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

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Goal: compute the electronic excitation energies of a finite electronic system (molecule).

Nuclear configuration (Born-Oppenheimer approximation): \( \{ \mathbf{R}_k \}_{1 \leq k \leq N} \):

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

Electronic problem with \( N \)-electrons

\[
H_N \Psi := \left( -\frac{1}{2} \sum_{i=1}^{N} \Delta r_i + \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|} + \sum_{i=1}^{N} \nu_{\text{ext}}(r_i) \right) \Psi(r_1, \ldots, r_N) = E \Psi(r_1, \ldots, r_N).
\]

\(|\Psi(r_1, \ldots, r_N)|^2\) is the probability density of observing electron 1 at \( r_1 \), electron 2 at \( r_2 \), ...

Pauli principle for fermions: \( \forall p \in S_N, \; \Psi(r_{p(1)}, \ldots, r_{p(N)}) = \epsilon(p) \Psi(r_1, \ldots, r_N) \).

State space

\[
\Psi \in \mathcal{H}_N := \bigwedge_{1}^{N} \mathcal{H}_1, \quad \mathcal{H}_1 = L^2(\mathbb{R}^3, \mathbb{C}).
\]

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

\[
\begin{align*}
E_N^0 & \quad E_N^1 & \quad E_N^2 & \cdots & \quad \sigma_{\text{ess}} \\
\end{align*}
\]

\( \sum_N \)

Ground state: \( \Psi_N^0 \in \mathcal{H}_N \) such that \( \| \Psi_N^0 \| = 1 \) and \( H_N \Psi_N^0 = E_N^0 \Psi_N^0 \).

Problem: \( \mathcal{H}_N \subset L^2(\mathbb{R}^{3N}) \) is a huge space. (Curse of dimensionality)

\[
H_2 \quad (N = 2) \quad H_2O \quad (N = 10) \quad C_8H_{10}N_4O_2 \quad (N = 102)
\]

\( \Rightarrow \) Several approximations were proposed in the last decades.

- Density functional theory (DFT): for ground state properties only
- 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.
The GW method (L. Hedin. Phys. Rev. 1965)

To calculate the electronic excitation energies of a system $\implies$ quantities of the form

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

Inverse photoemission spectroscopy (IPES)

System with $N$ electrons

System with $N + 1$ electrons

(HVZ theorem)

electronic excitation

$$E_N^0 \quad \Sigma_N$$

$$E_{N+1}^0 \quad E_{N+1}^1 \quad \Sigma_{N+1}$$
**The GW method** (L. Hedin. Phys. Rev. 1965)

To calculate the **electronic excitation energies** of a system $\Longrightarrow$ quantities of the form

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

**Photoemission spectroscopy (PES)**

- System with $N$ electrons
- System with $N - 1$ electrons

$\Sigma_N$ (HVZ theorem)

Electronic excitation

$E_N^0$, $E_{N-1}^0$, $E_{N-1}^1$, $\Sigma_{N-1}$
Definition of the Particle Green’s function in the time domain

Fock space

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

Annihilation and creation operators

\[ a \in \mathcal{B}(\mathcal{H}_1, \mathcal{B}(\mathbb{F})), \quad a^\dagger \in \mathcal{B}(\mathcal{H}_1, \mathcal{B}(\mathbb{F})), \]

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

\[ \forall \Psi \in \mathcal{H}_N, \quad (a(\phi)\Psi)(r_1, \ldots, r_{N-1}) = \sqrt{N} \int_{\mathbb{R}^3} \phi(r) \Psi(r, r_1, \ldots, r_{N-1}) \, dr. \]

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

\[ \forall \tau \in \mathbb{R}, \forall f, g \in \mathcal{H}_1, \quad \langle g | G_p(\tau) | f \rangle = -i \Theta(\tau) \left\langle \Psi^0_N \left| a(g)e^{-i\tau(H_{N+1}-E_0^N)}a^\dagger(f) \right| \Psi^0_N \right\rangle. \]

Annihilation and creation operators (bis)

\[ A^*_+ \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{N+1}) : f \mapsto a^\dagger(f) | \Psi^0_N \rangle, \quad A_+ = (A^*_+)^* \in \mathcal{B}(\mathcal{H}_{N+1}, \mathcal{H}_1). \]

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

\[ \forall \tau \in \mathbb{R}, \quad G_p(\tau) = -i \Theta(\tau) A_+ e^{-i\tau(H_{N+1}-E_0^N)} A^*_+. \]
Definition of the Particle Green’s function in the frequency domain

\[ \forall \tau \in \mathbb{R}, \quad G_p(\tau) = -i \Theta(\tau) A_+ e^{-i \tau (H_{N+1} - E_0^N)} A^*_+. \]

Normalization convention for the time-Fourier transform

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

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

\[ \hat{G}_p(\omega) = (\mathcal{F}_T G_p)(\omega), \quad \hat{G}_p \in H^{-1}(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)). \]

Key point

The support of the distribution \( \text{Im} \left( \hat{G}_p \right) \) is contained in the particle electronic excitation set \( S_p := \sigma(H_{N+1} - E_0^N) \).

