

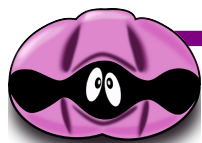
Beyond the Plasmon-Pole approximation: Real-axis GW & Lifetimes

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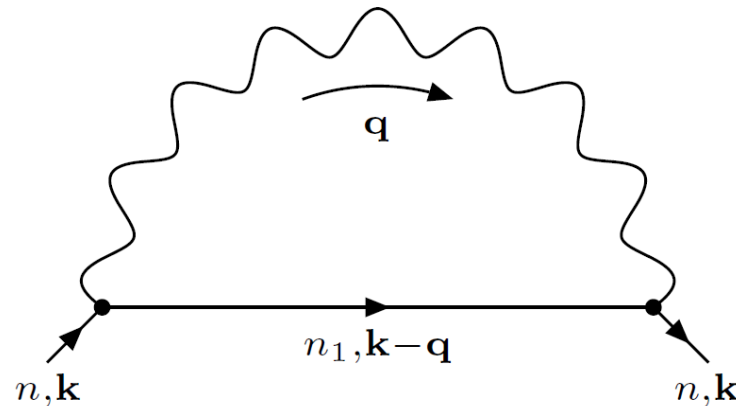
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The GW self-energy (I)

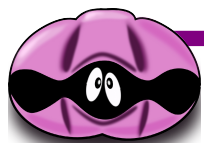


$$\Sigma(\mathbf{r}, \mathbf{r}', t) = \Sigma_x(\mathbf{r}, \mathbf{r}') + M(\mathbf{r}, \mathbf{r}', t)$$

$$\Sigma_x(\mathbf{r}, \mathbf{r}') = i\nu(\mathbf{r}, \mathbf{r}') G_0(\mathbf{r}, \mathbf{r}', t = 0^-)$$

$$M(\mathbf{r}, \mathbf{r}', t) = i\tilde{W}(\mathbf{r}, \mathbf{r}', t) G_0(\mathbf{r}, \mathbf{r}', t) = i \left[\int d\mathbf{r}'' \nu(\mathbf{r}, \mathbf{r}'') \bar{\epsilon}^{-1}(\mathbf{r}', \mathbf{r}'', t) \right] G_0(\mathbf{r}, \mathbf{r}', t)$$

The GW self-energy is defined in terms of a time product

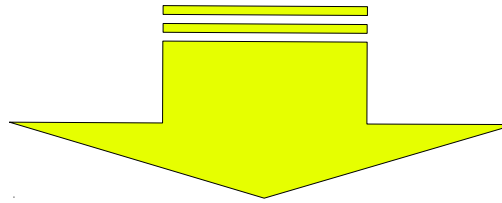


The GW self-energy (II)

$$G_0(\mathbf{r}_1, \mathbf{r}_2; \omega) = 2 \sum_n \sum_{\mathbf{k} \in BZ} \phi_{n\mathbf{k}}(\mathbf{r}_1) \phi_{n\mathbf{k}}^*(\mathbf{r}_2) \left[\frac{f_{n\mathbf{k}}}{\omega - \epsilon_{n\mathbf{k}} - i\delta} + \frac{1 - f_{n\mathbf{k}}}{\omega - \epsilon_{n\mathbf{k}} + i\delta} \right]$$

$$\tilde{\epsilon}_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega) = \frac{4\pi}{|\mathbf{q} + \mathbf{G}| |\mathbf{q} + \mathbf{G}'|} \chi_{\mathbf{G}, \mathbf{G}'}(\mathbf{q}, \omega) = \frac{|\mathbf{q} + \mathbf{G}|}{|\mathbf{q} + \mathbf{G}'|} \bar{\epsilon}_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega)$$

$$\tilde{\rho}_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) = \int d\mathbf{r} u_{n\mathbf{k}}^*(\mathbf{r}) u_{n_1(\mathbf{k}-\mathbf{q})}(\mathbf{r}) e^{i(\mathbf{G} + \mathbf{G}_{kq}) \cdot \mathbf{r}}$$



$$\langle n\mathbf{k} | M(\mathbf{r}_1, \mathbf{r}_2, \omega) | n'\mathbf{k}' \rangle$$

$$= i \sum_{n_1} \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \left\{ \sum_{\mathbf{G}, \mathbf{G}'} \frac{4\pi}{|\mathbf{q} + \mathbf{G}'|^2} \tilde{\rho}_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) [\tilde{\rho}_{n'n_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}')]^* \int \frac{d\omega'}{2\pi} \tilde{\epsilon}_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega') \left[\frac{f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega - \omega' - \epsilon_{n_1(\mathbf{k}-\mathbf{q})} - i\delta} + \frac{1 - f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega - \omega' - \epsilon_{n_1(\mathbf{k}-\mathbf{q})} + i\delta} \right] \right\}$$

