A mathematical study of the GW^0 method for computing electronic excited states of molecules

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Joint work with Eric Cancès and David Gontier

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Excited states of N-body Hamiltonians (1)

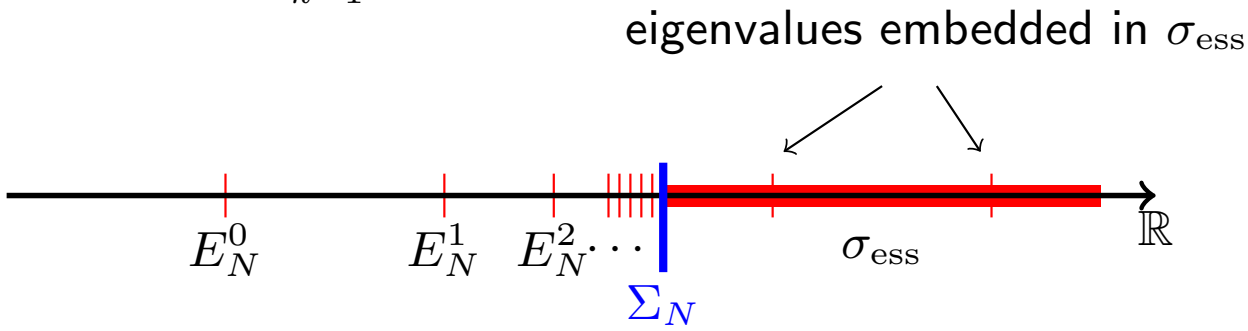
- Nuclei at positions $\mathbf{R}_k$ with charges z_k: $v_{\mathrm{ext}}(\mathbf{r}) := -\sum_{k=1}^{M} \frac{z_k}{|\mathbf{r}-\mathbf{R}_k|}$

Electronic problem with N-electrons

Find $\Psi \in \mathcal{H}_N := \bigwedge^N \mathcal{H}_1$ (with $\mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C})$) such that $\|\Psi\|_{L^2(\mathbb{R}^{3N})} = 1$ and

$$H_N \Psi := \left(-\frac{1}{2} \sum_{i=1}^{N} \Delta_{\mathbf{r}_i} + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i=1}^{N} v_{\mathrm{ext}}(\mathbf{r}_i) \right) \Psi = E \Psi(\mathbf{r}_1, \dots \mathbf{r}_N)$$

- HVZ theorm: if $N \leqslant Z := \sum_{k=1}^{M} z_k$, then $\sigma(H_N)$ is as follows:



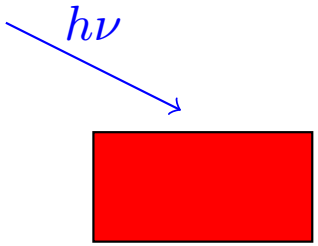
- **Assumptions**: E_N^0 is a simple eigenvalue of H_N and $2E_N^0 < E_{N+1}^0 + E_{N-1}^0$ (stability of the N-particle system)

Excited states of N-body Hamiltonians (2)

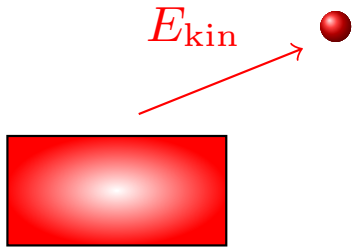
- Compute electronic excitation energies: quantities of the form

$$E_N^0 - E_{N+1}^k \quad \text{(gain of an electron)} \quad \text{and} \quad E_N^0 - E_{N-1}^k \quad \text{(loss of an electron)}.$$

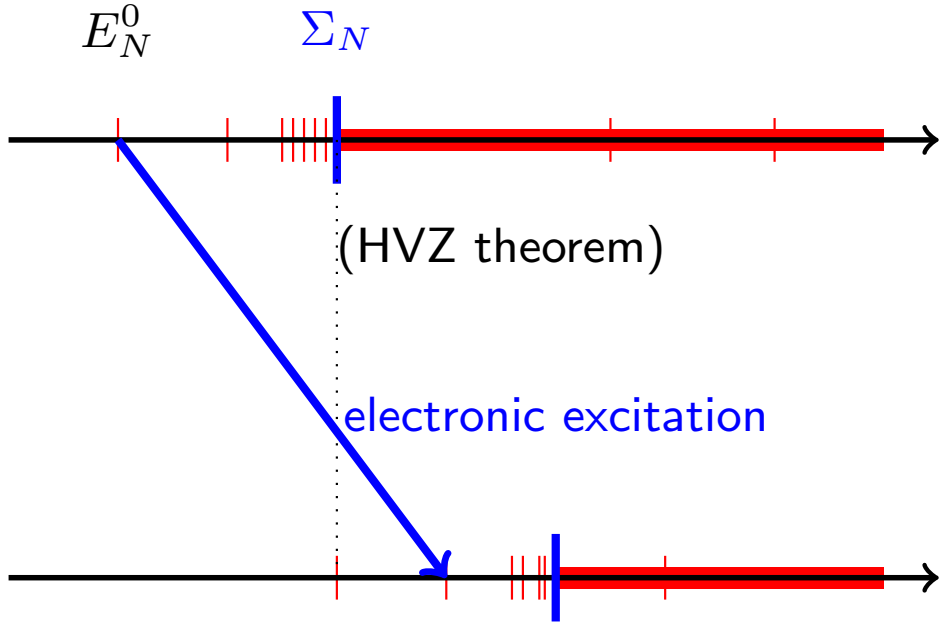
- Inverse photoemission spectroscopy (IPES)



