Phonons and more

M.A.L. Marques

Ruhr University Bochum, Germany

The Hamiltonian of everything

First, we have the kinetic energy:

$$\mathcal{T} = -\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2 - \frac{1}{2}\sum_{\mu=1}^{N}\frac{\nabla_\mu^2}{M_\mu} \tag{1}$$

And the electron-ion interaction

$$\mathcal{V}_{\mathrm{e-n}} = -\sum_{j=1}^{n}\sum_{\nu=1}^{N}\frac{Z_\nu}{|r_j - R_\nu|} \tag{2}$$

Finally, the electron-electron and ion-ion interactions

$$\mathcal{V}_{\mathrm{e-e}} = \sum_{j=1}^{n}\sum_{k=j+1}^{n}\frac{1}{|r_j - r_k|} \qquad \mathcal{V}_{\mathrm{n-n}} = \sum_{\nu=1}^{N}\sum_{\mu=\nu+1}^{N}\frac{Z_\nu Z_\mu}{|R_\mu - R_\nu|} \tag{3}$$

The Born-Oppenheimer approximation

We define the electronic Hamiltonian to be

$$\mathcal{H}_{\rm nf}(\bar{\boldsymbol{r}};\bar{\boldsymbol{R}}) = \mathcal{T}_{\rm e}(\bar{\boldsymbol{r}}) + \mathcal{V}_{\rm e-e}(\bar{\boldsymbol{r}}) + \mathcal{V}_{e-n}(\bar{\boldsymbol{r}};\bar{\boldsymbol{R}}) \tag{4}$$

with the eigenspectrum

$$\mathcal{H}_{\rm nf}(\bar{\boldsymbol{r}};\bar{\boldsymbol{R}})\Phi_m(\bar{\boldsymbol{r}},\bar{\sigma};\bar{\boldsymbol{R}}) = \mathcal{E}_m(\bar{\boldsymbol{R}})\Phi_m(\bar{\boldsymbol{r}},\bar{\sigma};\bar{\boldsymbol{R}}) \tag{5}$$

This equation will be “density-functionalized” in the following. We now expand the many-body wave-function in the complete basis set formed by the Φ_m

$$\Psi_i(\bar{\boldsymbol{r}},\bar{\sigma};\bar{\boldsymbol{R}}) = \sum_m \Theta_{im}(\boldsymbol{R})\Phi_m(\bar{\boldsymbol{r}},\bar{\sigma};\boldsymbol{R}) \tag{6}$$

If we restrict this sum just to the first term $m = 0$, we obtain for the ionic equation

$$\left[\mathcal{T}_N(\bar{\boldsymbol{R}}) + U(\bar{\boldsymbol{R}})\right]\Theta_i(\bar{\boldsymbol{R}}) = E_i\Theta_i(\bar{\boldsymbol{R}}) \tag{7}$$

The Harmonic expansion

We now assume that the ions are close to their equilibrium position $\bar{\boldsymbol{R}}_0$, and that they describe small oscillations around those positions. We can then expand the potential felt by the ions in a Taylor series:

$$U(\bar{\boldsymbol{R}}) = U(\bar{\boldsymbol{R}}_0) + \frac{1}{2} \sum_{l\mu, l'\nu} \left. \frac{\partial^2 U(\bar{\boldsymbol{R}})}{\partial \boldsymbol{u}(l\mu) \partial \boldsymbol{u}(l'\nu)} \right|_0 \boldsymbol{u}(l\mu)\boldsymbol{u}(l'\nu) + \cdots \tag{8}$$

where the displacements are defined as $\boldsymbol{R}(l\mu) = \boldsymbol{R}_0(l\mu) + \boldsymbol{u}(l\nu)$. We can also expand the electron-ion potential appearing in the electronic equation

$$\mathcal{V}_{e-n}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{R}}) = \mathcal{V}_{e-n}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{R}}_0) + \sum_{l\mu} \left. \frac{\partial \mathcal{V}_{e-n}(\bar{\boldsymbol{r}}; \bar{\boldsymbol{R}})}{\partial \boldsymbol{u}(l\mu)} \right|_0 \boldsymbol{u}(l\mu) + \cdots \tag{9}$$

The second term in the right-hand side is nothing more than the electron-phonon interaction.