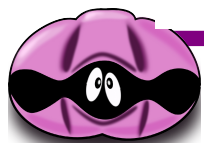
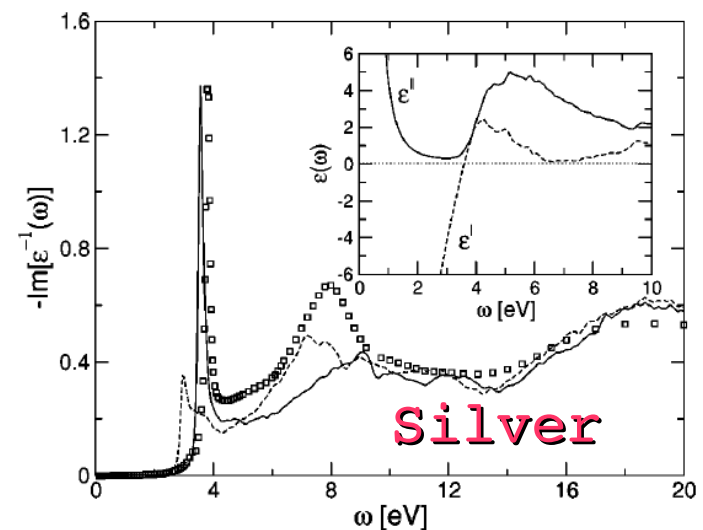
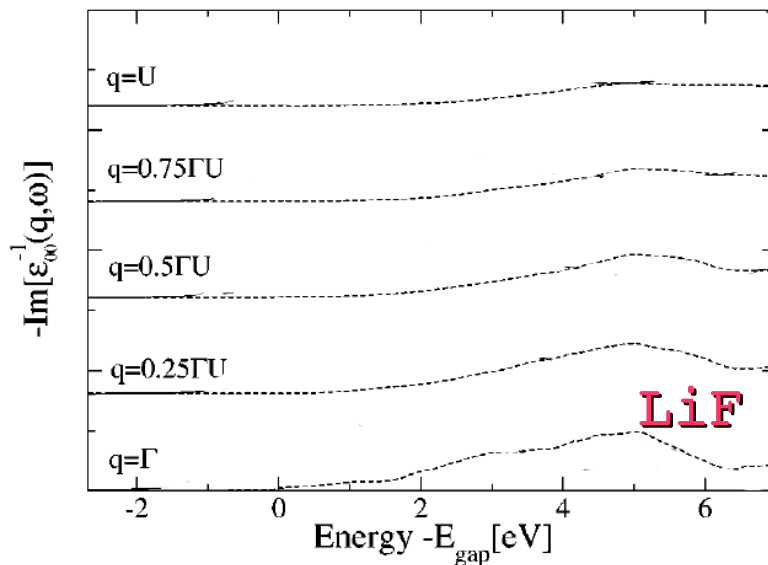


The Plasmon-Pole approximation

$$\tilde{\epsilon}_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q},\omega) = \sum_I \left[\frac{R_I^{(+)}(\mathbf{q},\mathbf{G},\mathbf{G}')}{\omega - E_I^N + i\delta} - \frac{R_I^{(-)}(\mathbf{q},\mathbf{G},\mathbf{G}')}{\omega + E_I^N - i\delta} \right],$$

$$\tilde{\epsilon}_{\mathbf{G},\mathbf{G}'}^{-1}(\mathbf{q},\omega) \approx \left[\frac{R_{\mathbf{G},\mathbf{G}'}(\mathbf{q})}{\omega - \tilde{\omega}_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) + i\delta} - \frac{R_{\mathbf{G},\mathbf{G}'}(\mathbf{q})}{\omega + \tilde{\omega}_{\mathbf{G},\mathbf{G}'}(\mathbf{q}) - i\delta} \right].$$

The PPA is expected to work well when the screening is dominated by few and high-energy poles.



Real-axis GW

The real-axis integral can be calculated once the inverse Dielectric function is calculated on a fine grid

```
% DmRngeXd  
0.10000 | 0.10000 | eV # [Xd] Damping range  
%  
ETStepsXd= 100 # [Xd] Total Energy steps
```

Yambo input file

$\langle nk | M(\mathbf{r}_1, \mathbf{r}_2, \omega) | n'k' \rangle$

$$= i \sum_{n_1} \int_{BZ} \frac{d\mathbf{q}}{(2\pi)^3} \left\{ \sum_{\mathbf{G}, \mathbf{G}'} \frac{4\pi}{|\mathbf{q} + \mathbf{G}'|^2} \tilde{\rho}_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) [\tilde{\rho}_{n'n_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}')]^* \right.$$

