Green's functions in N-body quantum mechanics
A mathematical perspective

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1. **Linear operators**

2. **Electronic Hamiltonians**

3. **One-body Green's function and self-energy**

4. **The dynamically screened Coulomb operator W**

5. **Hedin's equations and the GW approximation**

A1. Fourier transform

A2. Causal functions, Hilbert transform and Kramers-Kronig relations

1 - Linear operators

References:

- **E.B. Davies, *Linear operators and their spectra*, Cambridge University Press 2007.**
- **B. Helffer, *Spectral theory and its applications*, Cambridge University Press 2013.**
- **M. Reed and B. Simon, *Modern methods in mathematical physics*, Vol. 1, 2nd edition, Academic Press 1980.**

Notation: **in this section, $\mathcal{H}$ denotes a separable complex Hilbert space, $\langle\cdot|\cdot\rangle$ its scalar product, and $\|\cdot\|$ the associated norm.**

The finite dimensional case ($\mathcal{H} = \mathbb{C}^d$)

The spectrum of a matrix $A \in \mathbb{C}^{d\times d}$ is the finite set

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- **there exists a functional calculus for hermitian matrices.**

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Let A be a hermitian matrix of $\mathbb{C}^{d\times d}$ such that

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For any $f : \mathbb{R} \to \mathbb{C}$, the matrix

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Functional calculus can be extended to self-adjoint operators in Hilbert spaces.

Functional calculus is extremely useful in quantum physics, e.g. to define

- **the propagator e^{-itH} associated with a Hamiltonian H;**
- **the density matrix $\dfrac{1}{1+e^{(H-\varepsilon_F)/(k_B T)}}$ of a fermionic system at temperature T and chemical potential (Fermi level) ε_F.**

Bounded linear operators on Hilbert spaces

Definition-Theorem (bounded linear operator). A bounded operator on $\mathcal{H}$ is a linear map $A : \mathcal{H} \to \mathcal{H}$ such that

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Endowed with its norm $\|\cdot\|$ and the $*$ operation, $\mathcal{B}(\mathcal{H})$ is a C*-algebra.

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Definition (extensions of operators). Let A_1 and A_2 be operators on $\mathcal{H}$. A_2 is called an extension of A_1 if $D(A_1) \subset D(A_2)$ and if $\forall u \in D(A_1)$, $A_2 u = A_1 u$.

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Symmetric operators are not very interesting. Only self-adjoint operators represent physical observables and have nice mathematical properties:

- real spectrum;
- spectral decomposition and functional calculus.

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$$D(A^*) = \{v \in \mathcal{H} \mid \exists w_v \in \mathcal{H} \textbf{ s.t. } \forall u \in D(A),\ \langle Au|v\rangle = \langle u|w_v\rangle\}\,.$$

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Case of unbounded operators:

symmetric (easy to check) $\overset{\not\Rightarrow}{\Leftarrow}$ **self-adjoint (sometimes difficult to check)**

Some unbounded self-adjoint operators arising in quantum mechanics

- **position operator along the j axis:**
  - $\mathcal{H} = L^2(\mathbb{R}^d)$,
  - $D(\widehat{r}_j) = \left\{u \in L^2(\mathbb{R}^d) \mid r_j u \in L^2(\mathbb{R}^d)\right\}$, $(\widehat{r}_j \phi)(\mathbf{r}) = r_j \phi(\mathbf{r})$;
- **momentum operator along the j axis:**
  - $\mathcal{H} = L^2(\mathbb{R}^d)$,
  - $D(\widehat{p}_j) = \left\{u \in L^2(\mathbb{R}^d) \mid \partial_{r_j} u \in L^2(\mathbb{R}^d)\right\}$, $(\widehat{p}_j \phi)(\mathbf{r}) = -i\partial_{r_j} \phi(\mathbf{r})$;
- **kinetic energy operator:**
  - $\mathcal{H} = L^2(\mathbb{R}^d)$,
  - $D(T) = H^2(\mathbb{R}^d) := \left\{u \in L^2(\mathbb{R}^d) \mid \Delta u \in L^2(\mathbb{R}^d)\right\}$, $T = -\frac{1}{2}\Delta$;
- **Schrödinger operators in 3D: let $V \in L^2_{\rm unif}(\mathbb{R}^3, \mathbb{R})$ ($V(\mathbf{r}) = -\frac{Z}{|\mathbf{r}|}$ OK)**
  - $\mathcal{H} = L^2(\mathbb{R}^3)$,
  - $D(H) = H^2(\mathbb{R}^3)$, $H = -\frac{1}{2}\Delta + V$.