Semiclassical approach

We can rewrite the second order term in the standard way:

$$V = \frac{1}{2} \sum_{l\mu, l'\nu} \sum_{\alpha,\beta} \Phi_{\alpha,\beta}(l\mu, l'\nu) u_\alpha(l\mu) u_\beta(l'\nu) \tag{10}$$

The function Φ is called the **force constants matrix**, and is the 3D equivalent of the spring force constant in the harmonic oscillator. The equation of motion then reads:

$$M_\mu \ddot{u}_\alpha(l\mu) = - \sum_{l'\nu,\beta} \Phi_{\alpha,\beta}(l\mu, l'\nu) u_\alpha(l'\nu) \tag{11}$$

The function ϕ has a couple of very useful symmetries:

- **Lattice translational invariance**, which allows us to reduce the problem to $3s$ variables.
- **Infinitesimal translational invariance**, which means that there is no force when all atoms are displaced: $\sum_{l'\nu} \Phi_{\alpha,\beta}(l\mu, l'\nu) = 0$.

Normal modes

Using Bloch's theorem, we can write the *ansatz*

$$u_\alpha(l\mu) = \frac{1}{\sqrt{M_\mu}} \sum_{\boldsymbol{q}} \tilde{u}_\alpha(\boldsymbol{q};\mu) e^{\mathrm{i}(\boldsymbol{q}.\boldsymbol{r}(l)-\omega t)} \tag{12}$$

Inserting it in the equation of motion we arrive at

$$\omega^2_{j\boldsymbol{q}} \tilde{u}^j_\alpha(\boldsymbol{q}\mu) = \sum_{\nu\beta} D_{\alpha\beta}(\boldsymbol{q};\mu\nu) \tilde{u}^j_\beta(\boldsymbol{q}\nu) \tag{13}$$

where D, the dynamical matrix is essentially the Fourier transform of Φ

$$D_{\alpha\beta}(\boldsymbol{q};\mu\nu) = \frac{1}{\sqrt{M_\mu M_\nu}} \sum_{l'} \Phi_{\alpha\beta}(0\mu; l'\nu) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{r}(l')} \tag{14}$$

The relation between $\boldsymbol{q}$ and ω is called the **dispersion relation**. For a system with s atoms in the unit cell, there will be **3 acoustic branches** (where $w = 0$ for $\boldsymbol{q} = 0$) and **3s-3 optical branches**. From now we will call the (normalized) eigenvectors of the equation $\boldsymbol{e}_j(\boldsymbol{q};\mu)$. This are also called the polarization vectors of the phonons.

Quantum mechanical approach

The ionic Schrödinger equation can be written as

$$\sum_{l\mu} \frac{\boldsymbol{p}(l\mu)\cdot\boldsymbol{p}(l\mu)}{2M_\mu} + \frac{1}{2}\sum_{l\mu,l'\nu}\sum_{\alpha\beta}\Phi_{\alpha,\beta}(l\mu,l'\nu)u_\alpha(l\mu)u_\beta(l'\nu) \tag{15}$$

we now perform a canonical transformation to the so-called normal coordinates

$$\boldsymbol{u}(l\mu) = \frac{1}{\sqrt{N\Omega}}\sum_{\boldsymbol{q}}\boldsymbol{Q}(\boldsymbol{q}\mu)e^{\mathrm{i}\boldsymbol{q}\boldsymbol{r}(l)} \tag{16}$$

$$\boldsymbol{p}(l\mu) = \frac{1}{\sqrt{N\Omega}}\sum_{\boldsymbol{q}}\boldsymbol{P}(\boldsymbol{q}\mu)e^{\mathrm{i}\boldsymbol{q}\boldsymbol{r}(l)} \tag{17}$$

We make a further transformation, and include the polarization vector

$$Q_j(\boldsymbol{q}) = \sum_\mu \sqrt{M_\mu}\boldsymbol{e}_j^*(\boldsymbol{q};\mu)\cdot\boldsymbol{Q}(\boldsymbol{q}\mu) \tag{18}$$

$$P_j(\boldsymbol{q}) = \sum_\mu \frac{1}{\sqrt{M_\mu}}\boldsymbol{e}_j(\boldsymbol{q};\mu)\cdot\boldsymbol{P}(\boldsymbol{q}\mu) \tag{19}$$

