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

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June 17, 2015

Nuclear configuration $\{\mathbf{R}_k\}_{1\leq k\leq N}$:

$$v_{\text{ext}}(\mathbf{r}) := \sum_{k=1}^{M} \frac{-z_k}{|\mathbf{r}-\mathbf{R}_k|}.$$

Electronic problem with N-electrons

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

$|\Psi(\mathbf{r}_1,\dots\mathbf{r}_N)|^2$ is the probability density of observing electron 1 at $\mathbf{r}_1$, electron 2 at $\mathbf{r}_2$, ...

Pauli principle for fermions: $\forall p \in \mathfrak{S}_N,\ \Psi(\mathbf{r}_{p(1)},\dots\mathbf{r}_{p(N)}) = \epsilon(p)\Psi(\mathbf{r}_1,\dots\mathbf{r}_N)$.

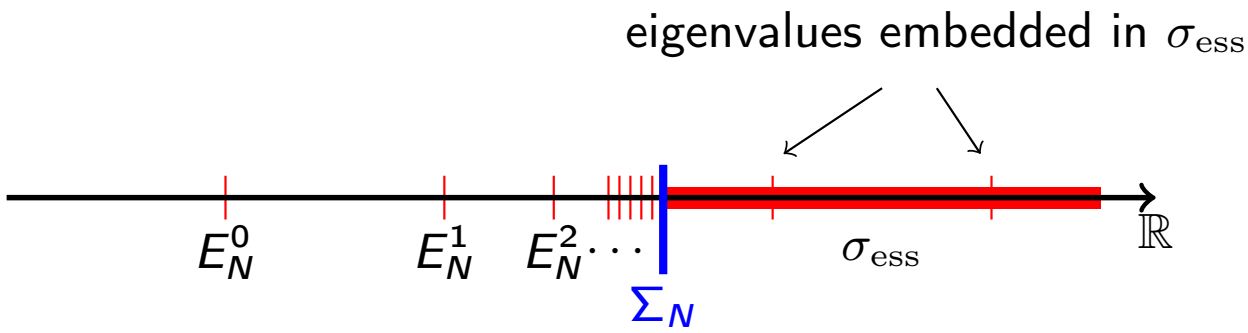
State space

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

Zhislin's theorem

G.M. Zhislin. Trudy Moskov. Mat. Obsc., 9, 1960.

If $N \leq Z := \sum_{k=1}^{M} z_k$, then $\sigma(H_N)$ is as follows:



Moreover, if $N \geq 2$, $\Sigma_N = E_{N-1}^0 < 0$ (HVZ theorem).

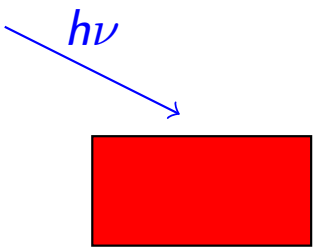
Assumptions

- E_N^0 is a simple eigenvalue of H_N, $H_N \Psi_N^0 = E_N^0 \Psi_N^0$, $\|\Psi_N^0\|_{L^2} = 1$
- Stability of the N-particle system: $2E_N^0 < E_{N+1}^0 + E_{N-1}^0$

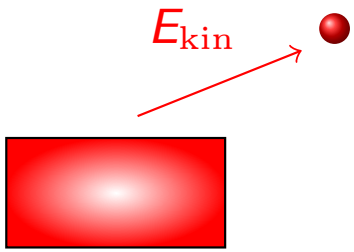
We would like to compute the electronic excitation energies of such a system:
$\Longrightarrow$ quantities of the form

