A mathematical study of the GW[1] method

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April 26, 2014

[1] Note: The name "GW" does not stand for anything

We consider a very big electronic system ($N \approx \infty$), with Hamiltonian

$$H_N := -\frac{1}{2}\sum_{i=1}^{N}\Delta_i + \sum_{1\le i<j\le N}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} + \sum_{i=1}^{N} V(\mathbf{x}_i)$$

acting on $\mathcal{H}_N := \bigwedge_{i=1}^{N}\mathcal{H}$, with $\mathcal{H} = L^2(\mathbb{R}^3)$.

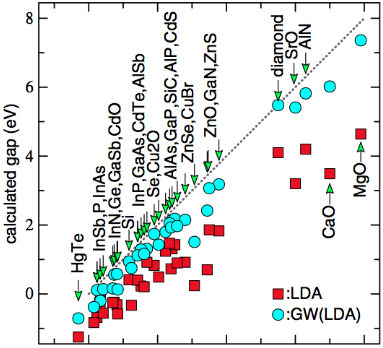
We would like to understand the optical properties of such a system.

System with N particles   System with $N-1$ particles

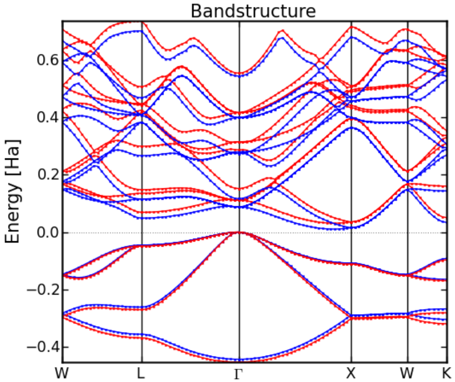
It holds $h\nu + E_N^0 = E_{\rm kin} + E_{N-1}^k$, from which we deduce the gap $E_{N-1}^k - E_N^0$.
There is a dynamical response due to the loss of a particle.

It is interesting to consider a dynamical system with a variable number of particles

In the limit $N \to \infty$, we expect to recover the correct band gap of crystals.



(a) Band gaps for LDA and GW.



(b) Band structure of Si for LDA, and GW.

A GW calculation gives better results with respect to band gaps.[2]
The GW method is based on Green's functions.

[2] M. van Schilfgaarde, T. Kotani and S. Faleev, Phys. Rev. Let. 96 (2006)

Definition of the Green's functions

We work with fermions, in spin-unpolarized systems.

- The 1-particle Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^3)$.
- The N-particle fermionic Hilbert space is $\mathcal{H}_N = \bigwedge_{i=1}^N L^2(\mathbb{R}^3)$.
- The fermionic Fock space is $\mathcal{F} = \mathbb{C} \oplus \mathcal{H} \oplus \mathcal{H}_2 \oplus \dots$

The Hamiltonian can be written in second quantization with

$$\mathbb{H} = \int_{\mathbb{R}^3} h(\mathbf{x})\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})\mathrm{d}\mathbf{x} + \iint_{\mathbb{R}^3\times\mathbb{R}^3} v(\mathbf{x},\mathbf{y})\Psi^\dagger(\mathbf{x})\Psi^\dagger(\mathbf{y})\Psi(\mathbf{y})\Psi(\mathbf{x})\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y},$$

where we separate the 1-body part of the Hamiltonian $h(\mathbf{x}) \approx -\frac{1}{2}\Delta + V(\mathbf{x})$, and the 2-body part $v(\mathbf{x},\mathbf{y}) = |\mathbf{x}-\mathbf{y}|^{-1}$.

We define the particle Green's function (here, Θ is the heavyside function):

$$G_p(\mathbf{x},t,\mathbf{x}',t') = -\mathrm{i}\Theta(t-t')\langle \Psi_N^0 | \Psi(\mathbf{x}) \mathrm{e}^{-\mathrm{i}(t-t')(H_{N+1}-E_N^0)} \Psi^\dagger(\mathbf{x}') | \Psi_N^0 \rangle.$$

Interpretation:

- start from the ground state
- create a particle at x'
- let the system evolves with its extra particle between t' and t $(t-t'>0)$
- annihilate a particle at x
- compare the new state with the ground state

"Describes the amplitude that a particle added at $(\mathbf{x},t)$ will be released at $(\mathbf{x}',t')$".