Linear operators and Green’s functions

Linear operators and Green's functions

Kernel of a linear operator on $L^2(\mathbb{R}^d)$

Let A be a linear operator on $L^2(\mathbb{R}^d)$ with domain $D(A)$.

The kernel of A, if it exists, is the distribution $A(\mathbf{x}, \mathbf{x}')$ such that

$$\forall \phi \in D(A), \quad (A\phi)(\mathbf{x}) = \text{"} \int_{\mathbb{R}^d} A(\mathbf{x}, \mathbf{x}')\, \phi(\mathbf{x}')\, d\mathbf{x}' \text{"}.$$

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If A is invertible, the kernel $G(\mathbf{x}, \mathbf{x}')$ of A^{-1}, if it exists, is called the Green's function of A. The solution u to the equation $Au = f$ then is

$$u(\mathbf{x}) = \text{"} \int_{\mathbb{R}^d} G(\mathbf{x}, \mathbf{x}')\, f(\mathbf{x}')\, d\mathbf{x}' \text{"} \quad \textbf{for a.a. } \mathbf{x} \in \mathbb{R}^d.$$

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Remark: **the Green's functions used in many-body perturbation theory are related to, but are not exactly, this kind of Green's functions.**

Definition-Theorem (spectrum of a linear operator). Let A be a closed[1] linear operator on $\mathcal{H}$.

- **The open set $\rho(A) = \{z \in \mathbb{C} \mid (z - A) \,:\, D(A) \to \mathcal{H}$ invertible$\}$ is called the resolvent set of A.**

[1] **The operator A is called closed if its graph $\Gamma(A) := \{(u, Au),\ u \in D(A)\}$ is a closed subspace of $\mathcal{H} \times \mathcal{H}$.**

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$$\rho(A) \ni z \mapsto R_z(A) := (z - A)^{-1} \in \mathcal{B}(\mathcal{H})$$

is called the resolvent of A. It holds $R_z(A) - R_{z'}(A) = (z' - z) R_z(A) R_{z'}(A)$.

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$$\sigma_{\mathrm{p}}(A) = \{z \in \mathbb{C} \mid (z - A) : D(A) \to \mathcal{H} \text{ non-injective}\} = \{\text{eigenvalues of } A\}$$

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$\mathcal{H}_\mathrm{p}$: **set of bound states,** $\mathcal{H}_\mathrm{c}$: **set of diffusive states**

Diagonalizable self-adjoint operators and Dirac's bra-ket notation

Let A be a self-adjoint operator that can be diagonalized in an orthonormal basis $(e_n)_{n\in\mathbb{N}}$ (this is not the case for many useful self-adjoint operators!).

Dirac's bra-ket notation: $$A = \sum_{n\in\mathbb{N}} \lambda_n |e_n\rangle\langle e_n|, \quad \lambda_n \in \mathbb{R}, \quad \langle e_m|e_n\rangle = \delta_{mn}.$$

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- $\mathcal{H}_{\mathrm{p}} = \mathcal{H}$ **and** $\mathcal{H}_{\mathrm{c}} = \{0\}$ **(no diffusive states);**
- **functional calculus for diagonalizable self-adjoint operators: for all $f:\mathbb{R}\to\mathbb{C}$, the operator $f(A)$ defined by**

$$D(f(A)) = \left\{|u\rangle = \sum_{n\in\mathbb{N}} u_n|e_n\rangle \mid \sum_{n\in\mathbb{N}}(1+|f(\lambda_n)|^2)|u_n|^2 < \infty\rangle\right\}, \quad f(A) = \sum_{n\in\mathbb{N}} f(\lambda_n)|e_n\rangle\langle e_n|$$

is independent of the choice of the spectral decomposition of A.