Second quantization

Finally, we can define creation and annihilation operators

$$\hat{a}_{\boldsymbol{q},j} = \frac{1}{\sqrt{2\omega_{\boldsymbol{q};j}}} P_j(\boldsymbol{q}) - \mathrm{i}\sqrt{\frac{\omega_{\boldsymbol{q},j}}{2}} Q_j^\dagger(\boldsymbol{q}) \tag{20}$$

$$\hat{a}_{\boldsymbol{q},j}^\dagger = \frac{1}{\sqrt{2\omega_{\boldsymbol{q};j}}} P_j^\dagger(\boldsymbol{q}) + \mathrm{i}\sqrt{\frac{\omega_{\boldsymbol{q},j}}{2}} Q_j(\boldsymbol{q}) \tag{21}$$

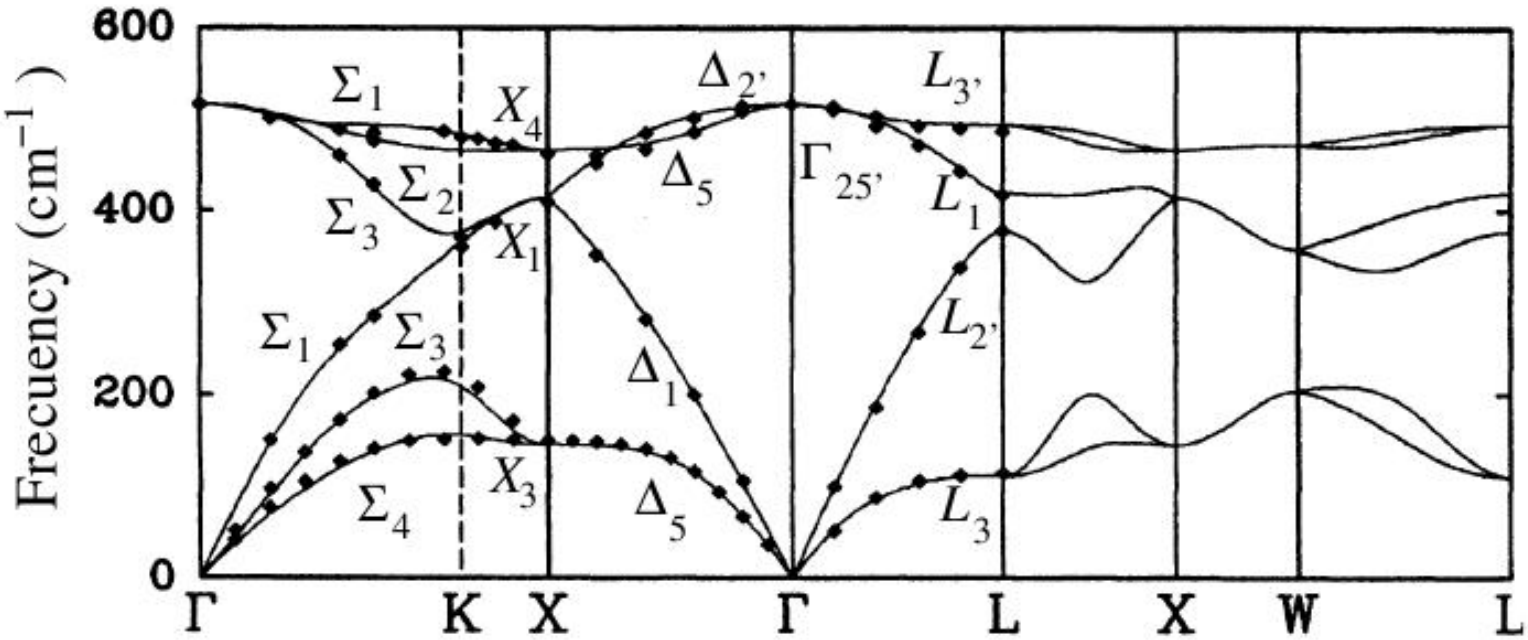
With these definitions, the Hamiltonian becomes diagonal

$$\mathcal{H}_{\text{ions}} = \sum_{\boldsymbol{q},j} \omega_{\boldsymbol{q},j} \left(a_{\boldsymbol{q},j}^\dagger a_{\boldsymbol{q},j} + \frac{1}{2} \right) \tag{22}$$