- Particle electronic excited energies can be recovered from \( \hat{G}_p \),
- \( \hat{G}_p \) is highly irregular.
Laplace transform of the Green’s function For \( z \in U = \{ z \in \mathbb{C}, \text{Im} \ (z) > 0 \} \), define

\[
\tilde{G}_p(z) := \int_0^\infty G_p(\tau)e^{iz\tau} \, d\tau.
\]

Remark

- \( \tilde{G}_p \) is an analytical continuation of \( \hat{G}_p \) on \( U \) (Titchmarsh’s theory).
- This continuation can be extended to \( \mathbb{C} \setminus S_p \).

\[
\forall z \in \mathbb{C} \setminus S_p, \quad \tilde{G}_p(z) = A_+ \left( \frac{1}{z - (H_{N+1} - E_0^N)} \right) A_+^*.
\]
Definition of the one-body hole Green’s function

Annihilation and creation operators (ter)

\[ A^- \in \mathcal{B}(\mathcal{H}_1, \mathcal{H}_{N-1}) : f \mapsto a(\bar{f})|\psi^0_N\rangle, \quad A^*^- \in \mathcal{B}(\mathcal{H}_{N-1}, \mathcal{H}_1). \]

In the time domain

\[
\forall \tau \in \mathbb{R}, \quad G_h(\tau) = i\Theta(-\tau)A^*^- e^{i\tau(H_{N-1} - E^0_N)} A^-.
\]

Properties

From the hole Green’s function, we can recover the following quantities:

- **One-body electronic ground-state density matrix:**

\[
\gamma^0_N = -iG_h(0^-) = A^*^- A^- \\
\gamma^0_N(\mathbf{r}, \mathbf{r}') = N \int_{\mathbb{R}^{3(N-1)}} \psi^0_N(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \psi^0_N(\mathbf{r}', \mathbf{r}_2, \cdots, \mathbf{r}_N) \, d\mathbf{r}_2 \cdots d\mathbf{r}_N,
\]

- **Electronic ground state density**

\[
\rho^0_N(\mathbf{r}) = N \int_{\mathbb{R}^{3(N-1)}} |\psi^0_N(\mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2 \, d\mathbf{r}_2 \cdots d\mathbf{r}_N,
\]

- **Ground state energy** (Galiskii-Migdal formula)


\[
E^0_N = \frac{1}{2} \mathrm{Tr}_{\mathcal{H}_1} \left[ \left( \frac{d}{d\tau} - i \left( -\frac{1}{2} \Delta + \nu_{\text{ext}} \right) \right) G_h(\tau) \right|_{\tau=0^-}.
\]
The hole Green’s function in the frequency domain

\[ \hat{G}_h(\omega) = (\mathcal{F}_T G_h)(\omega), \quad \hat{G}_h \in H^{-1}(\mathbb{R}\omega, \mathcal{B}(\mathcal{H})). \]

Key point

The support of the distribution \( \text{Im}(\hat{G}_h) \) is contained in the hole electronic excitation set \( S_h := \sigma(E^0_N - H^0_{N-1}) \).

In the complex frequency domain

\[ \forall z \in \mathbb{C} \setminus S_h, \quad \hat{G}_h(z) = A^* \left( \frac{1}{z - (E^0_N - H^0_{N-1})} \right) A_- . \]
Definition of the total Green’s function

Assumption: Stability condition

\[ 2E_N^0 < E_{N+1}^0 + E_{N-1}^0. \]

Chemical potential \( \mu \)

\[ E_N^0 - E_{N-1}^0 < \mu < E_{N+1}^0 - E_N^0. \]

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

\[ \forall z \in \mathbb{C} \setminus (S_h \cup S_p), \quad \tilde{G}(z) = \tilde{G}_h(z) + \tilde{G}_p(z). \]
Green’s function for non-interacting systems

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

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

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 $\mu_0$

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

Ground state of the non-interacting system

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

Green’s function of the non-interaction system

$$\widetilde{G}_{0,h}(z) = \gamma_{0,N}^0(z - h_1)^{-1}, \quad \widetilde{G}_{0,p}(z) = (1 - \gamma_{0,N}^0)(z - h_1)^{-1}, \quad \widetilde{G}_0(z) = (z - h_1)^{-1}.$$
Dynamical Hamiltonian

Non-interacting system: \( \tilde{G}_0(z) = (z - h_1)^{-1} \).