System with N particles



System with $N-1$ particles



A short review of methods and results

- Computation of excitation energies $E_N^0 - E_{N+1}^k$ or $E_N^0 - E_{N-1}^k$
  - Density functional theory (DFT) inadequate: only deals with ground state properties
  - Quantum Monte Carlo methods: idem
  - Wavefunction methods: scales from N_b^6 (CISD) to $N_b!$ (full CI)
  - Time-dependent DFT (TDDFT): does not work well for extended systems
  - Green's function method: in this talk, GW.

- Electronic excitations energies $\rightarrow$ band gap of perfect crystals as $N \rightarrow \infty$

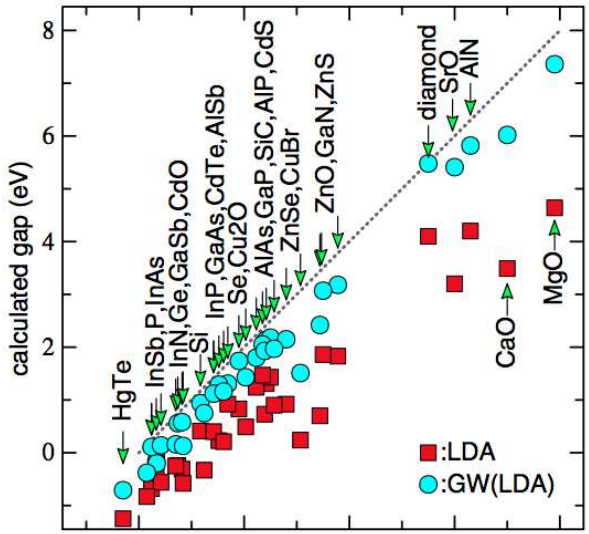


Figure : Band gaps for LDA and GW.

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

Definition of Green's functions,

self-energies, etc

The Particle Green's function in the time domain

- Fock space $\mathbb{F} := \bigoplus_{N=0}^{+\infty} \mathcal{H}_N$ with $\mathcal{H}_0 = \mathbb{C}$, $\mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C})$ and $\mathcal{H}_N = \bigwedge^N \mathcal{H}_1$
- Annihilation and creation operators $a^\dagger(\phi) = (a(\phi))^*$ for $\phi \in \mathcal{H}_1$

$$\forall \Psi_N \in \mathcal{H}_N, \qquad (a(\phi)\Psi_N)(\mathbf{r}_1, \cdots, \mathbf{r}_{N-1}) = \sqrt{N} \int_{\mathbb{R}^3} \overline{\phi(\mathbf{r})}\, \Psi_N(\mathbf{r}, \mathbf{r}_1, \cdots, \mathbf{r}_{N-1})\, d\mathbf{r}.$$

- Formal definition of the one-body particle Green's function (in the time domain)

$$\forall \tau \in \mathbb{R},\ \forall (f,g) \in \mathcal{H}_1 \times \mathcal{H}_1,\ \langle g | G_{\rm p}(\tau) | f \rangle = -\mathrm{i}\Theta(\tau) \left\langle \Psi_0^N \left| a(g) \mathrm{e}^{-\mathrm{i}\tau(H_{N+1} - E_N^0)} a^\dagger(f) \right| \Psi_0^N \right\rangle.$$

- Annihilation and creation operators (bis)

$$A_+^* \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{N+1}) : f \mapsto a^\dagger(f)|\Psi_N^0\rangle, \quad A_+ = (A_+^*)^* \in \mathcal{B}(\mathcal{H}_{N+1}, \mathcal{H}_1)$$

One-body particle Green's function (in the time domain)

$$\forall \tau \in \mathbb{R}, \quad G_{\rm p}(\tau) = -\mathrm{i}\Theta(\tau) A_+ \mathrm{e}^{-\mathrm{i}\tau(H_{N+1} - E_N^0)} A_+^*$$

- Note that $G_{\rm p} \in L^\infty(\mathbb{R}_\tau, \mathcal{B}(\mathcal{H}_1))$ and $G_{\rm p}(\tau) = 0$ for $\tau < 0$

The Particle Green's function in the frequency domain (1)

- Normalization convention for the time-Fourier transform

$$\forall f \in L^1(\mathbb{R}_\tau, X), \quad X \text{ Banach space}, \quad [\mathcal{F}_T f](\omega) = \widehat{f}(\omega) = \int_{-\infty}^{+\infty} f(\tau)\, e^{i\omega\tau}\, d\tau.$$

- Fourier representation of the one-body particle Green's function

$$\widehat{G_{\mathrm{p}}}(\omega) = (\mathcal{F}_T G_{\mathrm{p}})(\omega), \quad \widehat{G_{\mathrm{p}}} \in H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)).$$

Key point

The support of the distribution $\mathrm{Im}\left(\widehat{G_{\mathrm{p}}}\right)$ *is contained in the (particle) electronic excitation set* $S_{\mathrm{p}} := \sigma(H_{N+1} - E_N^0)$.