Finally, the atomic displacement vectors can be written in terms of the operators

$$\boldsymbol{u}(l\mu) = -\frac{\mathrm{i}}{\sqrt{N\Omega}} \sum_{\boldsymbol{q},j} \frac{1}{\sqrt{2M_\mu \omega_{\boldsymbol{q},j}}} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}(l)} \boldsymbol{e}_j(\boldsymbol{q};\mu) \left[\hat{a}_{\boldsymbol{q},j}^\dagger - \hat{a}_{-\boldsymbol{q},j} \right] \tag{23}$$

Phonon dispersions - an example



ab-initio phonon dispersion of Silicon (Giannozzi et al, PRB **43**, 7231 (1991)). The points represent experimental values (Nilson & Nelin, PRB **6**, 3777 (1972)).

Some definitions for the electron-phonon term

Moving also the electrons to second-quantization, we can write the electron-phonon term as

$$\sum_{\boldsymbol{q},j}\sum_{\sigma}\int \mathrm{d}^3 r\, \hat{\psi}^{\dagger}_{\sigma}(\boldsymbol{r})\psi_{\sigma}(\boldsymbol{r})\, V_{\boldsymbol{q},j}\left[a^{\dagger}_{\boldsymbol{q},j} - a_{-\boldsymbol{q},j}\right] \tag{24}$$

where the electron-phonon coupling constant is

$$V_{\boldsymbol{q},j}(\boldsymbol{r}) = \sum_{l\mu} \frac{1}{\sqrt{2M_{\mu}\omega_{\boldsymbol{q},j}}} e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}(l)} \boldsymbol{e}_j(\boldsymbol{q};\mu)\, \left.\frac{\partial \mathcal{V}_{e-n}(\bar{\boldsymbol{r}};\bar{\boldsymbol{R}})}{\partial \boldsymbol{u}(l\mu)}\right|_0 \tag{25}$$

what in the end will enter the equations are the matrix elements of this quantity between Kohn-Sham states

$$g^{\boldsymbol{q},j}_{\boldsymbol{k}+\boldsymbol{q},i';\boldsymbol{k}i} = < \boldsymbol{k}+\boldsymbol{q}, i' | V_{\boldsymbol{q},j}(\boldsymbol{r}) | \boldsymbol{k} i > \tag{26}$$

As we will see, often this quantity is averaged over the Fermi surface to yield the so-called life-times

$$\gamma_{\boldsymbol{q},j} = 2\pi\omega_{\boldsymbol{q},j} \sum_{\boldsymbol{k}ii'} |g^{\boldsymbol{q},j}_{\boldsymbol{k}+\boldsymbol{q},i';\boldsymbol{k}i}|^2 \delta(\epsilon_{\boldsymbol{k}i} - \epsilon_F)\delta(\epsilon_{\boldsymbol{k}+\boldsymbol{q}i'} - \epsilon_F) \tag{27}$$

and finally, the Eliashberg function

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(\epsilon_F)} \sum_{\boldsymbol{q},j} \frac{\gamma_{\boldsymbol{q},j}}{\omega_{\boldsymbol{q},j}} \delta(\omega - \omega_{\boldsymbol{q},j}) \tag{28}$$

Response functions

As we see, all these quantities are simply given by derivatives of either the total energy or the Kohn-Sham potential with respect to the displacement of the ions. They fall into the cathegory of the so-called linear response properties of the system, where one measures the response of the system to an external infinitesimal perturbation.
These perturbations can be

- Electric (e.g., polarizabilities, absorption, florescence ...)

$$V(\boldsymbol{r}) = \boldsymbol{r}_i$$

- Magnetic (e.g., susceptibilities, NMR ...)

$$V(\boldsymbol{r}) = \boldsymbol{L}_i$$

- Atomic Displacements (e.g., phonons ...)

$$V(\boldsymbol{r}) = \frac{\partial}{\partial \boldsymbol{R}_i}$$

These quantities can be calculated either from finite differences (e.g., frozen phonons), from molecular dynamics spectral analysis methods, or by perturbative approaches. This latter is by far the most efficient method, and is what is implemented in most software packages (ABINIT, PWSCF, etc.)