Theorem **(functional calculus for bounded functions). Let $\mathfrak{B}(\mathbb{R},\mathbb{C})$ be the $*$-algebra of bounded $\mathbb{C}$-valued Borel functions on $\mathbb{R}$ and let A be a self-adjoint operator on $\mathcal{H}$. Then there exists a unique map**

$$\Phi_A : \mathfrak{B}(\mathbb{R},\mathbb{C}) \ni f \mapsto f(A) \in \mathcal{B}(\mathcal{H})$$

satisfies the following properties:

1. **Φ_A is a homomorphism of $*$-algebras:**

   $$(\alpha f + \beta g)(A) = \alpha f(A) + \beta g(A), \quad (fg)(A) = f(A)g(A), \quad \overline{f}(A) = f(A)^*;$$

2. **$\|f(A)\| \le \sup_{x\in\mathbb{R}} |f(x)|$;**

3. **if $f_n(x) \to x$ pointwise and $|f_n(x)| \le |x|$ for all n and all $x \in \mathbb{R}$, then**

   $$\forall u \in D(A), \quad f_n(A)u \to Au \text{ in } \mathcal{H};$$

4. **if $f_n(x) \to f(x)$ pointwise and $\sup_n \sup_{x\in\mathbb{R}} |f_n(x)| < \infty$, then**

   $$\forall u \in \mathcal{H}, \quad f_n(A)u \to f(A)u \text{ in } \mathcal{H};$$

In addition, if $u \in \mathcal{H}$ is such that $Au = \lambda u$, then $f(A)u = f(\lambda)u$.

Theorem (spectral projections and functional calculus - general case -).

Let A be a self-adjoint operator on $\mathcal{H}$.

- **For all $\lambda \in \mathbb{R}$, the bounded operator $P_\lambda^A := \mathbb{1}_{]-\infty,\lambda]}(A)$, where $\mathbb{1}_{]-\infty,\lambda]}(\cdot)$ is the characteristic function of $]-\infty,\lambda]$, is an orthogonal projection.**

- **Spectral decomposition of A: for all $u \in D(A)$ and $v \in \mathcal{H}$, it holds**

$$\langle v|Au\rangle = \int_{\mathbb{R}} \lambda \, d\langle v|P_\lambda^A u\rangle, \quad \textbf{which we denote by} \quad A = \int_{\mathbb{R}} \lambda \, dP_\lambda^A.$$

- **Functional calculus: let f be a (not necessarily bounded) $\mathbb{C}$-valued Borel function on $\mathbb{R}$. The operator $f(A)$ can be defined by**

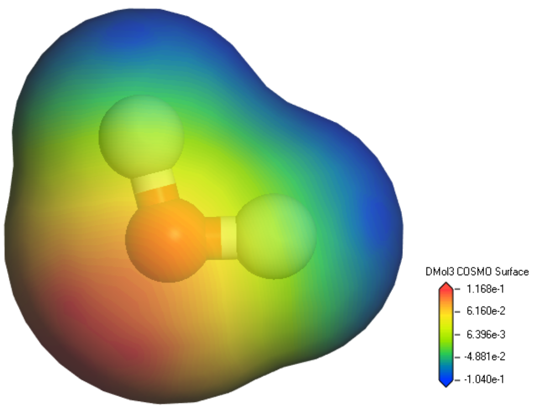
$$D(f(A)) := \left\{ u \in \mathcal{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2 \, d\langle u|P_\lambda^A u\rangle < \infty \right\}$$

and

$$\forall (u,v) \in D(f(A)) \times \mathcal{H}, \; \langle v|f(A)u\rangle := \int_{\mathbb{R}} f(\lambda) \, \langle v|P_{d\lambda}^A u\rangle.$$

2 - Electronic Hamiltonians

Electronic problem for a given nuclear configuration $\{\mathrm{R}_k\}_{1\le k\le M}$



Ex: water molecule H_2O

$M = 3$, $N = 10$, $z_1 = 8$, $z_2 = 1$, $z_3 = 1$

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

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

$|\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_N)|^2$ **probability density of observing electron 1 at r_1, electron 2 at r_2, ...**

$$\forall p \in \mathfrak{S}_N, \quad \Psi(\mathbf{r}_{p(1)},\cdots,\mathbf{r}_{p(N)}) = \varepsilon(p)\Psi(\mathbf{r}_1,\cdots,\mathbf{r}_N), \qquad \textbf{(Pauli principle)}$$