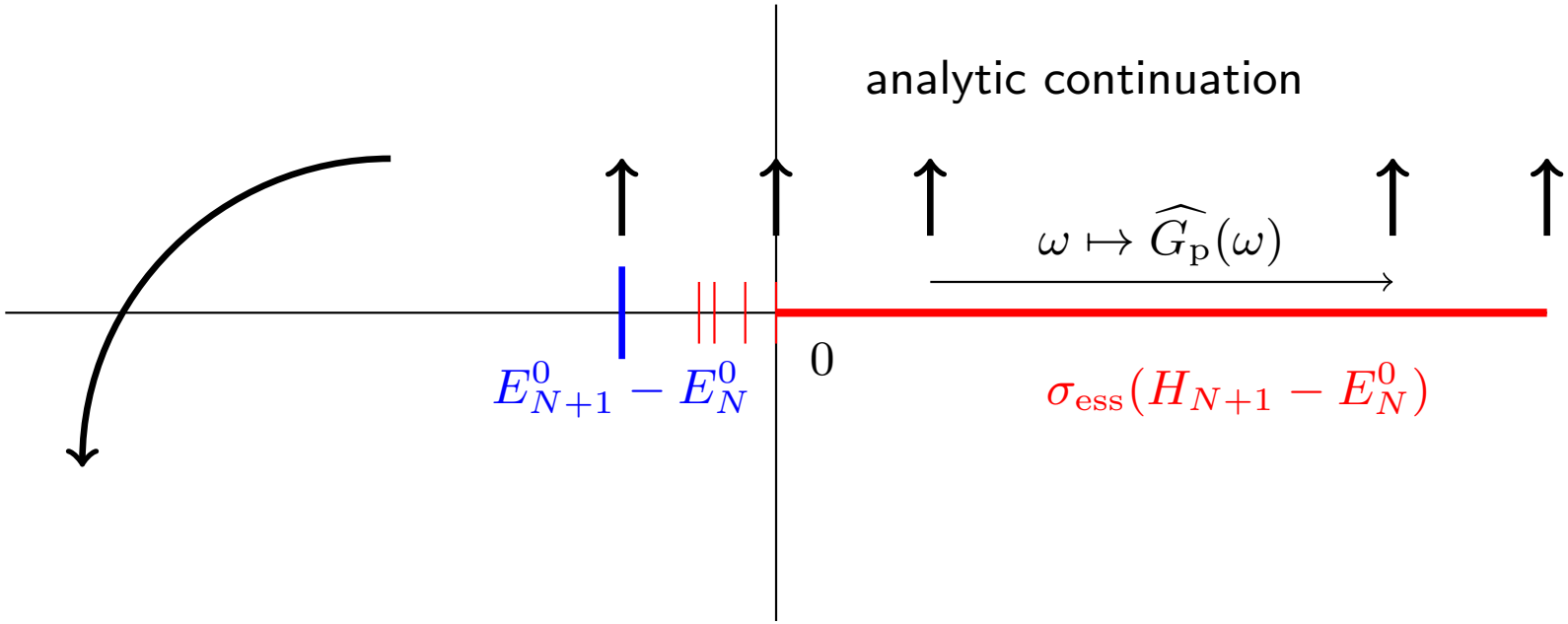
- Particle excited state energies recovered from $\widehat{G_{\mathrm{p}}}$ which is however highly irregular
- Analytic continuation through a Laplace transform on $\mathbb{U} := \{z \in \mathbb{C},\ \mathrm{Im}(z) > 0\}$

$$\forall f \in L^\infty(\mathbb{R}_\tau, X), \quad \forall z \in \mathbb{U}, \qquad \widetilde{f}(z) := \int_0^\infty f(\tau) \mathrm{e}^{\mathrm{i}z\tau} \mathrm{d}\tau$$

The Particle Green's function in the frequency domain (2)

- Complex frequency domain: analytical continuation $\widetilde{G_{\mathrm{p}}}$ of $\widehat{G_{\mathrm{p}}}$ on $\mathbb{U}$, extended to $\mathbb{C} \setminus S_{\mathrm{p}}$

$$\forall z \in \mathbb{C} \setminus S_{\mathrm{p}}, \quad \widetilde{G_{\mathrm{p}}}(z) = A_+ \left(\frac{1}{z - (H_{N+1} - E_N^0)} \right) A_+^*.$$