Perturbation theory - I

We want to study a system where we apply a small external perturbing potential. This can be expanded in a Taylor series

$$v(\lambda) = v^{(0)} + \lambda v^{(1)} + \lambda^2 v^{(2)} + \cdots \tag{29}$$

Likewise the Hamiltonian has the expansion

$$H(\lambda) = H^{(0)} + \lambda H^{(1)} + \lambda^2 H^{(2)} + \cdots \tag{30}$$

The (Kohn-Sham) equation for the perturbed system reads

$$H(\lambda)|\psi_i(\lambda)\rangle = \epsilon_i(\lambda)|\psi_i(\lambda)\rangle \tag{31}$$

we now Taylor expand both the eigenvalues and eigenfunctions

$$|\psi_i(\lambda)\rangle = |\psi_i^{(0)}\rangle + \lambda|\psi_i^{(1)}\rangle + \lambda^2|\psi_i^{(2)}\rangle + \cdots \tag{32}$$

$$\epsilon_i(\lambda) = \epsilon_i^{(0)} + \lambda\epsilon_i^{(1)} + \lambda^2\epsilon_i^{(2)} + \cdots \tag{33}$$

Inserting all these definitions in the Kohn-Sham equation, we obtain

$$\left[H^{(0)} - \epsilon_i^{(0)}\right]|\psi_i^{(0)}\rangle + \lambda\left\{\left[H^{(0)} - \epsilon_i^{(0)}\right]|\psi_i^{(1)}\rangle + \left[H^{(1)} - \epsilon_i^{(1)}\right]|\psi_i^{(0)}\rangle\right\} + \lambda^2\cdots = 0 \tag{34}$$

Perturbation theory - II

Separating the different powers of λ we obtain in 0th order

$$H^{(0)}|\psi_i^{(0)}\rangle = \epsilon_i^{(0)}|\psi_i^{(0)}\rangle \tag{35}$$

which is just the standard Kohn-Sham equation. In 1st order

$$\left[H^{(0)} - \epsilon_i^{(0)}\right]|\psi_i^{(1)}\rangle = -\left[H^{(1)} - \epsilon_i^{(1)}\right]|\psi_i^{(0)}\rangle \tag{36}$$

Now, expanding also the orthonormality condition $\langle\psi_i(\lambda)|\psi_i(\lambda)\rangle = 1$, we obtain

$$\langle\psi_i^{(0)}|\psi_i^{(0)}\rangle + \lambda\left(\langle\psi_i^{(1)}|\psi_i^{(0)}\rangle + \langle\psi_i^{(0)}|\psi_i^{(1)}\rangle\right) + \lambda^2\cdots = 1 \tag{37}$$

From which we get

$$\langle\psi_i^{(0)}|\psi_i^{(0)}\rangle = 1 \tag{38}$$

$$\langle\psi_i^{(1)}|\psi_i^{(0)}\rangle + \langle\psi_i^{(0)}|\psi_i^{(1)}\rangle = 0 \tag{39}$$

Perturbation theory - III

Multiplying by $\langle\psi_i^{(0)}|$ we obtain

$$\langle\psi_i^{(0)}|H^{(0)} - \epsilon_i^{(0)}|\psi_i^{(1)}\rangle = \langle\psi_i^{(0)}|H^{(1)} - \epsilon_i^{(1)}|\psi_i^{(0)}\rangle \tag{40}$$

$$\epsilon_i^{(0)}\langle\psi_i^{(0)}|\psi_i^{(1)}\rangle = \langle\psi_i^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle - \epsilon_i^{(1)} \tag{41}$$

from which we can get an expression for $\epsilon_i^{(1)}$

$$\epsilon_i^{(1)} = \langle\psi_i^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle \tag{42}$$

Using this in the equation for $|\psi_i^{(1)}\rangle$

$$\left[H^{(0)} - \epsilon_i^{(0)}\right]|\psi_i^{(1)}\rangle = -\left[H^{(1)} - \epsilon_i^{(1)}\right]|\psi_i^{(0)}\rangle \tag{43}$$

$$= -H^{(1)}|\psi_i^{(0)}\rangle + |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|H^{(1)}|\psi_i^{(0)}\rangle \tag{44}$$

$$= -\left(1 - |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|\right)H^{(1)}|\psi_i^{(0)}\rangle \tag{45}$$

This is the so-called Sternheimer equation. As an exercise, you can expand $|\psi_i^{(1)}\rangle$ in the complete basis set $|\psi_i^{(0)}\rangle$ and recover the sum-over-states formula of perturbation theory.

