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

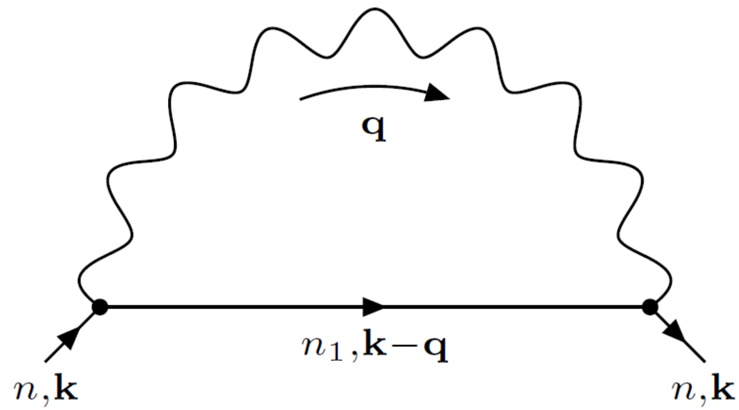
Andrea Marini

ikerbasque
Basque Foundation for Science

Condensed Matter Theory Group
University of Rome "Tor Vergata"

http://www.yambo-code.org/andrea

The GW self-energy (I)



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

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

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

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

The GW self-energy (II)

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

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

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

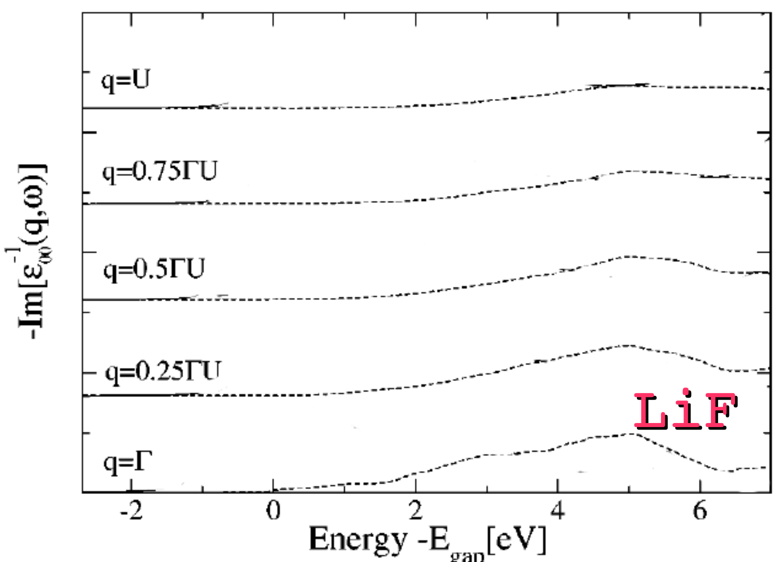
$$\langle n\mathbf{k}|M(\mathbf{r}_1,\mathbf{r}_2,\omega)|n'\mathbf{k}'\rangle$$
$$= i\sum_{n_1}\int_{BZ}\frac{d\mathbf{q}}{(2\pi)^3}\left\{\sum_{\mathbf{G},\mathbf{G}'}\frac{4\pi}{|\mathbf{q}+\mathbf{G}'|^2}\tilde{\rho}_{nn_1}(\mathbf{k},\mathbf{q},\mathbf{G})\left[\tilde{\rho}_{n'n_1}(\mathbf{k},\mathbf{q},\mathbf{G}')\right]^*\right.$$
$$\left.\int\frac{d\omega'}{2\pi}\tilde{\epsilon}^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega')\left[\frac{f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon_{n_1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon_{n_1(\mathbf{k}-\mathbf{q})}+i\delta}\right]\right\}$$