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

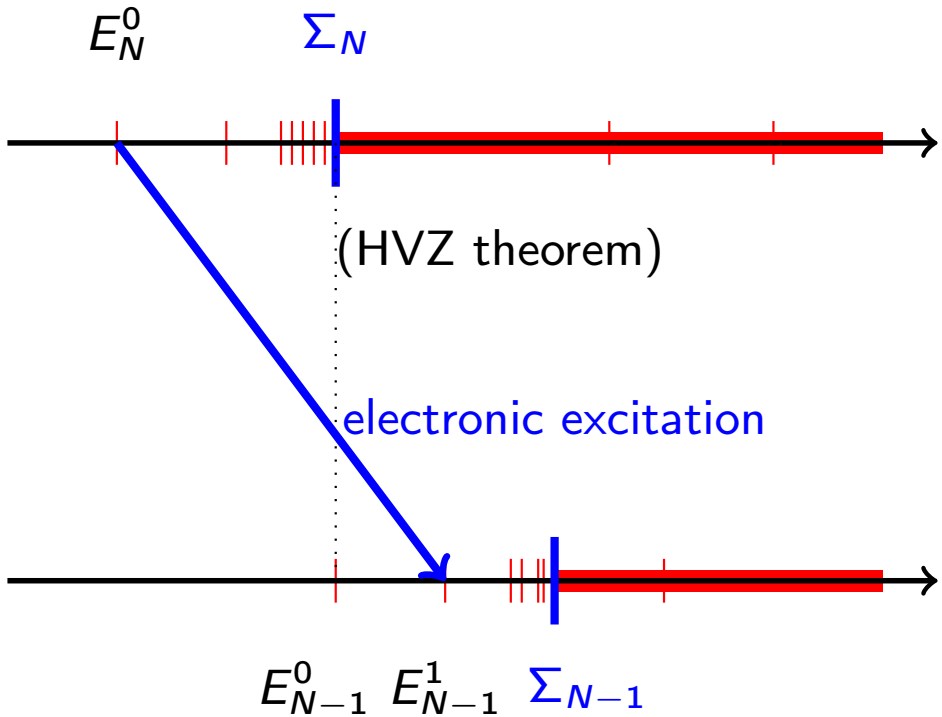
Inverse photoemission spectroscopy (IPES)



System with N particles



System with $N-1$ particles



Computation of the 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 $N \rightarrow \infty$

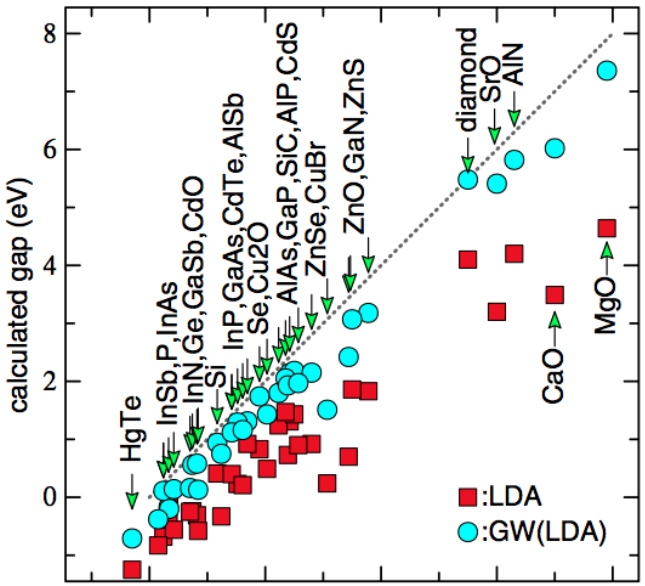


Figure: Band gaps for LDA and GW.

