Lecture 19: Microscopic Interactions

OUTLINE

1. **Motivation**
2. **Feedback & Electron Screening**
3. **Feedback & Phonon Screening**
4. **The electron-phonon interaction**

November 15, 2005

Motivation: Dielectric Constant

$$\Phi_{\text{tot}} = \frac{q}{4\pi\epsilon}\frac{1}{r}$$

Potential for point charge in a dielectric media

$$\Phi_{\text{tot}} = \frac{q}{4\pi\epsilon_o}\frac{1}{r}$$

Potential for point charge in free space

$$\Phi_{\text{tot}} = \frac{1}{\tilde{\epsilon}}\Phi_{\text{ext}}$$

Output = Transfer function * Input

Dielectric Constant $\epsilon(\mathbf{k})$

<u>Total Charge and Total Potential</u>

$$\nabla^2 \Phi_{\text{tot}}(\mathbf{r},t) = -\frac{\rho_{\text{tot}}(\mathbf{r},t)}{\epsilon_o}$$

<u>External Charge and External Potential</u>

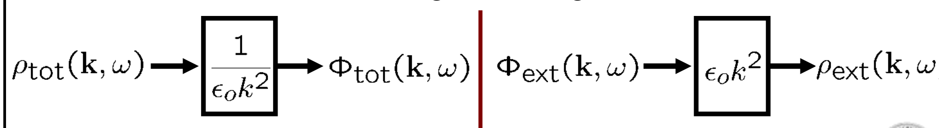
$$\nabla^2 \Phi_{\text{ext}}(\mathbf{r},t) = -\frac{\rho_{\text{ext}}(\mathbf{r},t)}{\epsilon_o}$$

Use Fourier Transform $f(\mathbf{r},t) = \int_{-\infty}^{+\infty} \frac{d\mathbf{k}}{(2\pi)^3} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} f(\mathbf{k},\omega) e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}$

$$\Phi_{\text{tot}}(\mathbf{k},\omega) = \frac{1}{\epsilon_o k^2} \rho_{\text{tot}}(\mathbf{k},\omega)$$

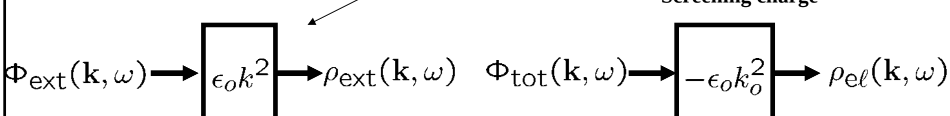
$$\rho_{\text{ext}}(\mathbf{k},\omega) = \epsilon_o k^2 \, \Phi_{\text{ext}}(\mathbf{k},\omega)$$

Block Diagrams of the Algebra

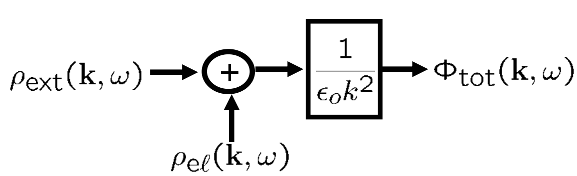


Screening Charge

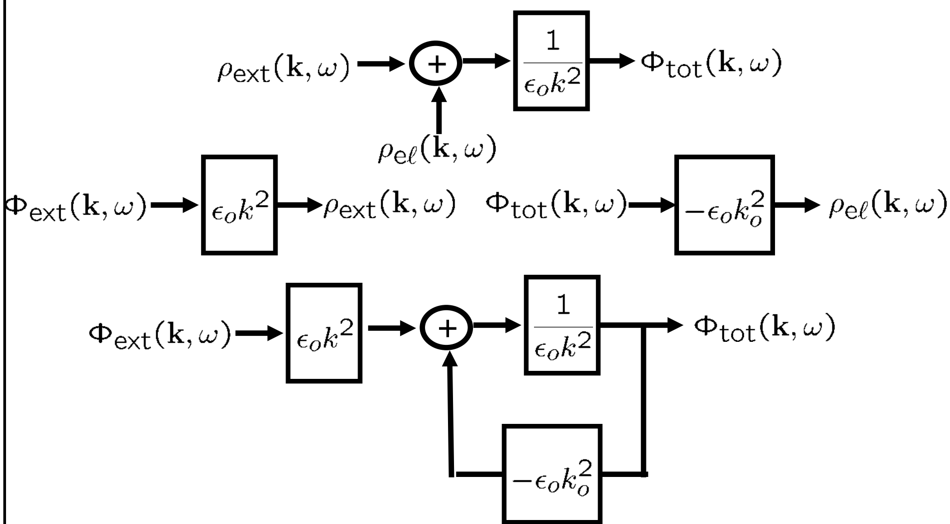
$$\rho_{\text{tot}}(\mathbf{r},t) = \rho_{\text{ext}}(\mathbf{r},t) + \underbrace{\rho_{\text{el}}(\mathbf{r},t)}_{\text{Screening charge}}$$