We also define the hole Green's function

$$G_h(\mathbf{x},t,\mathbf{x}',t') = \mathrm{i}\Theta(t'-t)\langle \Psi_N^0 | \Psi^\dagger(\mathbf{x}') \mathrm{e}^{\mathrm{i}(t-t')(H_{N-1}-E_N^0)} \Psi(\mathbf{x}) | \Psi_N^0 \rangle.$$

"Describes the amplitude that a hole added at $(\mathbf{x}',t')$ will be released at $(\mathbf{x},t)$".

We finally define the time-ordered Green's function

$$G(\mathbf{x},t,\mathbf{x}',t') = -\mathrm{i}\langle \Psi_N^0 | \mathcal{T}\left\{ \Psi_H(\mathbf{x},t)\Psi_H^\dagger(\mathbf{x}',t') \right\} | \Psi_N^0 \rangle$$
$$= G_p(\mathbf{x},t,\mathbf{x}',t') + G_h(\mathbf{x},t,\mathbf{x}',t'),$$

where $\mathcal{T}$ is the fermionic time-ordering operator.
Note that G contains all the information of G_p and G_h.
Finally, note that G_p, G_h and G only depends on $\tau := t - t'$.

The time-ordered Green's function has some interesting properties. We can recover:

- the 1-body density matrix from G:

$$-\mathrm{i}G(\mathbf{x},\mathbf{x}';0^-) = \gamma_N^0(\mathbf{x},\mathbf{x}') := \int_{\mathbb{R}^{3(N-1)}} \overline{\Psi_N^0(\mathbf{x},\mathbf{x}_2,\ldots\mathbf{x}_N)}\Psi_N^0(\mathbf{x}',\mathbf{x}_2,\ldots\mathbf{x}_N)\mathrm{d}\mathbf{x}_2\ldots\mathrm{d}\mathbf{x}_N.$$

- the electronic density $\rho_N^0(\mathbf{x}) = \gamma_N^0(\mathbf{x},\mathbf{x}) = -\mathrm{i}G(\mathbf{x},\mathbf{x},0^-)$.
- the ground-state energy (Galitskii-Migdal formula[3]).
- some information about the optical properties of the system, like $E_{N-1}^k - E_N^0$.

[3] V. M. Galitskii and A. B. Migdal, Sov. Phys.-JETP 7, 96 (1958).

Lemma

- *$\tau \mapsto G(\tau)$ is in $L^\infty(\mathcal{S}(\mathcal{H}))$, hence in the Schwartz class $\mathscr{S}'(\mathcal{S}(\mathcal{H}))$.*
- *Its time-Fourier transform exists (in the tempered-distributional sense), with*

$$\widehat{G}(\omega) = A_+ \left(\frac{1}{\omega - (H_{N+1} - E_N^0)} \right) A_+^* + A_-^\dagger \left(\frac{1}{\omega - (E_N^0 - H_{N-1})} \right) A_-$$

- *If $E_{N-2}^0 < E_N^0$, the analytic continuation of G into the physical Riemann sheet is*

$$\widetilde{G_p}(z) := A_+ \left(\frac{1}{z - (H_{N+1} - E_N^0)} \right) A_+^* + A_-^\dagger \left(\frac{1}{z - (E_N^0 - H_{N-1})} \right) A_-$$

  for $z \in \mathbb{C} \setminus \sigma(H_{N+1} - E_N^0)$.
- *It holds*

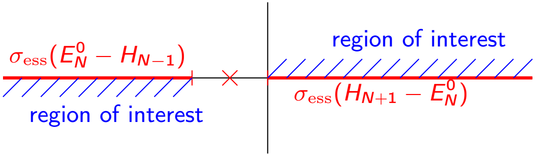
$$\widehat{G}(\omega) = \lim_{\eta \to 0+} \widetilde{G}(\omega + \mathrm{i}\eta) \quad \textit{for} \quad \omega > 0,$$

  and

$$\widehat{G}(\omega) = \lim_{\eta \to 0+} \widetilde{G}(\omega - \mathrm{i}\eta) \quad \textit{for} \quad \omega < 0.$$

Here, $A_+^\dagger : \mathcal{H} \to \mathcal{H}_{N+1}$ and $A_- : \mathcal{H} \to \mathcal{H}_{N-1}$ are the creation/annihilator operators.