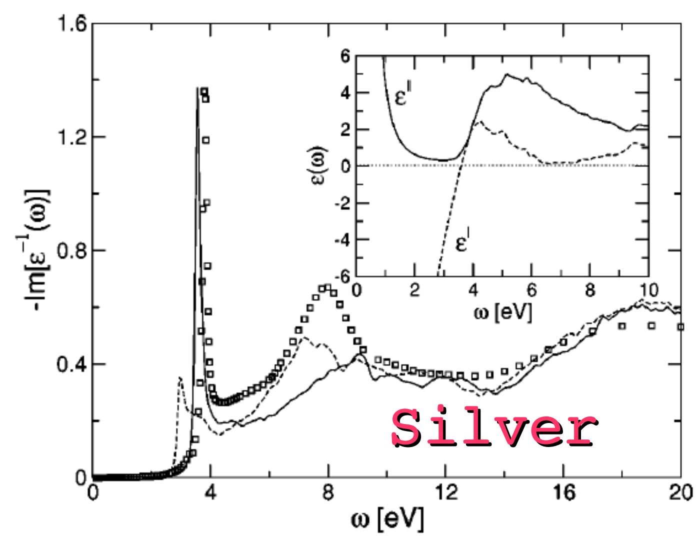
The Plasmon-Pole approximation

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

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

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
%
ETStpsXd= 100                  # [Xd] Total Energy steps
```

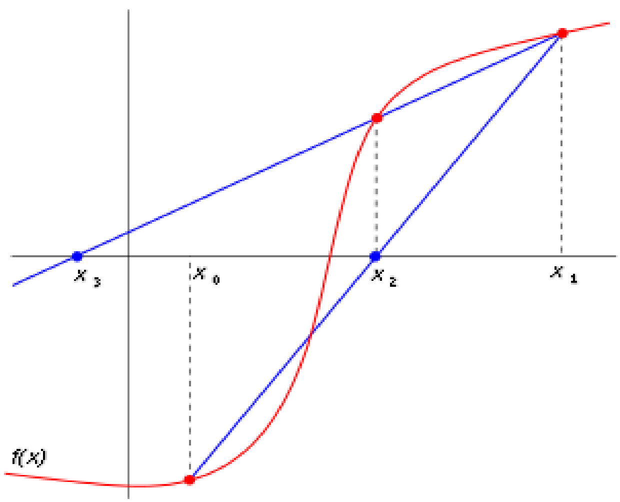
Yambo input file

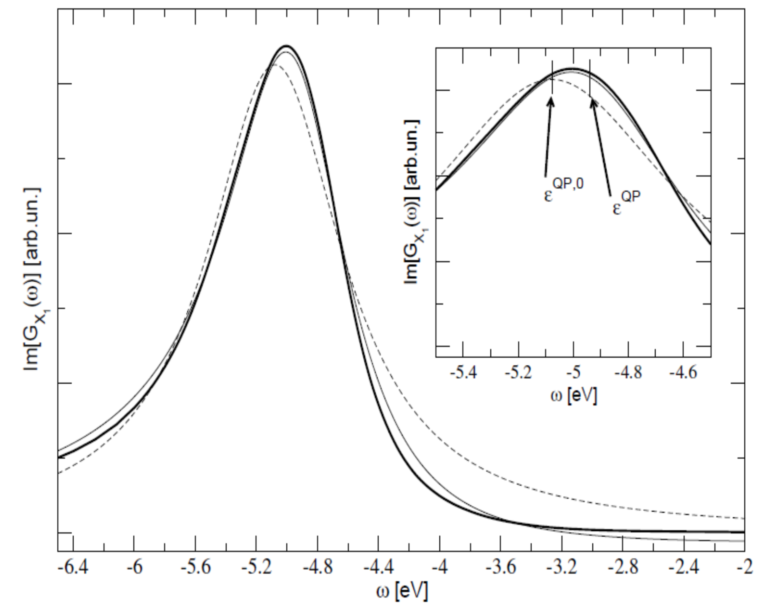
$$\langle n\mathbf{k}| M(\mathbf{r}_1,\mathbf{r}_2,\omega) |n'\mathbf{k}'\rangle = i\sum_{n_1}\int_{BZ}\frac{d\mathbf{q}}{(2\pi)^3}\left\{\sum_{\mathbf{G},\mathbf{G}'}\frac{4\pi}{|\mathbf{q}+\mathbf{G}'|^2}\tilde{\rho}_{nn_1}(\mathbf{k},\mathbf{q},\mathbf{G})\left[\tilde{\rho}_{n'n_1}(\mathbf{k},\mathbf{q},\mathbf{G}')\right]^* \int\frac{d\omega'}{2\pi}\tilde{\epsilon}^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega')\left[\frac{f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon_{n_1(\mathbf{k}-\mathbf{q})}-i\delta}+\frac{1-f_{n_1(\mathbf{k}-\mathbf{q})}}{\omega-\omega'-\epsilon_{n_1(\mathbf{k}-\mathbf{q})}+i\delta}\right]\right\}$$