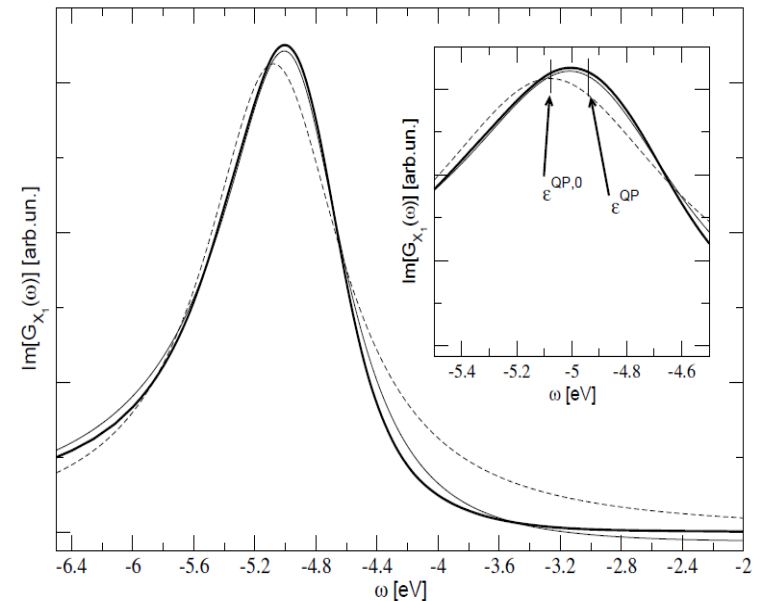
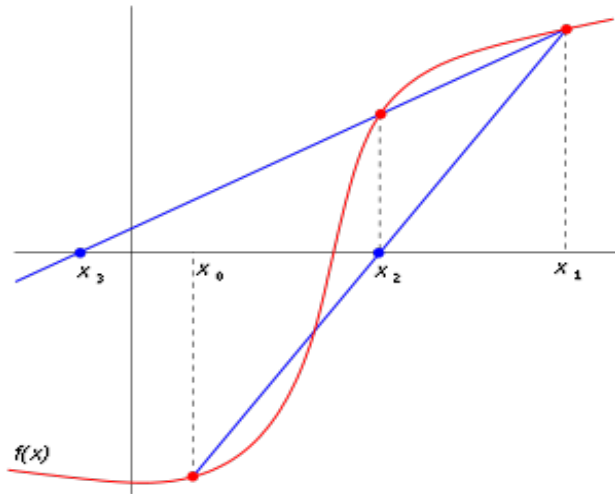
$$\left. \int \frac{d\omega'}{2\pi} \tilde{\epsilon}_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega') \left[\frac{f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega - \omega' - \epsilon_{n_1(\mathbf{k}-\mathbf{q})} - i\delta} + \frac{1 - f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega - \omega' - \epsilon_{n_1(\mathbf{k}-\mathbf{q})} + i\delta} \right] \right\}$$



Secant solver of Dyson equation

$$G_{nk}(\omega) = \frac{1}{\omega - \epsilon_{nk} - [\sum_x^{nk} + M_{nk}(\omega) - V_{xc}^{nk}]}$$

1 $\epsilon_{nk}^{QP,0} = \epsilon_{nk} - [\sum_x^{nk} + \Re [M_{nk}(\epsilon_{nk}^{QP,0})] - V_{xc}^{nk}]$



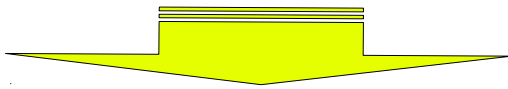
2 $M_{nk}(z) \approx M_{nk}(\epsilon_{nk}^{QP,0}) + M'_{nk}(\epsilon_{nk}^{QP,0})(z - \epsilon_{nk}^{QP,0})$

The Newton solution corresponds approximately to the result of the step 1.