- If $E_N^0 - E_{N-2}^0 < 0$, the physical Riemann sheet for G is connected.



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Similarly to $\widetilde{G_0}(z) = (z - H_0)^{-1}$ for a non-interacting Hamiltonian, we would like to define the (1-particle) dynamical Hamiltonian as

$$\widetilde{H}(z) := z - \left(\widetilde{G}(z)\right)^{-1}.$$

Lemma

For all $z \in \mathbb{C} \setminus \mathbb{R}$, $\widetilde{G}(z)$ is an invertible operator from $L^2(\mathbb{R}^3)$ to some dense set $D(z) \subset H^2(\mathbb{R}^3)$. In particular, $\widetilde{H}(z)$ is a well-defined operator with domain $D(z)$.

Question: Do we have $D(z) = H^2(\mathbb{R}^3)$?

Then, we look for solutions of $\widetilde{H}(z)\widetilde{u}(z) = \widetilde{E}(z)\widetilde{u}(z)$, with $\widetilde{E}(z) \in \mathbb{C}$ the quasi-energy.

- The real part of $\widetilde{E}(z)$ is the energy of the quasi-particle $\widetilde{u}(z)$
- The imaginary part of $\widetilde{E}(z)$ is the lifetime of the quasi-particle $\widetilde{u}(z)$
- There is no non-real solution on the physical Riemann sheet.
- Non real solutions can only be on the second Riemann sheet.

Question: How to calculate the time-ordered Green's function?

The GW approximation.

From the Schrödinger equation $H\Psi = \mathrm{i}\partial_t \Psi$, and the anti-commutation rules, we get an exact equation of motion for G:

$$(\mathrm{i}\partial_{t_1} - h(\mathbf{1}))\, G(\mathbf{12}) - \int \mathrm{d}\mathbf{3} v(\mathbf{13}) G^{(2)}(\mathbf{13}^{++}\mathbf{23}^{+}) = \delta(\mathbf{12}),$$

where $\mathbf{1} = (\mathbf{x}_1, t_1)$, $\mathbf{2} = (\mathbf{x}_2, t_2)$ ..., $v(\mathbf{13}) = |\mathbf{x}_1 - \mathbf{x}_3|^{-1}\delta_{t_1 t_3}$, $\mathrm{d}\mathbf{3} = \mathrm{d}\mathbf{x}_3 \mathrm{d}t_3$, ...

Remarks:

- We need to 2-body time-ordered Green's function $G^{(2)}$:

$$G^{(2)}(\mathbf{x}, t, \mathbf{x}', t', \mathbf{y}, s, \mathbf{y}', s') := -\mathrm{i}\langle \Psi_N^0 | \mathcal{T}\left\{ \Psi_H(\mathbf{x}, t)\Psi_H(\mathbf{x}', t')\Psi_H^\dagger(\mathbf{y}, s)\Psi_H^\dagger(\mathbf{y}', s')\right\} |\Psi_N^0\rangle.$$

- The equation of motion for $G^{(2)}$ uses $G^{(3)}$, and so on...
- In order to have a closed equation for G, we make an approximation.

After some manipulations, the equation of motion can be recast in the time-Fourier domain into

$$(\omega - H_0)\widehat{G}(\omega) - \widehat{\Sigma}(\omega)\widehat{G}(\omega) = \mathbb{1}_{\mathcal{H}}$$

where

$$H_0 = \sum_{i=1}^{N} \left(-\frac{1}{2}\Delta_i + V(\mathbf{x}_i) + \left(\rho_N^0 \star |\cdot|^{-1}\right)(\mathbf{x}_i) \right)$$

is the 1-body Hartree Hamiltonian.

We introduced the self-energy operator Σ which depends on $G^{(2)}$.