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

Definition of the Particle Green's function in the time domain

Fock space

$$\mathbb{F} := \bigoplus_{N=0}^{+\infty} \mathcal{H}_N, \qquad \mathcal{H}_0 = \mathbb{C}, \qquad \mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C}), \qquad \mathcal{H}_N = \bigwedge^N \mathcal{H}_1.$$

Annihilation and creation operators

$$a \in \mathcal{B}(\mathcal{H}_1, \mathcal{B}(\mathbb{F})), \qquad a^\dagger \in \mathcal{B}(\mathcal{H}_1, \mathcal{B}(\mathbb{F})),$$

$$\forall \phi \in \mathcal{H}_1, \qquad a(\phi) : \mathcal{H}_N \to \mathcal{H}_{N-1}, \qquad a^\dagger(\phi) : \mathcal{H}_N \to \mathcal{H}_{N+1}, \qquad a^\dagger(\phi) = (a(\phi))^*,$$

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

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

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

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) (bis)

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

Definition of the Particle Green's function in the frequency domain

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

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

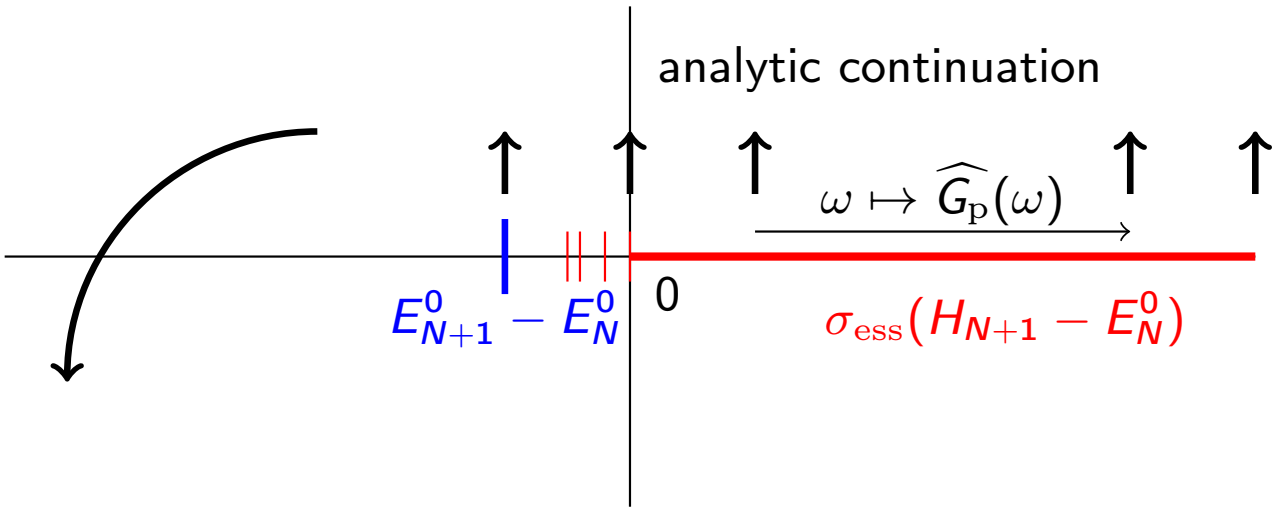
- Particle electronic excited state energies can be recovered from $\widehat{G_{\mathrm{p}}}$
- $\widehat{G_{\mathrm{p}}}$ is highly irregular
- $(\omega \mapsto \mathrm{Im}\ \left(\widehat{G_{\mathrm{p}}}(\omega)\right)$ is an observable)

Definition of the Particle Green's function in the complex frequency domain

Remark

There exists an analytical continuation $\widetilde{G_{\mathrm{p}}}$ *of* $\widehat{G_{\mathrm{p}}}$ *on* $\mathbb{U} = \{z \in \mathbb{C}, Im\,(z) > 0\}$. *This continuation can also be extended to* $\mathbb{C} \setminus S_{\mathrm{p}}$.