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

- Eigenvalues = quasi-energies,
- Eigenfunctions = quasi-particles.

Lemma

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

Assumption

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

\[
\mu = \mu_0.
\]

Self-energy

\( \forall z \in U \cup U \cup U (\mu - a, \mu + b) \), \( \tilde{\Sigma}(z) = \tilde{H}(z) - h_1 = \tilde{G}_0(z)^{-1} - \tilde{G}(z)^{-1} \) (Dyson equation).

\[
\tilde{H}(z) = h_1 + \tilde{\Sigma}(z).
\]
Dyson equation on the imaginary axis $\mu + i\mathbb{R}$

\[
\forall \omega \in \mathbb{R}, \quad \tilde{\Sigma} (\mu + i\omega) = \tilde{G}_0 (\mu + i\omega)^{-1} - \tilde{G} (\mu + i\omega)^{-1}
\]

Road map

- Construct a good non-interacting model for $\tilde{G}_0 (\mu + i\omega)$
  - Hartree Hamiltonian (in the original paper)
  - Kohn-Sham Hamiltonian (DFT)
- Use an approximation of the self-energy $\tilde{\Sigma} \approx \tilde{\Sigma}^{GW}$ on the axis $\mu + i\mathbb{R}$.
- Define $\tilde{G}^{GW} (\mu + i\omega)$ from the Dyson equation with $\tilde{\Sigma}^{GW} (\mu + i\omega)$

\[
\tilde{G}^{GW} (\mu + i\omega) = \left( \tilde{G}_0 (\mu + i\omega)^{-1} - \tilde{\Sigma}^{GW} (\mu + i\omega) \right)^{-1} = \left( \mu + i\omega - h_1 - \tilde{\Sigma}^{GW} (\mu + i\omega) \right)^{-1}.
\]
Choice of \( (\Sigma^{GW}, \tilde{G}^{GW}) \)? The Hedin’s equations (L. Hedin. Phys. Rev., 139, 1965.)

Kernel of a space-time operator \( A \)

\[
A(12) = A(r_1, t_1; r_2, t_2) = [A(t_1 - t_2)](r_1, r_2).
\]

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**
  
  \[
  \Gamma(12; 3) = \delta(12) \delta(13) + \int d(4567) \frac{\delta \Sigma(12)}{\delta G(45)} G(46) G(75) \Gamma(67; 3).
  \]
The $GW^0$ equations:

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

- Dyson equation

\[
G^{GW^0}(12) = G_0(12) + \int d(34) G_0(13) \Sigma^{GW^0}(34) G^{GW^0}(42),
\]

- Self-energy

\[
\Sigma^{GW^0}(12) = i G^{GW^0}(12) W^0(21).
\]

$W^0$ is the ($GW^0$ approximation of the) dynamically screened operator.

Flow chart of the self-consistent $GW^0$ scheme

\[
\begin{array}{c}
G_0 \\
\xrightarrow{G^{k=0} = G_0} \\
\xrightarrow{G^{k=0}} \\
\xrightarrow{W^0}
\end{array}
\]

Initialization
The $GW^0$ equations:
Find $\left( \Sigma^{GW^0}, G^{GW^0} \right)$ such that

- Dyson equation

$$G^{GW^0}(12) = G_0(12) + \int d(34) G_0(13) \Sigma^{GW^0}(34) G^{GW^0}(42),$$

- Self-energy

$$\Sigma^{GW^0}(12) = i G^{GW^0}(12) W^0(21).$$

$W^0$ is the ($GW^0$ approximation of the) dynamically screened operator.

Flow chart of the self-consistent $GW^0$ scheme

\[
\begin{array}{c}
G_0 \quad G^k \quad \text{Iteration k, step 1} \quad W^0 \\
\downarrow \quad \Sigma^k \quad \downarrow
\end{array}
\]
The $GW^0$ equations:
Find $\left(\Sigma^{GW^0}, G^{GW^0}\right)$ such that

- **Dyson equation**
  
  \[ G^{GW^0}(12) = G_0(12) + \int d(34)G_0(13)\Sigma^{GW^0}(34)G^{GW^0}(42), \]

- **Self-energy**
  
  \[ \Sigma^{GW^0}(12) = iG^{GW^0}(12)W^0(21). \]

$W^0$ is the ($GW^0$ approximation of the) dynamically screened operator.