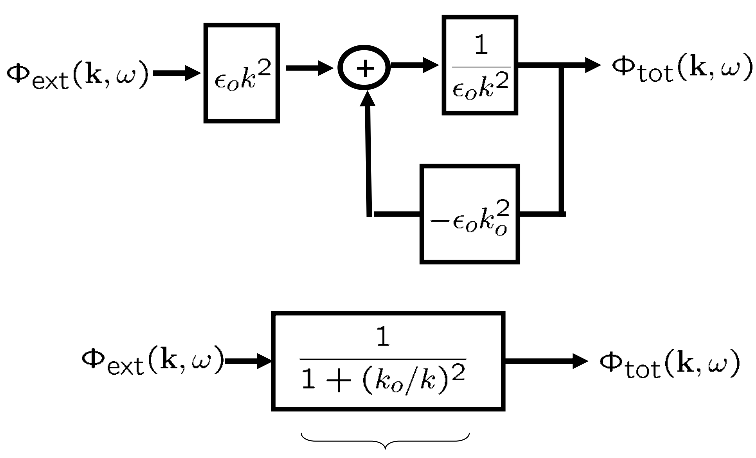
The screening effect is produced by the positive background charge and hence is of opposite sign.



Screening Charge

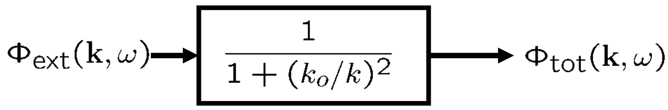


Screening Charge



Effective Dielectric function

Thomas-Fermi Screening



$$\Phi_{tot}(\mathbf{k},\omega) = \frac{1}{1+(k_o/k)^2}\,\Phi_{ext}(\mathbf{k},\omega)$$

For a point 'test' charge

$$\Phi_{tot}(\mathbf{k},\omega) = \frac{1}{1+(k_o/k)^2}\,\frac{q}{\epsilon_o k^2} = \frac{q}{\epsilon_o}\,\frac{1}{k^2+k_o^2}$$

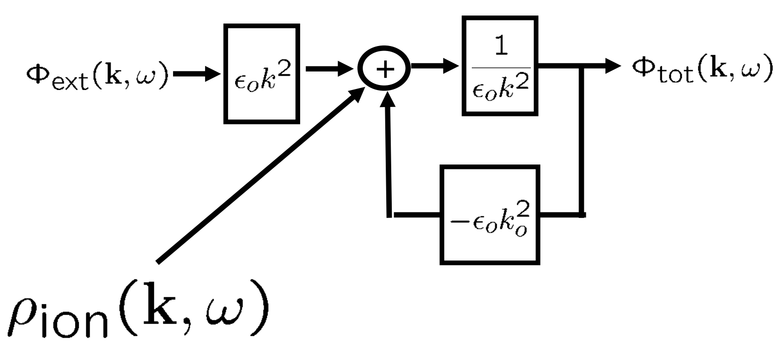
The inverse Fourier Transform gives

$$\Phi_{tot}(\mathbf{r},t) = \frac{q}{4\pi\epsilon_o}\,\frac{e^{-k_o r}}{r}$$

Thomas-Fermi Screening is like Debye-Hueckel screening k_0 is the thomas-fermi screeing length and is about one Angstrom

Dynamical Screening from the positive ions

$$\rho_{tot}(\mathbf{k},\omega) = \rho_{ext}(\mathbf{k},\omega) + \rho_{el}(\mathbf{k},\omega) + \rho_{ion}(\mathbf{k},\omega)$$



Need a simple model of the dynamics for the ion charge.

Model of Dynamics of Ions

Treat each positively charged ion as a free particle acted on by the <u>total</u> Electric Field

$$M \frac{d}{dt} \mathbf{v}_{\text{ion}}(\mathbf{r},t) = Q_{\text{ion}} \mathbf{E}(\mathbf{r},t)$$

And the resulting current density of the ions is

$$\mathbf{J}_{\text{ion}} = n Q_{\text{ion}} \mathbf{v}_{\text{ion}}(\mathbf{r},t)$$

$$\Rightarrow \quad \frac{d}{dt} \mathbf{J}_{\text{ion}}(\mathbf{r},t) = \frac{n Q_{\text{ion}}^2}{M} \mathbf{E}(\mathbf{r},t)$$

This looks just like our first London Equation for charged particles with no damping.

Model of Dynamics of Ions (cont.)