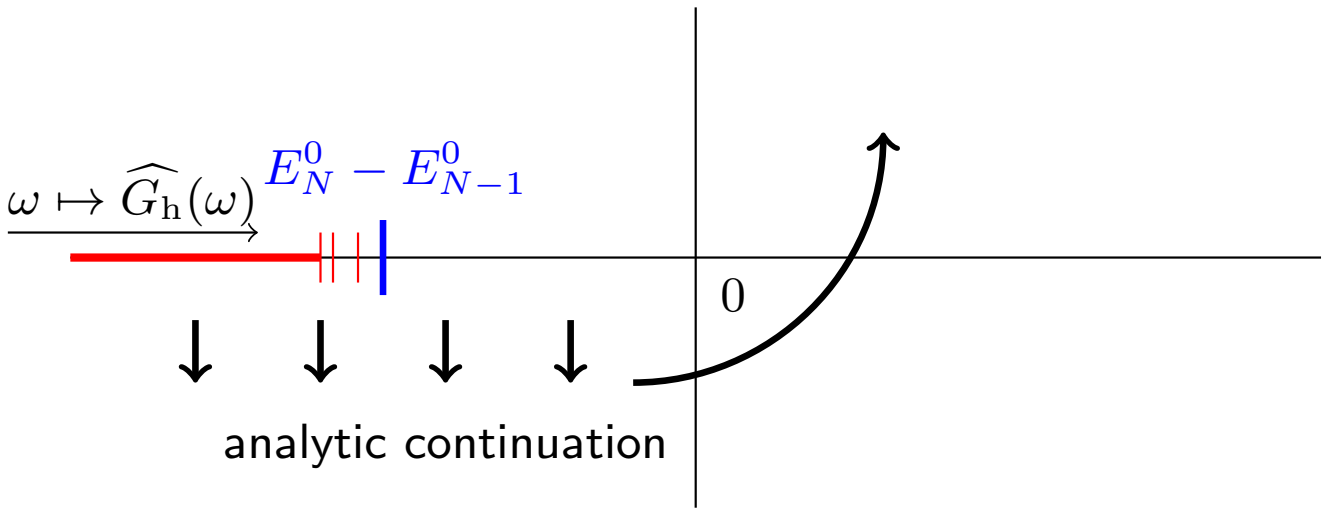
Hole Green's function

- Annihilation/creation operator $A_- \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{N-1}) : f \mapsto a(\overline{f})|\Psi_N^0\rangle$
- Time domain: $G_{\mathrm{h}}(\tau) = \mathrm{i}\Theta(-\tau) A_-^* \, \mathrm{e}^{\mathrm{i}\tau(H_{N-1} - E_N^0)} A_-$
- Recover the one-body ground-state density matrix as $\gamma_N^0 = -\mathrm{i}G_{\mathrm{h}}(0^-) = A_-^* A_-$

Key point

Support of $\mathrm{Im}\left(\widehat{G_{\mathrm{h}}}\right)$ *contained in (hole) electronic excitation set* $S_{\mathrm{h}} := \sigma(E_N^0 - H_{N-1}^0)$

- Complex frequency domain: $\forall z \in \mathbb{C} \setminus S_{\mathrm{h}}, \quad \widetilde{G_{\mathrm{h}}}(z) = A_-^* \left(\dfrac{1}{z - (E_N^0 - H_{N-1})} \right) A_-$



