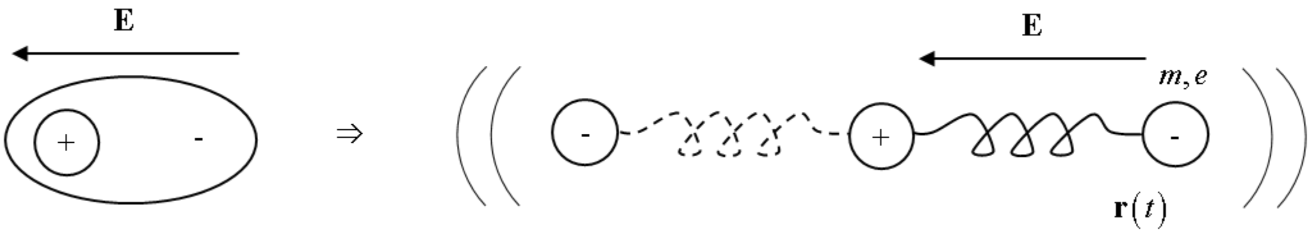
App.2. Classical Oscillator

Classical description of dielectric properties of semiconductors are for the valence electrons bound to the nuclei.

$\Rightarrow$ Classical Polarization



The classical EOM is given by

$$\left[m\frac{d^2}{dt^2} + 2m\gamma\frac{d}{dt} + m\omega_0{}^2 \right]\mathbf{r}(t) = e\mathbf{E}(t)$$

In frequency domain,

$$\left[\begin{array}{l} \mathbf{r}(\omega) = \int_{-\infty}^{\infty} dt\,\mathbf{r}(t)e^{i\omega t} \\ \mathbf{E}(\omega) = \int_{-\infty}^{\infty} dt\,\mathbf{E}(t)e^{i\omega t} \end{array}\right.$$

$$\Rightarrow \quad m\left(\omega^2 + i2\gamma\omega - \omega_0{}^2\right)\mathbf{r}(\omega) = -e\mathbf{E}(\omega)$$

Define the polarization $\mathbf{P}(\omega) = \chi(\omega)\mathbf{E}(\omega)$

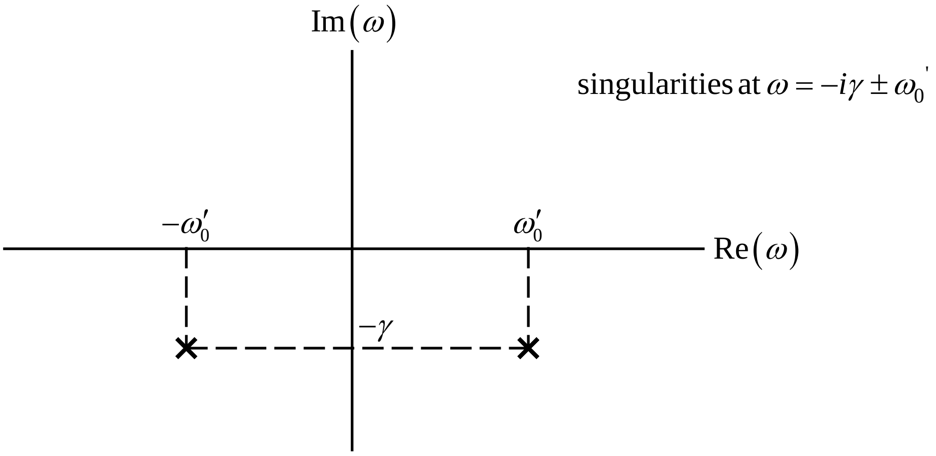
$$\mathbf{P} = \frac{\text{Total Dipole Moment}}{\text{Volume}} = \frac{N\mathbf{d}}{V} = ne\mathbf{r}$$