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



Definition of the one-body Hole Green's function

Annihilation and creation operators (ter)

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

In the time domain

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

Properties

From the hole or the total Green's function, we can recover the following quantities:

- One-body electronic ground-state density matrix: $\gamma_N^0 = -\mathrm{i}G_{\mathrm{h}}(0^-) = A_-^* A_-$

$$\gamma_N^0(\mathbf{r}, \mathbf{r}') = N \int_{\mathbb{R}^{3(N-1)}} \Psi_N^0(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \, \Psi_N^0(\mathbf{r}', \mathbf{r}_2, \cdots, \mathbf{r}_N) \, d\mathbf{r}_2 \cdots d\mathbf{r}_N,$$

- Electronic ground state density

$$\rho_N^0(\mathbf{r}) = N \int_{\mathbb{R}^{3(N-1)}} |\Psi_N^0(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2 \, d\mathbf{r}_2 \cdots d\mathbf{r}_N$$

- Ground state energy (Galiskii-Migdal formula)

  V.M. Galitskii and A.B. Midgal. Sov. Phys. JETP, 139, 1958.

$$E_N^0 = \frac{1}{2} \mathrm{Tr}_{\mathcal{H}_1} \left[\left(\frac{d}{d\tau} - \mathrm{i} \left(-\frac{1}{2}\Delta + v_{\mathrm{ext}} \right) \right) G_{\mathrm{h}}(\tau) \Big|_{\tau = 0^-} \right]$$

- Hole electronic excited state energies

The hole Green's function in the frequency domain

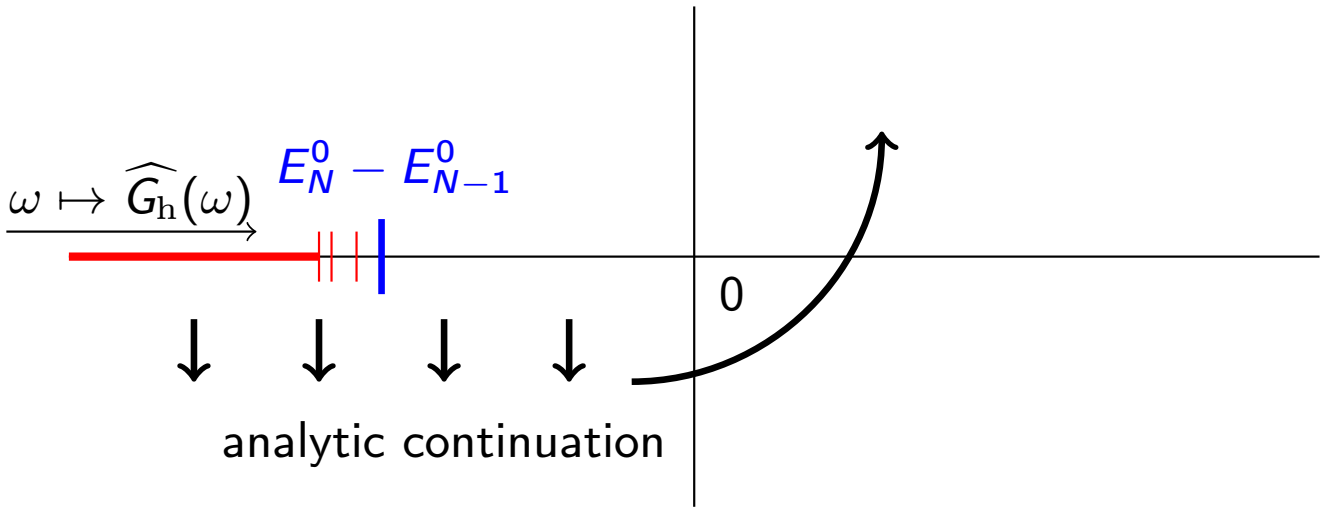
$$\widehat{G_{\mathrm{h}}}(\omega) = \left(\mathcal{F}_t G_{\mathrm{h}}\right)(\omega), \quad \widehat{G_{\mathrm{h}}} \in H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$$

