integrated, each total contraction yields the same result.

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

There are $(2k-1)(2k-3)\cdots 1 = \frac{(2k)!}{2^k k!}$ identical terms:

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

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

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

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:

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

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

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: $iG(1,2) = \langle F|\mathsf{T} S_{eff} \psi(1)\psi^\dagger(2)|F\rangle_\star$.
In momentum space the total e-e bare interaction is:

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

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:

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

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:

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

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

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 $\mathbf{k}$-space, i.e. a quartic interaction in $\mathbf{x}$-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

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

5. Dressed e-e interaction

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

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

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

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

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:

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

because $\epsilon - v_c\Pi^{\star} = 1$. Now insert U^0_{ep} to obtain the result for the dressed interaction mediated by phonons. □

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[11].

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

[11] W. Kohn, *Image of the Fermi surface in the vibration spectrum of a metal*, Phys. Rev. Lett. **2** (1959) 393

elements, such as lead, palladium, aluminum, chromium and niobium. 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).