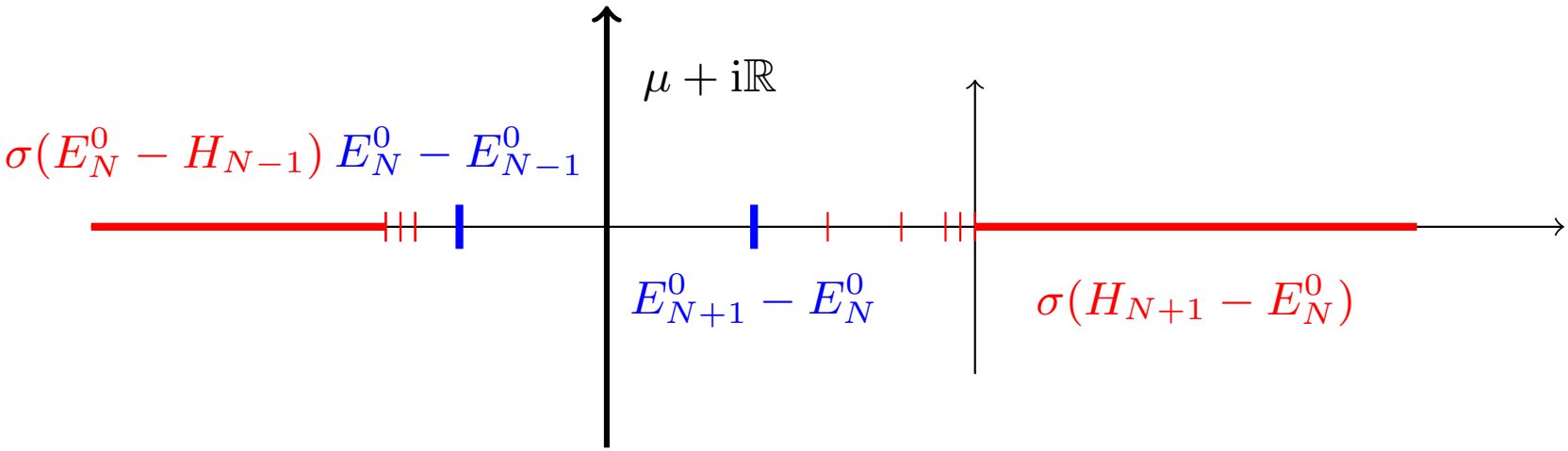
The one-body total Green's function

- **Chemical potential** μ: well defined by the stability condition

$$E_N^0 - E_{N-1}^0 < \mu < E_{N+1}^0 - E_N^0$$

One-body total Green's function in the complex frequency domain

$$\forall z \in \mathbb{C} \setminus (S_{\mathrm{h}} \cup S_{\mathrm{p}}), \quad \widetilde{G}(z) = \widetilde{G_{\mathrm{h}}}(z) + \widetilde{G_{\mathrm{p}}}(z).$$



Green's function for non-interacting systems

- System of non-interacting electrons subjected to an effective potential V

$$H_{0,N} = \sum_{i=1}^{N} \left(-\frac{1}{2}\Delta_{\mathbf{r}_i} + V(\mathbf{r}_i) \right) \text{ on } \mathcal{H}_N, \qquad h_1 = -\frac{1}{2}\Delta + V \text{ on } \mathcal{H}_1.$$

- **Assumptions**
  - h_1 has at least N negative eigenvalues $\varepsilon_1 \leqslant \varepsilon_2 \leqslant \cdots \leqslant \varepsilon_N$
  - Stability condition $\varepsilon_N < \varepsilon_{N+1}$

$\rightarrow$ Chemical potential of the non-interacting system $\varepsilon_N < \mu_0 < \varepsilon_{N+1}$

- Ground state $\Phi_N^0 = \phi_1 \wedge \cdots \wedge \phi_N$ and $\gamma_{0,N}^0 = \mathbb{1}_{(-\infty,\mu_0)}(h_1) = \sum_{i=1}^{N} |\phi_i\rangle\langle\phi_i|$

Green's function of the non-interaction system

Hole and particle Green's function

$$\widetilde{G_{0,\mathrm{h}}}(z) = \gamma_{0,N}^0 (z - h_1)^{-1}, \qquad \widetilde{G_{0,\mathrm{p}}}(z) = (1 - \gamma_{0,N}^0)(z - h_1)^{-1}$$

Total Green's function

$$\widetilde{G_0}(z) = (z - h_1)^{-1}$$

Dynamical Hamiltonian and self-energy

- Non-interacting system: $\widetilde{G_0}(z) = (z - h_1)^{-1}$
- Interacting system: in analogy with non-interacting systems, $\widetilde{G}(z) = (z - \widetilde{H}(z))^{-1}$

Dynamical Hamiltoninan $\widetilde{H}(z)$

For all $z \in \mathbb{C} \setminus (S_{\mathrm{h}} \cup S_{\mathrm{p}})$, $\widetilde{H}(z) = z - G(z)^{-1}$ is a well-defined closed operator on $\mathcal{H}_1$, with dense domain $\widetilde{D}(z)$ such that $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$.

- Eigenvalues = quasi-energies
- Eigenfunctions = quasi-particles

- Assume that chemical potentials of interacting/non-interacting systems equal

$$\mu = \mu_0$$

Definition of the self-energy

$$\forall z \in \mathbb{U} \cup \mathbb{L} \cup (\mu - a, \mu + b), \quad \widetilde{\Sigma}(z) = \widetilde{H}(z) - h_1 = \widetilde{G_0}(z)^{-1} - \widetilde{G}(z)^{-1} \quad \text{(Dyson equation)}$$

Some GW methods

The GW road map

- **Basis:** Dyson equation on the imaginary axis $\mu + \mathrm{i}\mathbb{R}$

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{\Sigma}(\mu + \mathrm{i}\omega) = \widetilde{G_0}(\mu + \mathrm{i}\omega)^{-1} - \widetilde{G}(\mu + \mathrm{i}\omega)^{-1}$$

- **Road map**
  - Construct a good non-interacting model for $\widetilde{G_0}(\mu + \mathrm{i}\omega)$
    - Hartree Hamiltonian (in the original paper)
    - Kohn-Sham Hamiltonian (DFT)
  - Use an approximation of the self-energy $\widetilde{\Sigma} \approx \widetilde{\Sigma^{\mathrm{GW}}}$ on the axis $\mu + \mathrm{i}\mathbb{R}$.
  - Define $\widetilde{G^{\mathrm{GW}}}(\mu + \mathrm{i}\omega)$ from the Dyson equation with $\widetilde{\Sigma^{\mathrm{GW}}}(\mu + \mathrm{i}\omega)$ as

$$\widetilde{G}(\mu + \mathrm{i}\omega) = \left(\widetilde{G_0}(\mu + \mathrm{i}\omega)^{-1} - \widetilde{\Sigma}(\mu + \mathrm{i}\omega)\right)^{-1} = \left(\mu + \mathrm{i}\omega - h_1 - \widetilde{\Sigma}(\mu + \mathrm{i}\omega)\right)^{-1}.$$

- **Choice of the approximations** $\left(\widetilde{\Sigma^{\mathrm{GW}}}, \widetilde{G^{\mathrm{GW}}}\right)$?