Finally, by introducing

$$\widehat{G_0}(\omega) = (\omega - H_0)^{-1}$$

the (time-Fourier transform of the) non-interacting Green's function, we get

$$\widehat{G}(\omega)^{-1} = \widehat{G_0}(\omega)^{-1} - \widehat{\Sigma}(\omega).$$

Remarks:

- In this equation, Σ is seen as a correction to the non-interacting GF.
- The GW approximation consists into approximating the self-energy Σ.

The Hedin's equations: [4]

$$G(\mathbf{12}) = G_0(\mathbf{12}) + \int \mathrm{d}\mathbf{34}\, G_0(\mathbf{13})\Sigma(\mathbf{34})G(\mathbf{42}) \qquad \text{(Dyson equation)}$$

$$\Sigma(\mathbf{12}) = \mathrm{i} \int \mathrm{d}\mathbf{34}\, G(\mathbf{13})W(\mathbf{14})\Gamma(\mathbf{423}) \qquad \text{(Self-energy)}$$

$$\Gamma(\mathbf{123}) = \delta(\mathbf{12})\delta(\mathbf{13}) + \int \mathrm{d}\mathbf{4567}\, \frac{\partial \Sigma(\mathbf{12})}{\partial G(\mathbf{45})} G(\mathbf{46})G(\mathbf{57})\Gamma(\mathbf{673}) \qquad \text{(Vertex function)}$$

$$W(\mathbf{12}) = \int \mathrm{d}\mathbf{3}\, \epsilon^{-1}(\mathbf{13})v(\mathbf{32}) \qquad \text{(Screening)}$$

$$\epsilon(\mathbf{12}) = \delta(\mathbf{12}) - \int \mathrm{d}\mathbf{3}\, v(\mathbf{13})P(\mathbf{32}) \qquad \text{(Dielectric)}$$

$$P(\mathbf{12}) = -\mathrm{i} \int \mathrm{d}\mathbf{34}\, G(\mathbf{13})G(\mathbf{41})\Gamma(\mathbf{342}) \qquad \text{(Irreducible polarizability)}$$

Remarks:

- Formulae based on Feynman diagram considerations (perturbation theory).
- The idea of Hedin is to develop the perturbation with respect to W, rather than V.

[4] L. Hedin, Phys. Rev. 139, 3A (1965).

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The GW approximation consists into setting

$$\frac{\partial \Sigma(\mathbf{12})}{\partial G(\mathbf{45})} = 0, \quad \text{or equivalently} \quad \Gamma(\mathbf{123}) = \delta(\mathbf{12})\delta(\mathbf{13}) \quad \text{(GW approximation)},$$

so that $\Sigma(\mathbf{12}) = \mathrm{i} \int \mathrm{d}\mathbf{34} G(\mathbf{13}) W(\mathbf{14}) \Gamma(\mathbf{423})$ simplifies into $\Sigma^{\mathrm{GW}}(\mathbf{12}) = \mathrm{i} G(\mathbf{12}) W(\mathbf{12}^+)$.

Remarks:

- We multiply the kernels of the operators, and not the operators!
- It is unclear *a priori* whether $\Sigma(\mathbf{12})$ is the kernel of some operators...
- If we replace W by v, we would get

$$\Sigma^{Gv}(\mathbf{x}, \mathbf{x}') = \mathrm{i} G(\mathbf{x}, \mathbf{x}', 0^-) v(\mathbf{x}, \mathbf{x}') = -\frac{\gamma_N^0(\mathbf{x}, \mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|},$$

  which is the Fock exchange term. We recover in this case the Hartree-Fock model.
- The self-energy can be seen as a "dynamically screened exchange operator".

Question: Is $\Sigma^{GW}(\mathbf{x}, t, \mathbf{x}', t')$ the kernel of a well-defined operator for all $t, t' \in \mathbb{R}^2$?

Lemma

For all $\tau := t - t'$, the operator $\Sigma^{\mathrm{GW}}(\tau)$ is a well defined operator on $\mathcal{H}$, which is uniformly bounded in τ.