Lifetimes

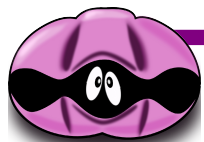
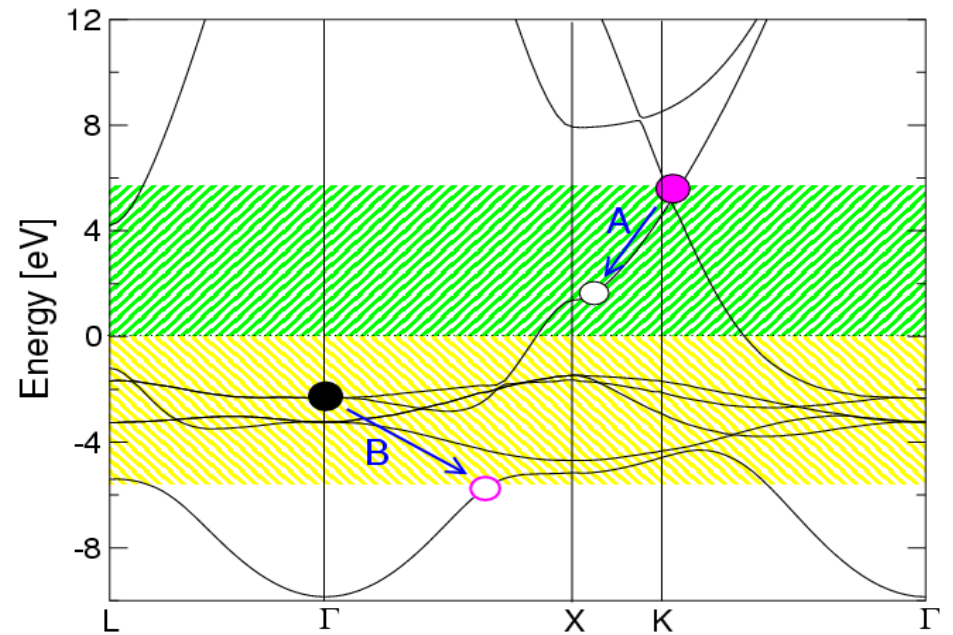
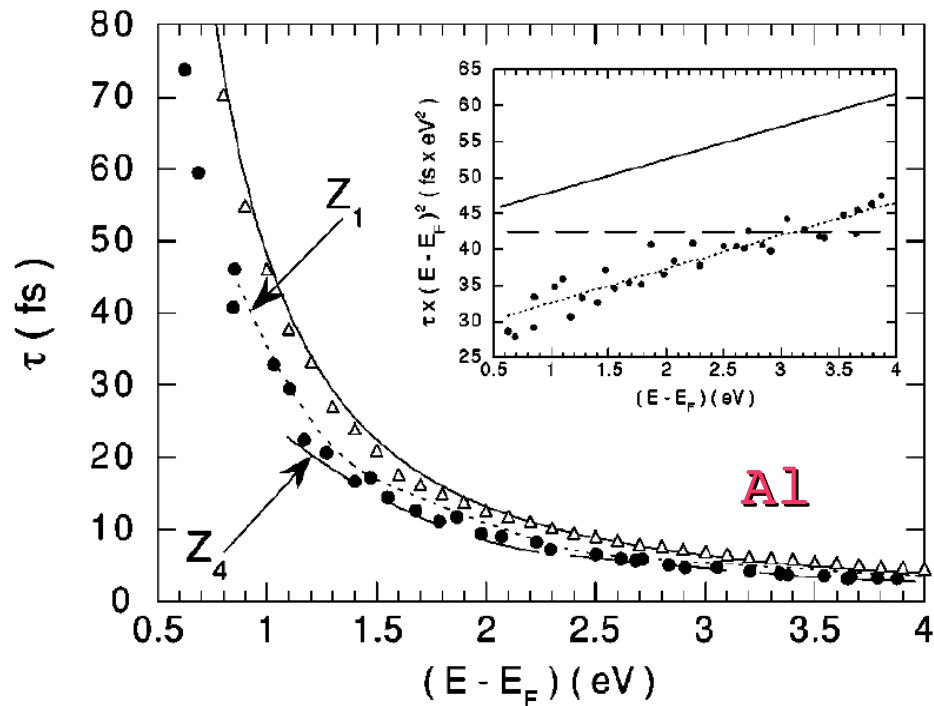
$$W(\omega) \sim \omega$$



$$\Gamma(\omega) \sim (\omega - E_{Fermi})^2$$

$$\tau(\omega) \sim (\omega - E_{Fermi})^{-2}$$

$$\Gamma_{nk} = \text{Im} [M_{nk}(\omega)] = 2\pi \sum_{n_1} \sum_{\mathbf{q}} \sum_{\mathbf{G}, \mathbf{G}'} \{ \tilde{\rho}_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}) [\tilde{\rho}_{nn_1}(\mathbf{k}, \mathbf{q}, \mathbf{G}')]^* \left(\int_{BZ'(\mathbf{q})} \frac{d\mathbf{q}'}{(2\pi)^3} \frac{1}{|\mathbf{q} + \mathbf{G}| |\mathbf{q} + \mathbf{G}'|} \right) \text{Im} [\tilde{\epsilon}_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{q}, \omega - \epsilon_{n_1}(\mathbf{k} - \mathbf{q}))] \left[\underbrace{(2 - f_{n_1}(\mathbf{k} - \mathbf{q})) \theta(\omega - \epsilon_{n_1}(\mathbf{k} - \mathbf{q}))}_A - \underbrace{f_{n_1}(\mathbf{k} - \mathbf{q}) \theta(\epsilon_{n_1}(\mathbf{k} - \mathbf{q}) - \omega)}_B \right] \}$$



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