$\rightarrow$ Hedin's equations[1]

[1] L. Hedin. Phys. Rev., 139, 1965

Hedin's equations[2]

- **Kernel** of a space-time operator A

$$A(12) = A(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \left[A(t_1 - t_2)\right](\mathbf{r}_1, \mathbf{r}_2)$$

- Coulomb operator $v_c(\mathbf{r}, \mathbf{r}') = \dfrac{1}{|\mathbf{r} - \mathbf{r}'|}$

Hedin's equations

- Dyson equation $G^{\mathrm{GW}}(12) = G_0(12) + \int d(34) G_0(13) \Sigma(34) G^{\mathrm{GW}}(42)$
- Self-energy $\Sigma^{\mathrm{GW}}(12) = \mathrm{i} G^{\mathrm{GW}}(12) W^{\mathrm{GW}}(21^+)$
- Screened interaction $W^{\mathrm{GW}}(12) = v_{\mathrm{c}}(12) + \int d(34) v_{\mathrm{c}}(13) P^{\mathrm{GW}}(34) W^{\mathrm{GW}}(42)$
- Irreducible polarization $P^{\mathrm{GW}}(12) = -\mathrm{i} G^{\mathrm{GW}}(12) G^{\mathrm{GW}}(21)$

[2] As written by physicists... as horrible this may be!

Hedin's equation: self-consistent solutions

- Find $\left(\Sigma^{\mathrm{GW}}, G^{\mathrm{GW}}\right)$ such that
  - Dyson equation $G^{\mathrm{GW}}(12) = G_0(12) + \int d(34) G_0(13) \Sigma(34) G^{\mathrm{GW}}(42)$
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- **Flow chart of the self-consistent GW scheme**

$$G_0 \xrightarrow{G^{k=0} = G_0} G^{k=0}$$

Initialization

Hedin's equation: self-consistent solutions

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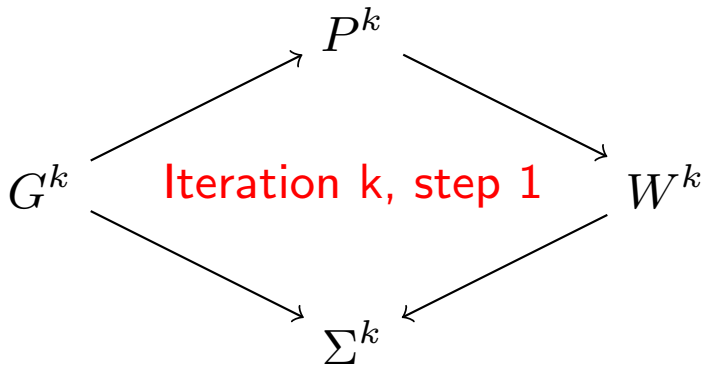
G_0



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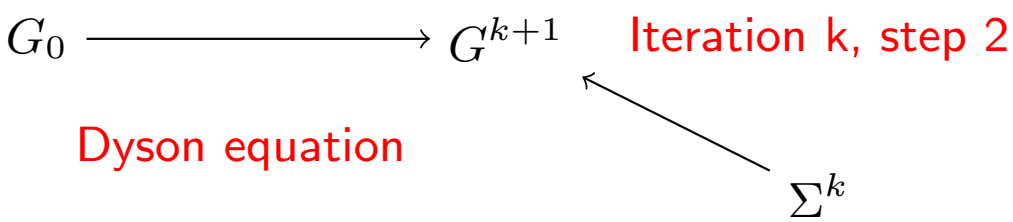

Hedin's equation: the GW^0 method

- Mathematical difficulties in the study of the fully self-consistent GW method
- Simplification: fix the screened interaction to W^0

The GW^0 method

Find $\left(\Sigma^{\mathrm{GW}^0}, G^{\mathrm{GW}^0}\right)$ such that

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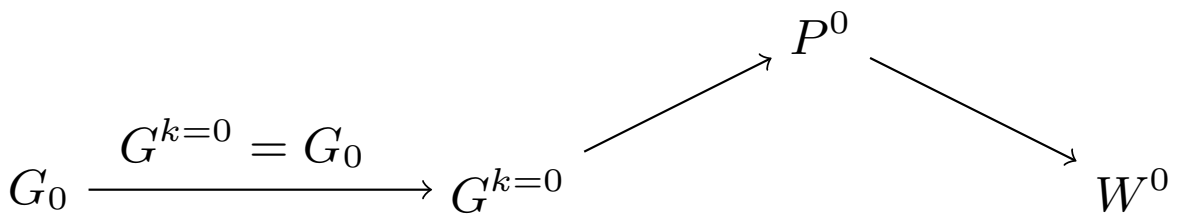