Key point

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

In the complex frequency domain

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



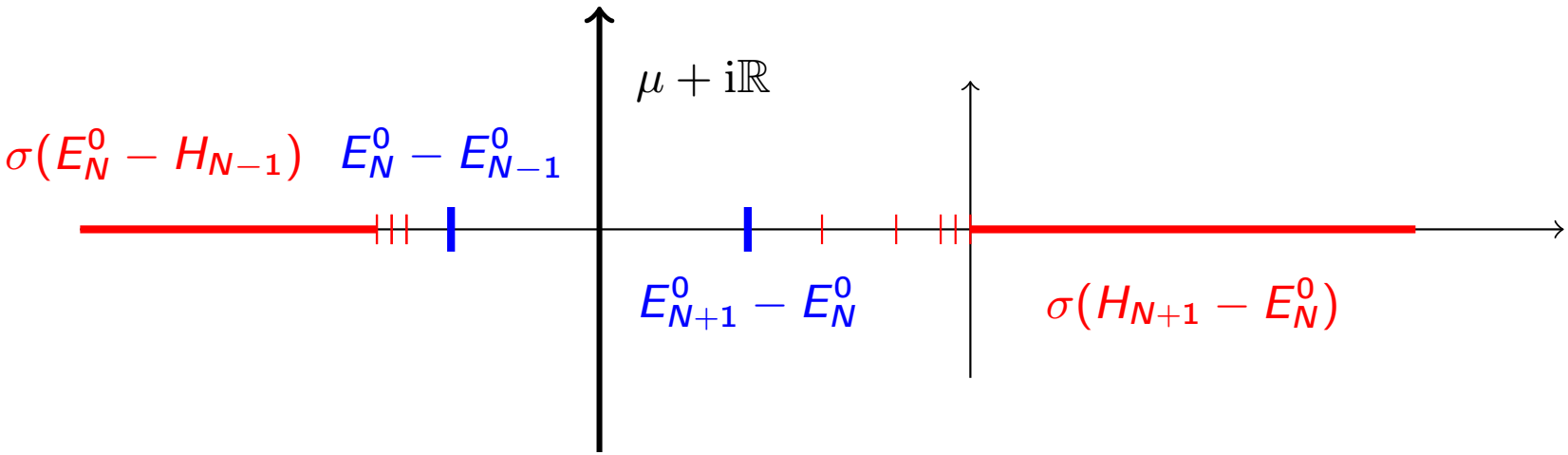
Definition of the total Green's function

Chemical potential μ

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

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 $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_N$
- Stability condition: It holds $\varepsilon_N < \varepsilon_{N+1}$

Chemical potential of the non-interacting system μ_0

$$\varepsilon_N < \mu_0 < \varepsilon_{N+1}.$$

Ground state of the non-interacting system

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

Green's function of the non-interaction system

$$\widetilde{G_{0,\mathrm{h}}}(z) = \gamma_{0,N}^0 (z - h_1)^{-1}, \quad \widetilde{G_{0,\mathrm{p}}}(z) = (1 - \gamma_{0,N}^0)(z - h_1)^{-1}, \quad \boxed{\widetilde{G_0}(z) = (z - h_1)^{-1}.}$$

Dynamical Hamiltonian

Non-interacting system: $\widetilde{G_0}(z) = (z - h_1)^{-1}$

Interacting system: $\widetilde{G}(z) = (z - \widetilde{H}(z))^{-1}$, $\widetilde{H}(z)$: dynamical Hamiltonian

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

Lemma

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 $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$.

Assumption

- The chemical potential of the interacting system and of the non-interacting system can be chosen equal:

$$\boxed{\mu = \mu_0.}$$

Self-energy

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

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

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

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 $\widetilde{\Sigma^{\mathrm{GW}}}(\mu + \mathrm{i}\omega)$

$$\forall \omega \in \mathbb{R}_\omega, \quad \widetilde{G}(\mu + \mathrm{i}\omega) = \left(\widetilde{G_0}(\mu + \mathrm{i}\omega)^{-1} - \widetilde{\Sigma}(\mu + \mathrm{i}\omega)\right)^{-1} = \left(\mu + \mathrm{i}\omega - h_1 - \widetilde{\Sigma}(\mu + \mathrm{i}\omega)\right)^{-1}.$$

Choice of $\left(\widetilde{\Sigma^{\mathrm{GW}}}, \widetilde{G^{\mathrm{GW}}}\right)$: The Hedin's equations (L. Hedin. Phys. Rev., 139, 1965.)