What is $H^{(1)}$

Do not forget that we are doing Kohn-Sham, so the variation of the Hamiltonian is

$$H^{(1)} = \frac{\partial H(\lambda)}{\partial \lambda} \tag{46}$$

$$= v^{(1)} + v^{(1)}_{\mathrm{Hxc}} \tag{47}$$

as the Hartree and exchange-correlation potential is a functional of the density, we can use the chain rule to calculate $v^{(1)}_{\mathrm{Hxc}}$

$$v^{(1)}_{\mathrm{Hxc}}(\boldsymbol{r}) = \int \mathrm{d}^3 r' \left.\frac{\delta v^{\lambda}_{\mathrm{Hxc}}(\boldsymbol{r})}{\delta n^{\lambda}(\boldsymbol{r}')}\right|_{\lambda=0} \frac{\partial n^{\lambda}(\boldsymbol{r}')}{\partial \lambda} \tag{48}$$

The first derivative is usually written as

$$\frac{\delta v^{\lambda}_{\mathrm{Hxc}}(\boldsymbol{r})}{\delta n^{\lambda}(\boldsymbol{r}')} = \frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|} + f_{\mathrm{xc}}(\boldsymbol{r},\boldsymbol{r}') \tag{49}$$

And the derivative of the density is simply

$$\frac{\partial n^{\lambda}(\boldsymbol{r})}{\partial \lambda} = n^{(1)}(\boldsymbol{r}) = \sum_i \psi^{(1)*}_i(\boldsymbol{r})\psi^{(0)}_i(\boldsymbol{r}) + \psi^{(0)*}_i(\boldsymbol{r})\psi^{(1)}_i(\boldsymbol{r}) \tag{50}$$

Eliashberg Theory - I

We write the Hamiltonian in the basis of electronic eigen-states. We will also ignore the band index.

$$\hat{H} = \sum_{\boldsymbol{k}} \xi_k : \hat{\Psi}^\dagger_{\boldsymbol{k}} \tau_3 \hat{\Psi}_{\boldsymbol{k}} : + \sum_{\boldsymbol{k}\boldsymbol{k}'} \sum_{\boldsymbol{q}\lambda} g^{\boldsymbol{k}\boldsymbol{k}'}_{\lambda\boldsymbol{q}} : \hat{\Psi}^\dagger_{\boldsymbol{k}} \tau_3 \hat{\Psi}_{\boldsymbol{k}'} : \hat{\Phi}_{\lambda\boldsymbol{q}} \quad , \tag{51}$$

Where we defined the field-operators in Nambu-Gorkov space

$$\hat{\Psi}(\boldsymbol{r}, \tau) = \begin{pmatrix} \hat{\psi}_\uparrow(\boldsymbol{r}, \tau) \\ \hat{\psi}^\dagger_\downarrow(\boldsymbol{r}, \tau) \end{pmatrix} , \tag{52}$$

and the (matrix) Green's function reads

$$\bar{G}(12) = -\langle \hat{T} \hat{\Psi}(1) \otimes \hat{\Psi}^\dagger(2) \rangle \tag{53}$$

Now we perform perturbation theory. The unperturbed Green's function is

$$\bar{G}_0^{-1}(k, \omega_n) = \mathrm{i}\omega_n \tau_0 - \xi_k \tau_3 \, , \tag{54}$$

where $\xi_k = \varepsilon_k - \mu$, and τ_i are the Pauli matrices. Dyson's equation is, as usual

$$\bar{G}^{-1}(\boldsymbol{k}, \omega_n) = \bar{G}_0^{-1}(\boldsymbol{k}, \omega_n) - \bar{\Sigma}(\boldsymbol{k}, \omega_n) \, . \tag{55}$$