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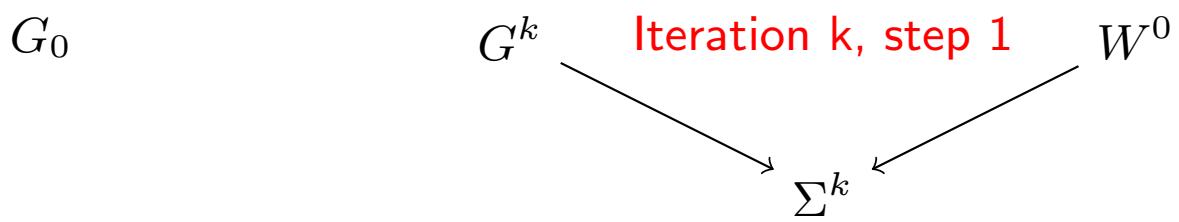

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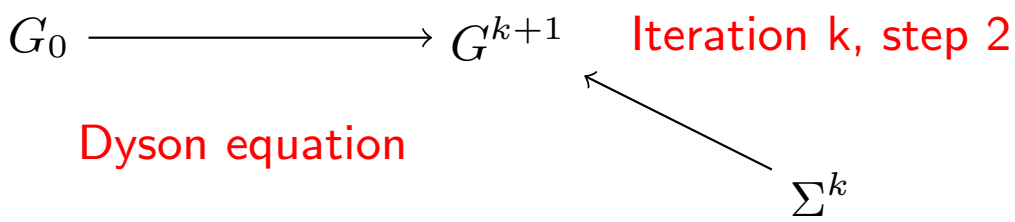


- **Mathematical analysis?**

The dynamically screened operator W

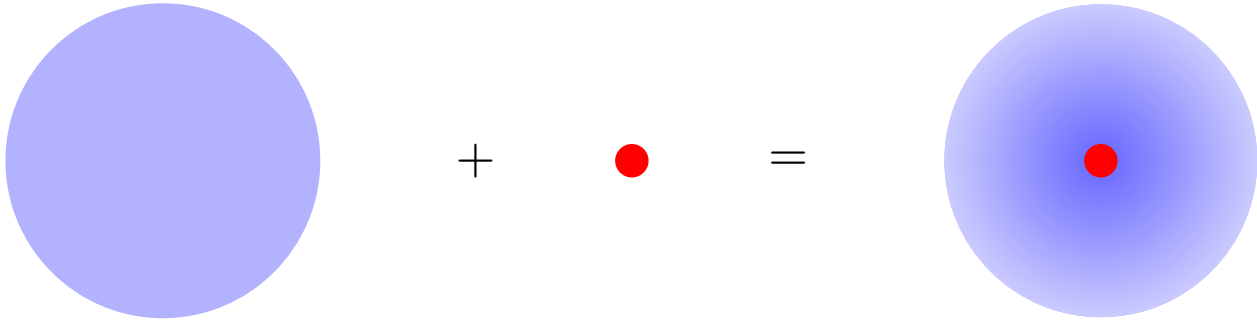
- In the vacuum, a time-dependent charge $\delta\rho(\mathbf{r},t)$ creates a potential

$$\delta V(\mathbf{r}',t) = \int_{\mathbb{R}^3} \frac{1}{|\mathbf{r}-\mathbf{r}'|}\delta\rho(\mathbf{r},t)\mathrm{d}\mathbf{r}, \quad \text{or} \quad \delta V = \delta_0(t) v_{\mathrm{c}}(\delta\rho)$$

- In a molecule, a time-dependent charge $\delta\rho(\mathbf{r},t)$ creates a potential

$$\begin{aligned}\delta V(\mathbf{r}',t) &= \int_{\mathbb{R}^3}\int_{-\infty}^{t} W(\mathbf{r}t,\mathbf{r}'t')\delta\rho(\mathbf{r},t')\,\mathrm{d}\mathbf{r}\,\mathrm{d}t' \\ &= \delta_0(t) v_c\left(\delta\rho\right) + \int_{\mathbb{R}^3}\int_{-\infty}^{t} W_c(\mathbf{r}t,\mathbf{r}'t')\delta\rho(\mathbf{r},t')\,\mathrm{d}\mathbf{r}\,\mathrm{d}t'\end{aligned}$$

- Screening effect



- Dynamically screened operator W^0 calculated from Hartree Hamiltonian (RPA):

$$W^0(\tau) = \delta_0(\tau) v_c + W_c^0(\tau)$$

The GW^0 approximation of the self-energy

- Formally $\Sigma^{\mathrm{app}}(12) = \mathrm{i}G^{\mathrm{app}}(12)W^0(21^+)$

$$\Sigma^{\mathrm{app}}(\mathbf{r},\mathbf{r}';\tau) = \mathrm{i}\delta_0(\tau)G_{\mathrm{h}}^{\mathrm{app}}(\mathbf{r},\mathbf{r}';0^-)v_c(\mathbf{r},\mathbf{r}') + \mathrm{i}G^{\mathrm{app}}(\mathbf{r},\mathbf{r}';\tau)W_c^0(\mathbf{r}',\mathbf{r};-\tau)$$
$$= \underbrace{-\frac{\gamma_N^{\mathrm{app}}(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\delta_0(\tau)}_{\text{Fock term}} + \mathrm{i}G^{\mathrm{app}}(\mathbf{r},\mathbf{r}';\tau)W_c^0(\mathbf{r}',\mathbf{r};-\tau).$$