Secant solver of Dyson equation

$$G_{n\mathbf{k}}(\omega) = \frac{1}{\omega - \epsilon_{n\mathbf{k}} - \left[\Sigma_x^{n\mathbf{k}} + M_{n\mathbf{k}}(\omega) \; - V_{xc}^{n\mathbf{k}}\right]}$$

1 $\epsilon_{n\mathbf{k}}^{QP,0} = \epsilon_{n\mathbf{k}} - \left[\Sigma_x^{n\mathbf{k}} + \Re\left[M_{n\mathbf{k}}\left(\epsilon_{n\mathbf{k}}^{QP,0}\right)\right] - V_{xc}^{n\mathbf{k}}\right]$





2 $M_{n\mathbf{k}}(z) \approx M_{n\mathbf{k}}\left(\epsilon_{n\mathbf{k}}^{QP,0}\right) + M'_{n\mathbf{k}}\left(\epsilon_{n\mathbf{k}}^{QP,0}\right)\left(z - \epsilon_{n\mathbf{k}}^{QP,0}\right)$

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

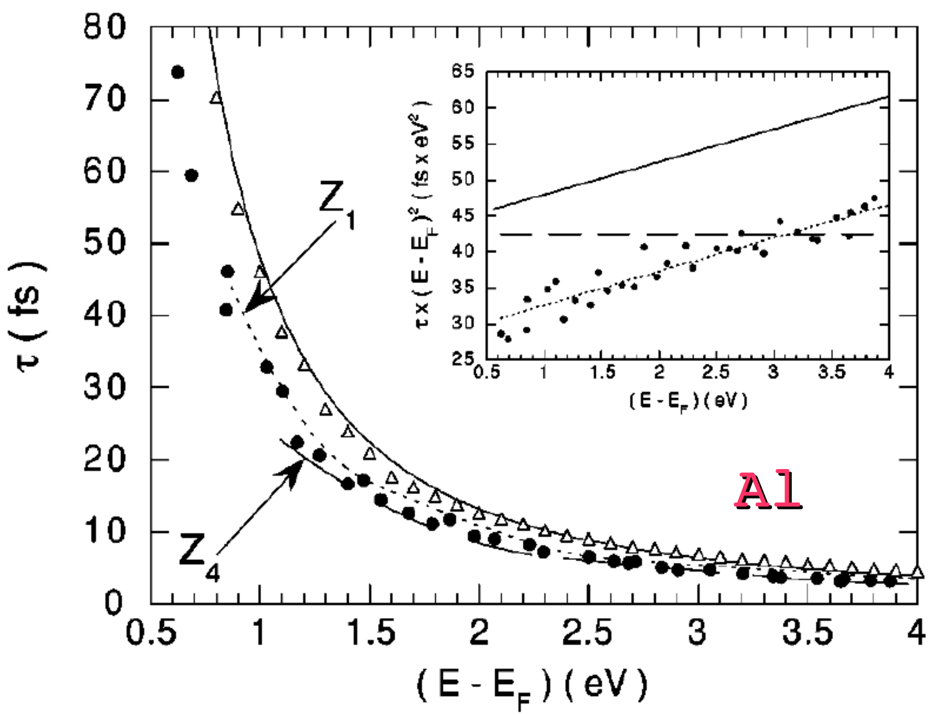
Lifetimes

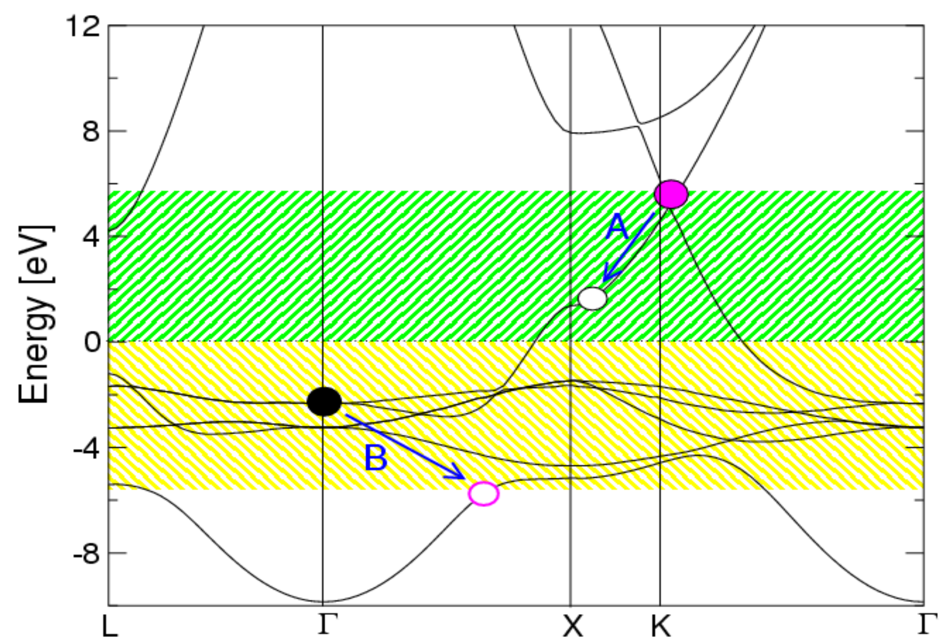
$$W(\omega) \sim \omega$$

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

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

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





Let's play with Yambo