Flow chart of the self-consistent $GW^0$ scheme

\[ G_0 \rightarrow G^{k+1}_{G0} \quad \text{Iteration k, step 2} \]

Dyson equation

\[ \Sigma^k \]
The GW\(^0\) equations:
Find \((\Sigma^{GW\(^0\)}, G^{GW\(^0\)})\) such that

- Dyson equation
  \[
  G^{GW\(^0\)}(12) = G_0(12) + \int d(34) G_0(13) \Sigma^{GW\(^0\)}(34) G^{GW\(^0\)}(42),
  \]

- Self-energy
  \[
  \Sigma^{GW\(^0\)}(12) = i G^{GW\(^0\)}(12) W^0(21).
  \]

\(W^0\) is the \((GW\(^0\) approximation of the) dynamically screened operator.

Next step: give a sense to these equations

- Define the multiplication \(A(12)B(21)\),
- Study the operator \(W^0\),
- Transform the GW\(^0\) equations on the time axis \(\mathbb{R}_\tau\) into formally equivalent GW\(^0\) equations on the imaginary frequency axis \(\mu + i\mathbb{R}_\omega\).
The kernel product (infinite dimensional Hadamard product)

How to define an operator \( C \) such that \( C(r, r') = A(r, r')B(r', r) \)?

Associated quadratic form

\[
\forall f, g \in \mathcal{H}_1, \quad \langle f|C|g \rangle_{\mathcal{H}_1} = \iint_{\mathbb{R}^2} \overline{f}(r)C(r, r')g(r')drdr'
= \iint_{\mathbb{R}^2} A(r, r')g(r')B(r', r)\overline{f}(r)drdr' = \text{Tr}_{\mathcal{H}_1}(AgB\overline{f})
\]

Definition

The kernel-product of \( A \) and \( B \) is the operator \( A \odot B \), defined by the quadratic form

\[
\forall f, g \in \mathcal{H}_1, \quad \langle f|A \odot B|g \rangle = \text{Tr}_{\mathcal{H}_1}(AgB\overline{f})
\]

Lemma

If \( A \in \mathcal{B}(\mathcal{H}_1) \) and \( B \) is such that,

\[
\forall f, g \in \mathcal{H}_1, \quad gB\overline{f} \in \mathfrak{S}_1(\mathcal{H}_1) \quad \text{with} \quad \|gB\overline{f}\|_{\mathfrak{S}_1} \lesssim \|f\|_{\mathcal{H}_1}\|g\|_{\mathcal{H}_1},
\]

then \( A \odot B \) is a well-defined bounded operator on \( \mathcal{H}_1 \).
The dynamically screened operator $W$

**The Coulomb operator**

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

$$\delta V(r', t) = \int_{\mathbb{R}^3} \frac{1}{|r - r'|} \delta \rho(r, t) \, dr,$$

or

$$\delta V = \delta_0(t) v_c(\delta \rho).$$

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

**The dynamically screened operator**

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

$$\delta V(r', t) = \int_{\mathbb{R}^3} \int_{-\infty}^{t} W(rt, r't') \delta \rho(r, t') \, dr \, dt'$$

$$= \delta_0(t) v_c(\delta \rho) + \int_{\mathbb{R}^3} \int_{-\infty}^{t} W_c(rt, r't') \delta \rho(r, t') \, dr \, dt'.$$

**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

$$\Sigma^{\text{app}}(12) = i G^{\text{app}}(12) W^0(21).$$

$$\Sigma^{\text{app}}(r, r'; \tau) = i \delta_0(\tau) G^{\text{app}}_h(r, r'; 0^-) v_c(r, r') + i G^{\text{app}}(r, r'; \tau) W^0_c(r', r; -\tau)$$

$$= -\frac{\gamma^{\text{app}}_{N}(r, r')}{|r - r'|} \delta_0(\tau) + i G^{\text{app}}(r, r'; \tau) W^0_c(r', r; -\tau).$$

In practice

$$\Sigma^{\text{app}}(\tau) = K_x \delta_0(\tau) + i G^{\text{app}}(\tau) \otimes W^0_c(-\tau), \quad \text{with} \quad K_x(r, r') := -\frac{\gamma^{\text{app}}_{0,N}(r, r')}{|r - r'|}.$$
Analytical continuation method