Kernel of a space-time operator A

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

The Hedin's equations

- Dyson equation

$$G(12) = G_0(12) + \int d(34) G_0(13) \Sigma(34) G(42)$$

- Self-energy

$$\Sigma(12) = i \int d(34) G(13) W(41^+) \Gamma(32; 4)$$

- Screened interaction

$$W(12) = v_c(12) + \int d(34) v_c(13) P(34) W(42)$$

- Irreducible polarization

$$P(12) = -i \int d(34) G(13) G(41^+) \Gamma(34; 2)$$

- Vertex function

$$\Gamma(12; 3) = \delta(12)\delta(13) + \int d(4567) \frac{\delta \Sigma(12)}{\delta G(45)} G(46) G(75) \Gamma(67; 3)$$

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The GW equations

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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$$\Sigma^{\mathrm{GW}}(12) = iG^{\mathrm{GW}}(12) W^{\mathrm{GW}}(21^+)$$

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$$P^{\mathrm{GW}}(12) = -iG^{\mathrm{GW}}(12) G^{\mathrm{GW}}(21)$$

Flow chart of the self-consistent GW scheme

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

Initialization

The GW equations

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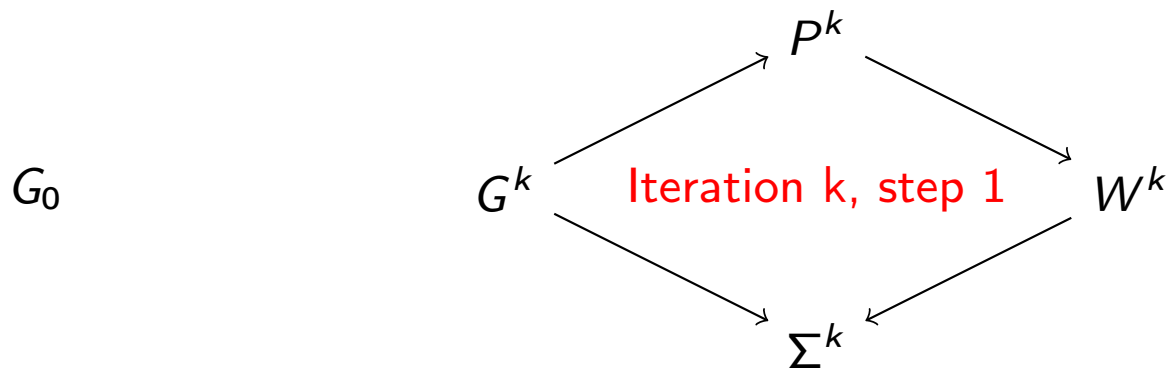

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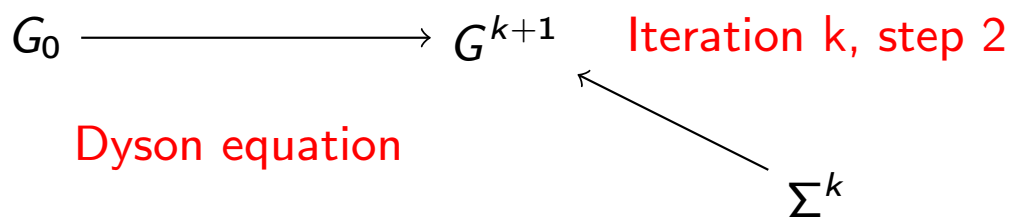