Idea of the proof

It holds, for $f, g \in \mathcal{H} \times \mathcal{H}$,

$$\begin{aligned}
\langle f | \Sigma^{\mathrm{GW}}(\tau) | g \rangle &= \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \overline{f(\mathbf{x})} \Sigma^{\mathrm{GW}}(\mathbf{x}, \mathbf{x}', \tau)) g(\mathbf{x}') \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x} \\
&= \mathrm{i} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \overline{f(\mathbf{x})} G(\mathbf{x}, \mathbf{x}', \tau) g(\mathbf{x}') W^*(\mathbf{x}', \mathbf{x}, \tau) \mathrm{d}\mathbf{x} \mathrm{d}\mathbf{x}' \\
&= \mathrm{Tr} \left(\overline{f} G(\tau) g W^*(\tau) \right).
\end{aligned}$$

Here, f and g are seen as multiplicative operators.

In some sense, $\sqrt{W(\tau)} f \in \mathfrak{S}_2$, with $\| \sqrt{W(\tau)} f \|_{\mathfrak{S}_2} \leq C \| f \|_{L^2}$. Hence

$$\begin{aligned}
\langle f | \Sigma^{\mathrm{GW}}(\tau) | g \rangle &\leq \| \sqrt{W} \, \overline{f} G(\tau) g \sqrt{W(\tau)} \|_{\mathfrak{S}_1} \leq \| G(\tau) \|_{\mathcal{S}(\mathcal{H})} \| \sqrt{W(\tau)} f \|_{\mathfrak{S}_2} \| \sqrt{W(\tau)} g \|_{\mathfrak{S}_2} \\
&\leq C \| G(\tau) \|_{\mathcal{S}(\mathcal{H})} \| f \|_{\mathcal{H}} \| g \|_{\mathcal{H}}.
\end{aligned}$$

In practice

$$\Sigma^{\mathrm{GW}}(\mathbf{12}) = \mathrm{i}G(\mathbf{12})W(\mathbf{12}^+) \quad \text{and} \quad \widehat{G^{\mathrm{GW}}}(\omega)^{-1} := \widehat{G_0}(\omega)^{-1} - \widehat{\Sigma^{\mathrm{GW}}}(\omega).$$

Problem: We need to know G to compute Σ^{GW} (and W).

Idea 1: One-shot GW, or $G_0 W_0$ approximation:
Set

$$\Sigma^{\mathrm{GW},00}(\mathbf{12}) = \mathrm{i}G_0(\mathbf{12})W_0(\mathbf{12}^+) \quad \text{and} \quad \widehat{G^{\mathrm{GW},00}}(\omega)^{-1} := \widehat{G_0}(\omega)^{-1} - \widehat{\Sigma^{\mathrm{GW},00}}(\omega).$$

Idea 2: Self-consistent GW:
Repeat on k:

$$\Sigma_{k+1}^{\mathrm{GW}}(\mathbf{12}) = \mathrm{i}G_k(\mathbf{12})W_k(\mathbf{12}^+) \quad \text{and} \quad \widehat{G_{k+1}}(\omega)^{-1} := \widehat{G_0}(\omega)^{-1} - \widehat{\Sigma_{k+1}^{\mathrm{GW}}}(\omega)$$

until convergence.

Questions:

- What does "convergence" mean?
- Does the self-consistent loop converge?

The periodic case.

- It is not obvious in what sense some thermodynamic limit must be made for G.
- However, the thermodynamic limit for the Hartree model (*i.e.* G_0) has a meaning.[5]

IDEA: study the Green's function given by the $G_0 W_0$ approximation:

- From G_0, calculate W_0, and $\Sigma^{00}(\mathbf{1},\mathbf{2}) = \mathrm{i} G_0(\mathbf{12}) W_0(\mathbf{12})$.
- Define the time-ordered Green's function with

$$\widetilde{G^{\mathrm{GW},00}}(z)^{-1} := \widetilde{G_0}(z)^{-1} - \widetilde{\Sigma^{00}}(z).$$

We will therefore consider the (non-interacting) Hamiltonian defined by (from the Bloch transformation)

$$H_0 := \int_{q \in \Gamma^*}^{\oplus} H_q \mathrm{d}q \quad \text{where} \quad H_q := (-\mathrm{i}\nabla + q)^2 + V_{\mathrm{per}} + \rho_0 \star |\cdot|^{-1} \quad \text{is acting on } L^2_{\mathrm{per}}(\Gamma).$$