- Definition of $C = A \odot B$ by the kernel product $C(\mathbf{r},\mathbf{r}') = A(\mathbf{r},\mathbf{r}')B(\mathbf{r}',\mathbf{r})$?

$$\langle f|C|g\rangle = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \overline{f}(\mathbf{r})C(\mathbf{r},\mathbf{r}')g(\mathbf{r}')\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \overline{f}(\mathbf{r})A(\mathbf{r},\mathbf{r}')g(\mathbf{r}')B(\mathbf{r}',\mathbf{r})\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'$$
$$= \mathrm{Tr}_{\mathcal{H}_1}\left(AgB\overline{f}\right)$$

Kernel-product (infinite dimensional Hadamard product)

For $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_1)$, the operator $A \odot B$ defined by the quadratic form

$$(f,g) \mapsto \langle f|A \odot B|g\rangle := \mathrm{Tr}_{\mathcal{H}_1}\left(AgB\overline{f}\right)$$

- In practice, $\Sigma^{\mathrm{app}}(\tau) = K_x\delta_0(\tau) + \mathrm{i}G^{\mathrm{app}}(\tau) \odot W_c^0(-\tau)$ with $K_x(\mathbf{r},\mathbf{r}') := -\dfrac{\gamma_{0,N}^0(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$

Reformulation by an analytical continuation

- The equation $\Sigma^{\mathrm{app}}(\tau) := K_x \delta_0(\tau) + \mathrm{i} G^{\mathrm{app}}(\tau) \odot W_c^0(-\tau)$ is formally equivalent to

$$\widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) = K_x - \frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{app}}}\big(\mu_0 + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\, \mathrm{d}\omega'$$

The GW^0 equations on the imaginary frequency axis

Find $G^{\mathrm{GW}^0} \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ solution to the system

$$(\mathrm{GW}^0) \quad \begin{cases} \widetilde{\Sigma^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega) = K_x - \dfrac{1}{2\pi} \displaystyle\int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{GW}^0}}\big(\mu_0 + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\, \mathrm{d}\omega', \\ \widetilde{G^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega) = \left[\mu_0 + \mathrm{i}\omega - \left(h_1 + \widetilde{\Sigma^{\mathrm{GW}^0}}(\mu_0 + \mathrm{i}\omega)\right)\right]^{-1} \end{cases}$$

- For all $\widetilde{G^{\mathrm{app}}} \in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$ and all $\omega \in \mathbb{R}_\omega$, the operator

$$\widetilde{\Sigma_c^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{app}}}\big(\mu_0 + \mathrm{i}(\omega + \omega')\big) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\, \mathrm{d}\omega'$$

is a well-defined bounded operator on $\mathcal{H}_1$

The GW^0 approximation in a perturbative regime

- **Problem:** for $\widetilde{G^{\mathrm{app}}}(\mu_0 + \mathrm{i}\cdot)$ close to $\widetilde{G_0}(\mu_0 + \mathrm{i}\cdot)$ in $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$, is the operator

$$\mu_0 + \mathrm{i}\omega - \left(h_1 + \widetilde{\Sigma^{\mathrm{app}}}(\mu_0 + \mathrm{i}\omega)\right)$$

invertible? Replace v_{c} by λv_{c}...

$$(\mathrm{GW}^0_\lambda) \quad \begin{cases} \widetilde{\Sigma^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega) = K_x - \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{+\infty} \widetilde{G^{\mathrm{GW}^0_\lambda}}\left(\mu_0 + \mathrm{i}(\omega+\omega')\right) \odot \widetilde{W_c^0}(\mathrm{i}\omega')\,\mathrm{d}\omega', \\ \widetilde{G^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega) = \left[\mu_0 + \mathrm{i}\omega - \left(h_1 + \lambda\widetilde{\Sigma^{\mathrm{GW}^0_\lambda}}(\mu_0 + \mathrm{i}\omega)\right)\right]^{-1} \end{cases}$$

Theorem (Gontier, Cancs, Stoltz)

There exists $\lambda_* > 0$ such that, for all $0 \leqslant \lambda \leqslant \lambda_*$, there is a unique solution $\widetilde{G^{\mathrm{GW}^0_\lambda}}$ to the problem (GW^0_λ) in the vicinity of $\widetilde{G_0}$.
Moreover, the self-consistent procedure starting from $\widetilde{G_0}$ converges geometrically fast toward $\widetilde{G^{\mathrm{GW}^0_\lambda}}$ in $L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$.

Conclusion and perspectives

Conclusion and perspectives

- **Current results**
  - The fundamental objects (G, G_0, Σ, W_0) involved in GW^0 formalism are mathematically well-defined
  - Some of their properties have been rigorously proved
  - The GW^0 equations are well-posed in a perturbative regime

- **Work in progress**
  - Analysis of the fully self-consistent GW method for periodic crystals

E. Cancès, D. Gontier and G. Stoltz, A mathematical analysis of the GW0 method for computing electronic excited state energies of molecules, *ar*Xiv preprint **1506.01737** (2015)