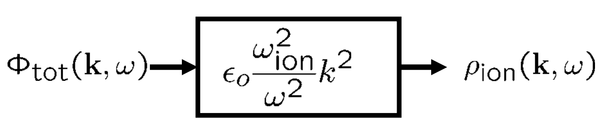
The continuity equation gives

$$\frac{\partial}{\partial t} \rho_{\text{ion}} + \nabla \cdot \mathbf{J}_{\text{ion}} = 0$$

Combine with previous equation to give:

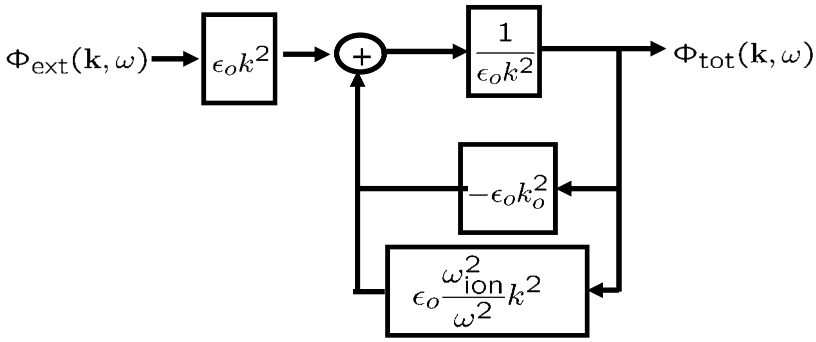
$$\frac{\partial^2}{\partial t^2} \rho_{\text{ion}} = -\frac{n Q_{\text{ion}}^2}{M} \nabla \cdot \mathbf{E} = \frac{n Q_{\text{ion}}^2}{M} \nabla^2 \Phi_{\text{tot}}(\mathbf{r},t)$$

$$\Rightarrow \quad \rho_{\text{ion}}(\mathbf{k},\omega) = \epsilon_o \frac{\omega_{\text{ion}}^2}{\omega^2} k^2 \, \Phi_{\text{tot}}(\mathbf{k},\omega)$$



Dynamical Screening from the positive ions

$$\rho_{\text{tot}}(\mathbf{k},\omega) = \rho_{\text{ext}}(\mathbf{k},\omega) + \rho_{\text{el}}(\mathbf{k},\omega) + \rho_{\text{ion}}(\mathbf{k},\omega)$$



$$\Phi_{\text{ext}}(\mathbf{k},\omega) \rightarrow \boxed{\frac{1}{1+(k_o/k)^2-(\omega_{\text{ion}}/\omega)^2}} \rightarrow \Phi_{\text{tot}}(\mathbf{k},\omega)$$

Effective Dynamical Dielectric function $\epsilon(\mathbf{k},\omega)$

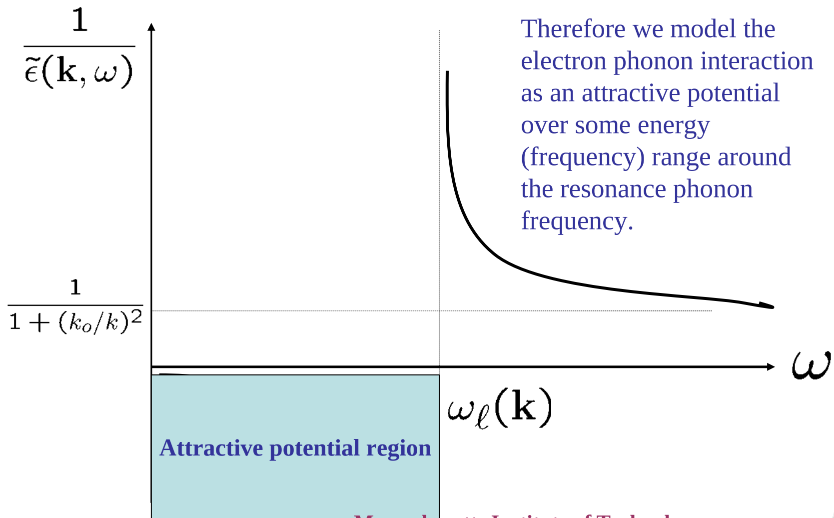
$$\Phi_{\text{ext}}(\mathbf{k},\omega) \rightarrow \boxed{\frac{1}{1+(k_o/k)^2-(\omega_{\text{ion}}/\omega)^2}} \rightarrow \Phi_{\text{tot}}(\mathbf{k},\omega)$$

$$\frac{1}{\tilde{\epsilon}(\mathbf{k},\omega)} = \frac{1}{1+(k_o/k)^2}\left(\frac{\omega^2}{\omega^2-\omega_\ell^2(\mathbf{k})}\right)$$

$$\omega_\ell(\mathbf{k}) \equiv \sqrt{\frac{\omega_{\text{ion}}^2}{1+(k_o/k)^2}} \quad \xrightarrow[k \ll k_o]{} \quad \frac{\omega_{\text{ion}}}{k_o} k$$

Sound waves with the velocity of sound $\quad u = \omega_{\text{ion}}/k_o$

Effective Dynamical Dielectric function $\epsilon(\mathbf{k}, \omega)$



Therefore we model the electron phonon interaction as an attractive potential over some energy (frequency) range around the resonance phonon frequency.