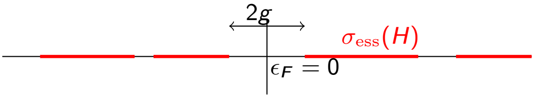
We will write in the sequel

$$H_q = \sum_{n=1}^{\infty} \epsilon_{nq} |u_{nq}\rangle\langle u_{nq}| \quad \text{with} \quad u_{nq} \in L^2_{\mathrm{per}}(\Gamma).$$

[5] I. Catto, C. Le Bris and P.L. Lions, Ann. I. H. Poincaré 19, 2 (2002)

We suppose that the crystal is a semi-conductor with gap $2g$.
We set the Fermi level $\epsilon_F = 0$, and suppose that

$$\forall q \in \Gamma^* \quad \epsilon_{N,q} \leq -g \quad \text{and} \quad \epsilon_{N+1,q} \geq g.$$

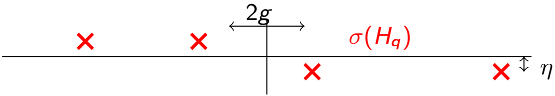


We can work at q fixed, for every operator commutes with translation. For instance,

$$\widetilde{G_0}(q,z) = \sum_{n=1}^{N} \frac{|u_{nq}\rangle\langle u_{nq}|}{z - \epsilon_{nq} - \mathrm{i}\eta} + \sum_{m=N+1}^{\infty} \frac{|u_{mq}\rangle\langle u_{mq}|}{z - \epsilon_{mq} + \mathrm{i}\eta}.$$

Remark:

- Here, $\eta > 0$ allows to force the region of interest (shift poles in the correct direction).
- Indeed, we are only working with $z = \omega \in \mathbb{R}$ in the sequel.

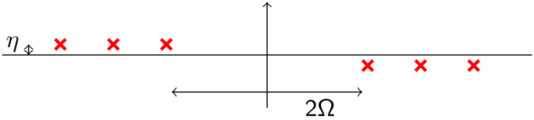


To calculate W_0, we use the Hedin's equation

$$\widehat{W_0}(q,\omega) = v + \sqrt{v(q)}\widehat{P_0}(q,\omega)\sqrt{v(q)}.$$

Usually, $\widehat{P_0}(q,\omega)$ is very expensive to calculate.
It is approximated via a Plasmon-Pole interpolation:

$$\widehat{P_0^{\mathrm{PP}}}(q,\omega) = \sum_{p\in\mathbb{N}} \frac{|u_p(q)\rangle\langle u_p(q)|}{\omega^2 - (\omega_p(q) - \mathrm{i}\eta)^2}$$



- In this last expression, $u_p(q)$ is not necessarily an orthonormal basis, and $\omega_p(q) > 0$.
- It holds $\widehat{P_0}(q,-\omega) = \widehat{P_0}(q,\omega)$, and there exists a gap $2\Omega >> 2g$.
- There exists several Plasmon-Pole approximations.
- We worked with the one by Engel and Farid[6] (good mathematical properties).

[6] G. Engel and B. Farid, Phys. Rev. B 47, 23 (1993)

Lemma

In the periodic case, with the Engel and Farid plasmon-pole, for all $\omega \in]-\Omega - g, \Omega + g[$, $\widehat{\Sigma^{00}}(q, \omega)$ *is a well-defined symmetric operator. It is in the Schatten class* $\mathfrak{S}_p(L^2_{\rm per}(\Gamma))$, *for all* $p > 3$.

- This theorem in valid in the limit $\eta \to 0$.
- The small gap g has been opened by $\Omega >> g$.

Finally, we want to find the (real) solutions of

$$\widehat{G^{\mathrm{GW},00}}^{-1}(q,\omega)u = 0 \quad \text{or} \quad \left(H_q + \widehat{\Sigma^{00}}(q,\omega)\right) u = \omega u.$$

Perturbative approach: look for solutions $\omega = E_{nq} \approx \epsilon_{nq}$