The GW^0 equations:

$$\boxed{\text{Fix } W^k = W^0}$$

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

- Dyson equation

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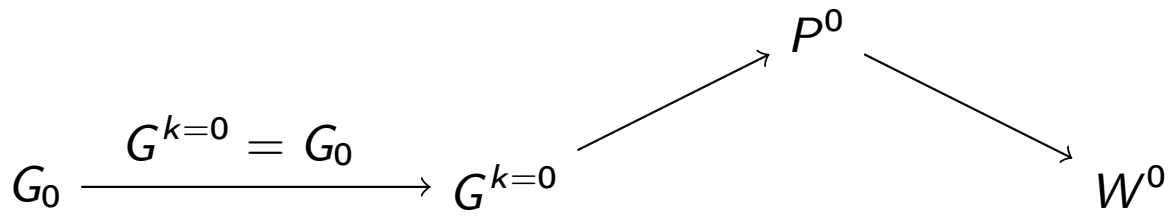

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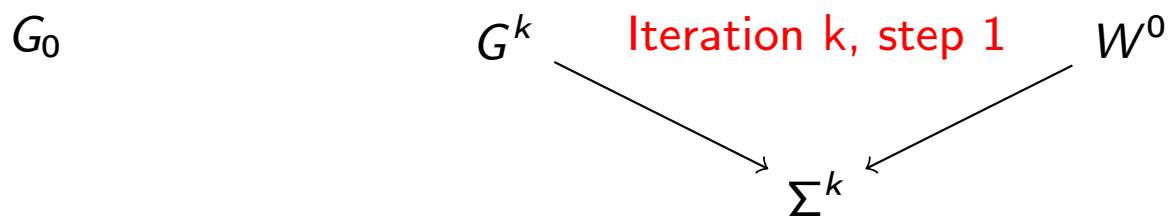

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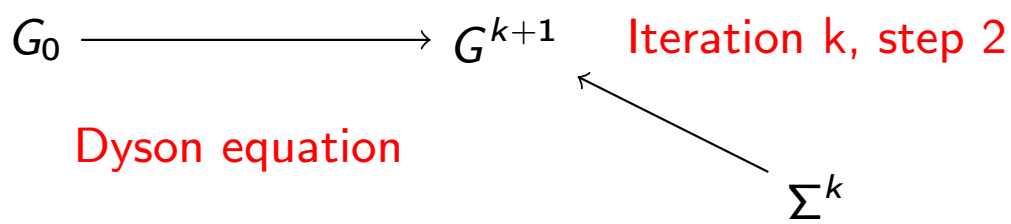

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Next part of the talk

- Explain the operator W and W^0
- Explain the "multiplication" of type $A(12)B(21)$
- Transform the GW^0 equations on the time axis $\mathbb{R}_\tau$ into formally equivalent GW^0 equations on the imaginary frequency axis $\mu + \mathrm{i}\mathbb{R}_\omega$

The dynamically screened operator W

The Coulomb operator

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

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

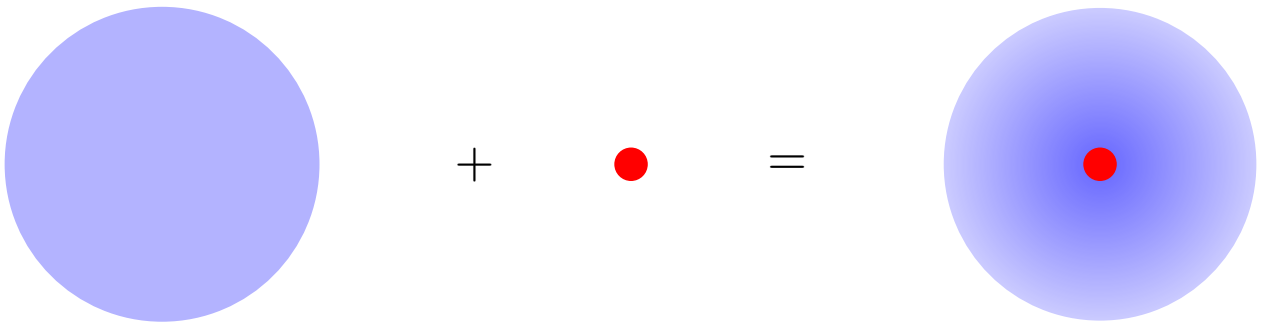
$$\boxed{v_c(\mathbf{r}, \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|} \quad \text{Coulomb operator}}$$