Equation

\[ \forall \tau \in \mathbb{R}, \quad \Sigma^{\text{app}}(\tau) := K_x \delta_0(\tau) + i G^{\text{app}}(\tau) \otimes W_c^0(-\tau) \]

is formally equivalent to

\[ \Sigma^{\text{app}}(\mu_0 + i \omega) = K_x - \frac{1}{2\pi} \int_{-\infty}^{+\infty} G^{\text{app}}(\mu_0 + i(\omega + \omega')) \otimes \tilde{W}_c^0(i\omega') d\omega'. \]

The \( GW^0 \) equations in the imaginary frequency axis

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

\[
\begin{cases}
\Sigma^{GW^0}(\mu_0 + i \omega) = K_x - \frac{1}{2\pi} \int_{-\infty}^{+\infty} G^{GW^0}(\mu_0 + i\omega + \omega') \otimes \tilde{W}_c^0(i\omega') d\omega', \\
G^{GW^0}(\mu_0 + i \omega) = \left[ \mu_0 + i \omega - \left( h_1 + \Sigma^{GW^0}(\mu_0 + i \omega) \right) \right]^{-1},
\end{cases}
\]

with

\[ K_x(r, r') = -\frac{\gamma_{\mu, \nu}^0(r, r')}{|r - r'|}. \]
\[
\begin{align*}
\Sigma_{GW^0}(\mu_0 + i\omega) &= K_x - \frac{1}{2\pi} \int_{-\infty}^{+\infty} G_{GW^0}(\mu_0 + i(\omega + \omega')) \odot \tilde{W}_c^0(i\omega') \, d\omega', \\
G_{GW^0}(\mu_0 + i\omega) &= \left[ \mu_0 + i\omega - \left( h_1 + \Sigma_{GW^0}(\mu_0 + i\omega) \right) \right]^{-1}
\end{align*}
\]

**Lemma**

*For all \( \tilde{G}_{app}(\mu_0 + i\cdot) \in L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) * and all \( \omega \in \mathbb{R}_\omega *, the operator

\[
\Sigma_{c_{app}}(\mu_0 + i\omega) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \tilde{G}_{app}(\mu_0 + i(\omega + \omega')) \odot \tilde{W}_c^0(i\omega') \, d\omega'
\]

is a well-defined bounded operator on \( \mathcal{H}_1 \).*

**Problem**

*For \( \tilde{G}_{app}(\mu_0 + i\cdot) close to \( \tilde{G}_0(\mu_0 + i\cdot) in L^\infty(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1)) * , is the operator

\[
\mu_0 + i\omega - \left( h_1 + \Sigma_{app}(\mu_0 + i\omega) \right)
\]

invertible?*
The $\text{GW}^0$ approximation in a perturbative regime

\[
\begin{cases}
\Sigma_{\text{GW}^0}^\lambda (\mu_0 + i\omega) = K_x - \frac{1}{2\pi} \int_{-\infty}^{+\infty} G_{\text{GW}^0}^\lambda (\mu_0 + i(\omega + \omega')) \odot \tilde{W}_c^0(i\omega') d\omega',
\end{cases}
\]

\[
\begin{aligned}
G_{\text{GW}^0}^\lambda (\mu_0 + i\omega) &= \left[ \mu_0 + i\omega - \left( h_1 + \lambda \Sigma_{\text{GW}^0}^\lambda (\mu_0 + i\omega) \right) \right]^{-1}.
\end{aligned}
\]

**Theorem (Éric Cancès, DG, Gabriel Stoltz)**

- There exists $\lambda_* > 0$ such that, for all $0 \leq \lambda \leq \lambda_*$, there exists a unique solution $\tilde{G}_{\text{GW}^0}^\lambda$ to the problem $(\text{GW}^0_\lambda)$ which is close to $\tilde{G}_0$.
- Moreover, the self-consistent procedure starting from $\tilde{G}_0$ converges toward $G_{\text{GW}^0}^\lambda$ in $L^2(\mathbb{R}_\omega, \mathcal{B}(\mathcal{H}_1))$. 

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The $\text{GW}^0$ method
Current results

- The fundamental objects \((G, G_0, \Sigma, W_0)\) 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.

Future work

- Perform the same work for periodic systems.
  - with Éric Cancès and Gabriel Stoltz
- Study the speed of convergence with respect to numerical parameters.
- Understand the Bethe-Salpeter equations.

Reference