$$\text{with} \quad \left(\begin{array}{lll} \mathbf{d} = e\mathbf{r} & : & \text{Dipole Moment per atom} \\ N & : & \text{total \# of dipoles} \\ V & : & \text{sample volume} \end{array}\right.$$

$$\Rightarrow \quad \mathbf{P}(\omega) = -\frac{ne^2}{m}\frac{1}{\omega^2 + i2\gamma\omega - \omega_0{}^2}\mathbf{E}(\omega) = \chi(\omega)\mathbf{E}(\omega)$$

$$\Rightarrow \quad \boxed{\chi(\omega) = -\frac{ne^2}{2m\omega_0}\left(\frac{1}{\omega - \omega_0{}' + i\gamma} - \frac{1}{\omega + \omega_0 + i\gamma}\right)} \quad : \quad \text{Electron Susceptiblity}$$

$$\text{with} \quad \boxed{\omega_0{}' = \sqrt{\omega_0{}^2 - \gamma^2}} \quad : \quad \text{Renormalized Resonance Frequency}$$



$\Rightarrow \quad \chi(\omega) \quad : \quad$ Analytic Function at $\operatorname{Im}(\omega) \geq 0 \ \left(\text{as}\ \gamma \to 0^{+}\right)$

According to the Causality Principle, "Cause and (then) Effect"

Dielectric Response $\chi(t)$ can only be influenced by the External Stimulation $\mathbf{E}(t-\tau)$ for $\tau \geq 0$

$$\Rightarrow \quad \boxed{\mathbf{P}(t) = \int_{-\infty}^{t} dt' \chi(t-t') \mathbf{E}(t')} \quad (\text{or from the convolution theorem})$$

Let $t - t' = \tau$, then

$$\boxed{\mathbf{P}(t) = \int_{0}^{\infty} d\tau \chi(\tau) \mathbf{E}(t-\tau)} \quad \text{with} \ \boxed{\chi(\tau) = 0 \ \text{for} \ \tau < 0} \quad (\text{or}\ t < t')$$

$$\Rightarrow \quad \chi(\omega) = \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{i\omega\tau} = \int_{0}^{\infty} \chi(\tau) e^{i\omega\tau}$$

From the Cauchy relation for $\delta \to 0^{+}$

$$\chi(\omega) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\nu \frac{\chi(\nu)}{\nu - \omega - i\delta}$$

Instead of the contour method,

$$\text{use} \quad \boxed{\frac{1}{\omega \pm i\delta} = \underline{P}\left(\frac{1}{\omega}\right) \mp i\pi\delta(\omega)} \quad : \quad \text{Dirac identity}$$

Where $\underline{P}$ denotes the "Cauchy Principle Value"

$$\Rightarrow \quad \chi(\omega) = \frac{1}{2\pi i} \underline{P} \int_{-\infty}^{\infty} d\nu \frac{\chi(\nu)}{\nu - \omega} + \frac{1}{2} \underbrace{\int_{-\infty}^{\infty} d\nu \chi(\nu) \delta(\nu - \omega)}_{\chi(\omega)}$$

$$\Rightarrow \boxed{\begin{aligned} \chi'(\omega) &= \frac{1}{\pi}\underline{P}\int_{-\infty}^{\infty} d\nu \, \frac{\chi''(\nu)}{\nu-\omega} \\ \chi'(\omega) &= -\frac{1}{\pi}\underline{P}\int_{-\infty}^{\infty} d\nu \, \frac{\chi'(\omega)}{\nu-\omega} \end{aligned}} \quad : \quad \text{Kramers-Kronig Relation}$$

Changing from $\int_{-\infty}^{\infty} d\nu$ to $\int_{0}^{\infty} d\nu$,

$$\boxed{\chi'(\omega) = \frac{2}{\pi}\int_{0}^{\infty} d\nu \, \frac{\nu}{\nu^2-\omega^2} \chi''(\nu)}$$

How about $\varepsilon(\omega)$ and $n(\omega)$?