- Solve $E_{nq} = \epsilon_{nq} + \langle u_{nq} | \widehat{\Sigma^{00}}(q, E_{nq}) | u_{nq} \rangle$.
- $\widehat{\Sigma^{00}}(q, E_{nq}) \approx \widehat{\Sigma^{00}}(q, \epsilon_{nq}) + (E_{nq} - \epsilon_{nq}) \dfrac{\partial \widehat{\Sigma^{00}}}{\partial \omega}(q, \varepsilon_{nq})$.
- Hence,

$$E_{nq} = \epsilon_{nq} + \frac{\langle u_{nq} | \widehat{\Sigma^{00}}(q,\epsilon_{nq}) | u_{nq} \rangle}{1 - \left\langle u_{nq} \left| \dfrac{\partial \widehat{\Sigma^{00}}}{\partial \omega}(q,\epsilon_{nq}) \right| u_{nq} \right\rangle}$$

Lemma

For all $\omega \in]-\Omega - g, \Omega + g[$, $\dfrac{\partial \widehat{\Sigma^{00}}}{\partial \omega}(q,\omega)$ is a non-positive symmetric operator.

Remark: Because of the opening of the gap, this lemma is valid for a wide range of ϵ_{nq}.

Conclusions:

- We gave a mathematical meaning to the operators in GW.
- In particular, we proved that the self-energy is a well-defined operator in both finite systems and crystals (within the plasmon-pole approximation).
- We proved the well-posedness of the resulting numerical models.

Perspectives

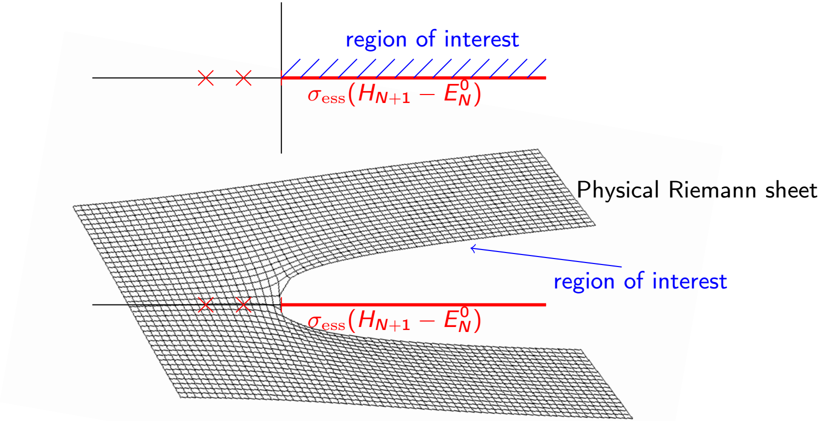
- Understand the resonances (= quasi-energies on the second Riemann sheet).
- Is the following non-linear eigenvalue problem well-posed?

$$\det\left(H_q + \widehat{\Sigma^{00}}(q,\omega) - \omega\right) = 0.$$

- Investigate on the self-consistent GW method (convergence,...)

$$\widetilde{G_p}(z) := A_+ \left(\frac{1}{z - (H_{N+1} - E_N^0)} \right) A_+^\dagger \quad \text{for} \quad z \in \mathbb{C} \setminus \sigma(H_{N+1} - E_N^0)$$

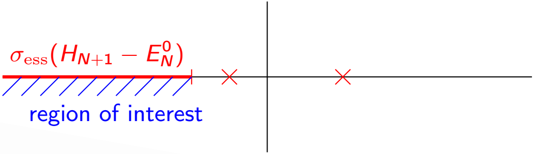
- The eigenvalues of $H_{N+1} - E_N^0$ are poles of $\widetilde{G}_p$.
- The essential spectrum of $H_{N+1} - E_N^0$ is a branch cut of $\widetilde{G}_p$.
- The essential spectrum of $H_{N+1} - E_N^0$ is $[0, +\infty[$ due to the HVZ theorem.



We can perform a similar work for the hole Green's function:

$$\widetilde{G}_h(z) := A_-^\dagger \left(\frac{1}{z - (E_N^0 - H_{N-1})} \right) A_- \quad \text{for} \quad z \in \mathbb{C} \setminus \sigma(H_{N+1} - E_N^0)$$

- The essential spectrum of $E_N^0 - H_{N-1}$ is $]-\infty, E_N^0 - E_{N-2}^0]$ due to the HVZ theorem.



Physical Riemann sheet