

# Band Gap Renormalization - Plasmon Pole Approximation

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The objective is to evaluate the Band Gap Renormalization (BGR) using the single plasmon pole approximation (SPPA) for the dielectric constant.

BGR can be simply estimated through the change in energy dispersion due to interaction i.e. Self energy. Considering the screened interaction  $W(q, iq_n)$  (in Matsubara formalism), we can simply compute the self energy using the  $G_0W$  approximation.

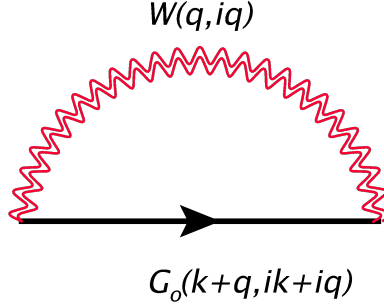


FIG. 1. Self Energy Diagram

$$\Sigma(k, ik_n) = -\frac{1}{\beta} \sum_{q, iq_n} W(q, iq_n) G_0(k+q, ik_n + iq_n) \quad (1)$$

where the non-interacting Green function

$$G_0(k+q, ik_n + iq_n) = \frac{1}{ik_n + iq_n - \varepsilon_{k+q}} \quad (2)$$

and the screened interaction  $W(q, iq_n)$  is

$$W(q, iq_n) = \frac{V(q)}{\varepsilon(q, iq_n)} = V(q) + V(q) \left[ \frac{1}{\varepsilon(q, iq_n)} - 1 \right] \quad (3)$$

The plasmon-pole approximation is used to construct the full dielectric function  $\varepsilon(q, iq_n)$  which replaces the continuum of poles in the Lindhard function by one effective plasmon-pole  $\omega_q$ . Therefore

$$\frac{1}{\varepsilon(q, iq_n)} = 1 + \frac{\omega_p^2}{(iq_n)^2 - \omega_q^2} \quad (4)$$

Therefore

$$\begin{aligned} \Sigma(k, ik_n) &= -\frac{1}{\beta} \sum_{q, iq_n} \left[ V(q) + V(q) \left[ \frac{1}{\varepsilon(q, iq_n)} - 1 \right] \right] G_0(k+q, ik_n + iq_n) \\ &= -\frac{1}{\beta} \sum_{q, iq_n} V(q) G_0(k+q, ik_n + iq_n) - \frac{1}{\beta} \sum_{q, iq_n} V(q) \left[ \frac{1}{\varepsilon(q, iq_n)} - 1 \right] G_0(k+q, ik_n + iq_n) \\ &= \Sigma_x(k, ik_n) + \Sigma_c(k, ik_n) \end{aligned} \quad (5)$$

where the exchange and correlation self energy terms can be evaluated.

$$\Sigma_x(k, ik_n) = -\frac{1}{\beta} \sum_{q, iq_n} V(q) G_0(k+q, ik_n + iq_n) = -\sum_q V(q) f_{k+q} \quad (6)$$

where  $f_{k+q}$  is the Fermi-Dirac distribution function,

$$\begin{aligned}\Sigma_c(k, ik_n) &= -\frac{1}{\beta} \sum_{q, iq_n} V(q) \left[ \frac{1}{\varepsilon(q, iq_n)} - 1 \right] G_0(k+q, ik_n + iq_n) \\ &= -\frac{1}{\beta} \sum_{q, iq_n} V(q) \frac{\omega_p^2}{(iq_n)^2 - \omega_q^2} G_0(k+q, ik_n + iq_n) \\ &= \sum_q V(q) \frac{\omega_p^2}{2\omega_q} \left[ \frac{f_{k+q} + g_q}{ik_n - \varepsilon_{k+q} + \omega_q} + \frac{1 - f_{k+q} + g_q}{ik_n - \varepsilon_{k+q} - \omega_q} \right]\end{aligned}\quad (7)$$

and  $g_q = 1/(\exp(\omega_q/T) - 1)$ . Thus the renormalization of band edge due to carriers can be evaluated by analytic continuation of the self energy and setting momenta to the band extrema location:  $\omega = \varepsilon_k$  and  $k = 0$  here.

$$\Delta E = \Sigma(k, \varepsilon_k)|_{k=0} \quad (8)$$

This is also referred to as the rigid band shift.