Eliashberg Theory - II

We expand the self-energy using the Pauli matrices

$$\bar{\Sigma}(\boldsymbol{k},\omega_n) = [1 - Z(\boldsymbol{k},\omega_n)]\,\mathrm{i}\omega_n\tau_0 + \phi_1(\boldsymbol{k},\omega_n)\tau_1 + \phi_2(\boldsymbol{k},\omega_n)\tau_2 + \chi(\boldsymbol{k},\omega_n)\tau_3\,, \tag{56}$$

and solve Dyson's equation to get $\bar{G}(Z,\phi,\chi)$.
Migdal's theorem tells use that vertex corrections are unimportant, so we approximate the self-energy by

$$\bar{\Sigma}(\boldsymbol{k},\omega_n) =$$

$$= -\frac{1}{\beta}\sum_{\boldsymbol{k}'\omega_n'}\sum_{\lambda\boldsymbol{q}}\left|g^{\boldsymbol{k}\boldsymbol{k}'}_{\lambda\boldsymbol{q}}\right|^2 \tau_3\bar{G}(\boldsymbol{k}',\omega_n')\tau_3 D_{\lambda\boldsymbol{q}}(\omega_n-\omega_n') \tag{57}$$

Putting everything together, we arrive at 4 coupled integral equations. E.g., the equation for Z reads ($\Xi = [Z\omega]^2 + [\xi+\chi]^2 + \phi_1^2 + \phi_2^2$)

$$[1 - Z(\boldsymbol{k},\omega_n)]\,\omega_n = \frac{1}{\beta}\sum_{\boldsymbol{k}'\omega_n'}\sum_{\lambda\boldsymbol{q}}\frac{Z(\boldsymbol{k}',\omega_n')\omega_n'}{\Xi(\boldsymbol{k}',\omega_n')}\left|g^{\boldsymbol{k}\boldsymbol{k}'}_{\lambda\boldsymbol{q}}\right|^2\frac{-2\Omega_{\lambda\boldsymbol{q}}}{(\omega_n-\omega_n')^2+\Omega^2_{\lambda\boldsymbol{q}}} \tag{58}$$

Eliashberg Theory - III

These equations are too complicated to solve. Let's do some approximations

- Neglect χ, as it only gives a correction to μ.
- k dependence of Z and $\phi_{1,2}$ is small compared to ξ_k, so replace them by their value at the Fermi surface.
- Average the electron-phonon coupling constants over the Fermi surface.

A bit of algebra, and we arrive at the Eliashberg equations in frequency space

$$\Delta(\omega_n)Z(\omega_n) = \frac{\pi}{\beta}\sum_{\omega'_n}\lambda(\omega_n-\omega'_n)\frac{\Delta(\omega'_n)}{\sqrt{\omega'^2_n+|\Delta(\omega_n)|^2}} \tag{59}$$

$$[1-Z(\omega_n)]\,\omega_n = -\frac{\pi}{\beta}\sum_{\omega'_n}\lambda(\omega_n-\omega'_n)\frac{\omega'_n}{\sqrt{\omega'^2_n+|\Delta(\omega_n)|^2}} \quad , \tag{60}$$

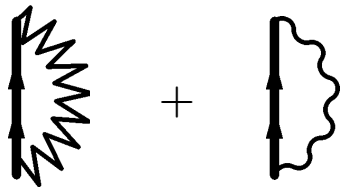
with

$$\lambda(\nu_n) = \int d\Omega\,\alpha^2F(\Omega)\frac{2\Omega}{\nu_n^2+\Omega^2} \quad \text{and} \quad \Delta(\omega_n) = \frac{\phi_1(\omega_n)+\mathrm{i}\phi_2(\omega_n)}{Z(\omega_n)} \tag{61}$$

What about the Coulomb repulsion?

We can include the Coulomb repulsion in the self-energy

$$\bar{\Sigma}(\boldsymbol{k}, \omega_n) = \quad + \qquad (62)$$



But

- What do we write for the interaction, v, W_{static}, W_{dynamic}?
- But in this case, all the approximations fail, and we are stuck with 4 integral equations in 4 dimensions.
- Solution: phenomenological interaction, with strength μ and a certain range.

In this way we arrive at McMillan's formula

$$T_c = \frac{\langle \Omega \rangle}{1.20} e^{-1.04 \frac{1+\lambda}{\lambda - \mu^*}} \qquad (63)$$

Thanks!

- Jorge Serrano, PhD Thesis
- Savrasov & Savrasov, Phys. Rev. B **54**, 16487 (1996)
- Gonze and Baroni stuff for DFPT
- Scalapino and Allen & Mitrovic reviews