The dynamically screened operator

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

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

Screening effect



The dynamically screened operator W^0

Calculated from the Hartree Hamiltonian:

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

GW^0 approximation of the self-energy

$$\Sigma^{\mathrm{app}}(12) = iG^{\mathrm{app}}(12)W^0(21^+)$$

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

Kernel-product (infinite dimensional Hadamard product)

For $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_1)$,

$$C = A \odot B \quad \text{with} \quad C(\mathbf{r},\mathbf{r}') = A(\mathbf{r},\mathbf{r}')B(\mathbf{r}',\mathbf{r}).$$

In practice

$$\boxed{\Sigma^{\mathrm{app}}(\tau) = K_x \delta_0(\tau) + \mathrm{i}G^{\mathrm{app}}(\tau) \odot W_c^0(-\tau), \quad \text{with} \quad K_x(\mathbf{r},\mathbf{r}') := -\frac{\gamma_{0,N}^0(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}.}$$

Analytical continuation method

Equation

$$\forall \tau \in \mathbb{R}_\tau, \quad \Sigma^{\mathrm{app}}(\tau) := K_x \delta_0(\tau) + \mathrm{i} G^{\mathrm{app}}(\tau) \odot W_c^0(-\tau)$$

is formally equivalent to

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

The GW^0 equations in the imaginary frequency axis

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

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

with

$$K_x(\mathbf{r}, \mathbf{r}') = -\frac{\gamma_{0,N}^0(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}.$$

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

Lemma

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 $\mathcal{H}_1$.

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?

The GW^0 approximation in a perturbative regime

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

Theorem (DG, Cancès, Stoltz)

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

Conclusion

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
- How to recover $\mathrm{Im}\ \widehat{G_{\mathrm{p}}^{\mathrm{GW}^0}}$ and $\mathrm{Im}\ \widehat{G_{\mathrm{h}}^{\mathrm{GW}^0}}$ from $\omega \mapsto \widetilde{G^{\mathrm{GW}^0}}(\mu + \mathrm{i}\omega)$

Infinite dimensional Hadamard product

Hadamard product for matrices

If $A = (a_{ij})_{1\leq i,j\leq N} \in \mathcal{M}_{N\times N}(\mathbb{C})$ and $B = (b_{ij})_{1\leq i,j\leq N} \in \mathcal{M}_{N\times N}(\mathbb{C})$,

$$C := A \odot B = (c_{ij})_{1\leq i,j\leq N} \quad \text{with} \quad c_{ij} = a_{ij} b_{ji}$$

Hadamard product for operators, the formal definition

$A = A(\mathbf{r}, \mathbf{r}') \in \mathcal{B}(\mathcal{H}_1)$ and $B = B(\mathbf{r}, \mathbf{r}') \in \mathcal{B}(\mathcal{H}_1)$

$$C = A \odot B \quad \text{with} \quad C(\mathbf{r}, \mathbf{r}') = A(\mathbf{r}, \mathbf{r}') B(\mathbf{r}', \mathbf{r}).$$

Formally, for $f, g \in \mathcal{H}_1$,

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

Definition

The kernel-product of $A \in \mathcal{B}(\mathcal{H}_1)$ and $B \in \mathcal{B}(\mathcal{H}_1)$ is the operator $A \odot B$ defined by the quadratic form

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