### BGR IN 2D ELECTRON-HOLE SYSTEM

In 2D, considering an electron hole plasma with a reduced mass  $m$ :  $m^{-1} = m_e^{-1} + m_h^{-1}$ , the electrons cause shift in the CB minima and the holes cause shift of the VB maxima. Thus the BGR will have contribution from both the species of charge carriers

$$\begin{aligned}\Delta E_G &= \Sigma_e(k, \varepsilon_k)|_{k=0} + \Sigma_h(k, \varepsilon_k)|_{k=0} \\ &= - \sum_{q, i=\{e, h\}} V(q) f_{i, q} + \sum_{q, i=\{e, h\}} V(q) \frac{\omega_p^2}{2\omega_q} \left[ \frac{f_{i, q} + g_q}{\varepsilon_{i, 0} - \varepsilon_{i, q} + \omega_q} + \frac{1 - f_{i, q} + g_q}{\varepsilon_{i, 0} - \varepsilon_{i, q} - \omega_q} \right]\end{aligned}\quad (9)$$

In accordance with Schmitt-Rink et. al [Solid State Communications, Vol.52, No.2, pp.123-125, 1984], we express all lengths and energies in units of exciton Bohr radius and Rydberg.

$$a_0 = \frac{\varepsilon_0}{2me^2} \quad E_0 = \frac{1}{2ma_0^2} = \frac{e^2}{\varepsilon_0 a_0} \quad (10)$$

Therefore

- Interaction potential  $V(q) = \frac{2\pi e^2}{\varepsilon_0 q} = \frac{2\pi a_0^2}{qa_0} E_0$
- Plasma Frequency  $\omega_p^2 = \frac{2\pi n e^2 q}{\varepsilon_0 m} = 4\pi (na_0^2)(qa_0) E_0^2$
- Energy dispersion  $\varepsilon_i = \frac{k^2}{2m_i} = \frac{m}{m_i} (ka_0)^2 E_0$  where  $i = \{e, h\}$  [Spin Degenerate]
- Number Density  $n = 2 \sum_k f_{i, k} \Rightarrow na_0^2 = \frac{\bar{T}}{2\pi} \frac{m_i}{m} \text{Ln}(1 + \exp(\bar{\mu}_i/\bar{T}))$  where  $T = \bar{T} E_0$
- Chemical Potential  $\bar{\mu}_i = \bar{T} \text{Ln} \left[ \exp \left( \frac{2\pi n (na_0^2)}{\bar{T} m_i} \right) - 1 \right]$
- Thomas Fermi Screening wavenumber  $\kappa = \frac{2\pi e^2}{\varepsilon_0} \sum_i \frac{\partial n}{\partial \mu_i}$  where  $\mu_i = \bar{\mu}_i E_0$  is the chemical potential  $\Rightarrow \kappa a_0 = 2\pi \left[ \frac{\partial (na_0^2)}{\partial \bar{\mu}_e} + \frac{\partial (na_0^2)}{\partial \bar{\mu}_h} \right] = \frac{m_e}{m} \frac{1}{1 + e^{-\bar{\mu}_e/\bar{T}}} + \frac{m_h}{m} \frac{1}{1 + e^{-\bar{\mu}_h/\bar{T}}}$ .
- Plasmon Pole with Lundquist correction  $\omega_q^2 = \omega_p^2(1 + q/\kappa) + (\varepsilon_{e, q} + \varepsilon_{h, q})^2/4$

Thus computing the BGR for Coulomb interaction in 2D where the expression  $-3.1(na_0^2)^{1/3} E_0$  is a good approximation to BGR for  $T=0$ .

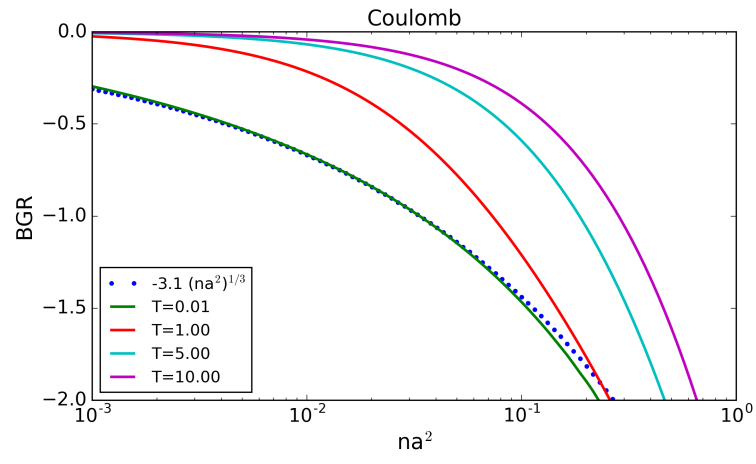


FIG. 2. BGR - Coulomb in 2D - in units of  $E_0$ . Temperatures are in units of  $E_0$ .