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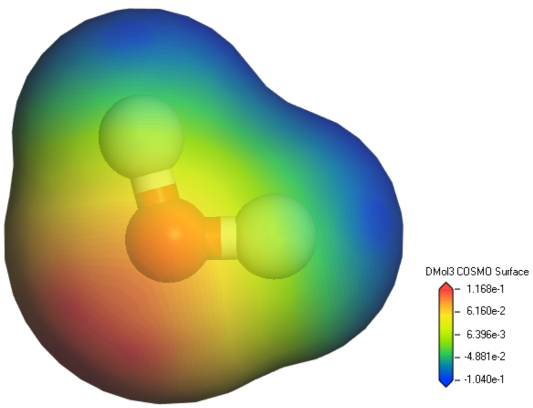

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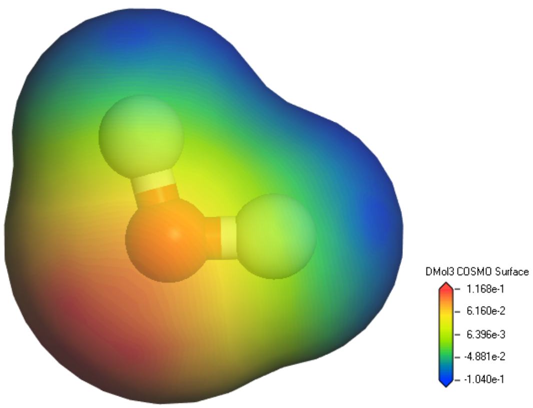

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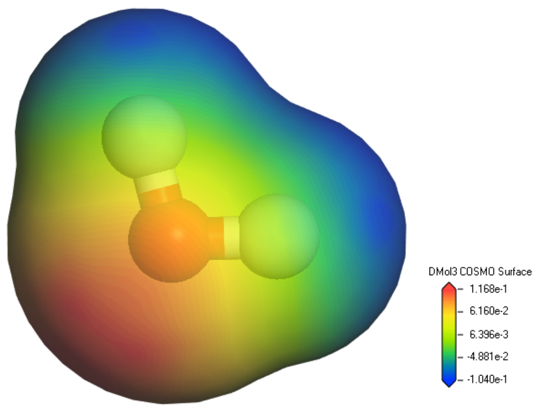

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Theorem (Kato '51). The operator $H_N := -\frac{1}{2}\sum_{i=1}^N \Delta_{\mathbf{r}_i} + \sum_{i=1}^N v_{\rm ext}(\mathbf{r}_i) + \sum_{1\le i<j\le N}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}$ **with domain** $D(H_N) := \mathcal{H}_N \cap H^2(\mathbb{R}^{3N})$ **is self-adjoint on** $\mathcal{H}_N$**.**

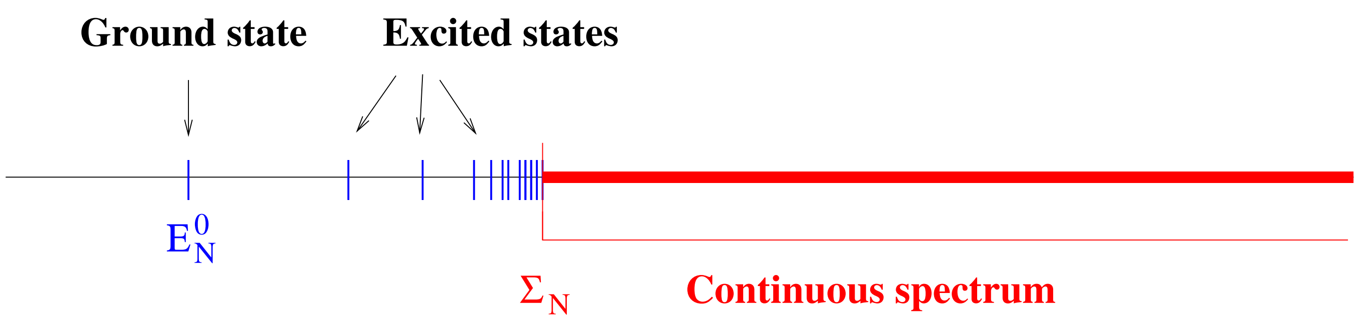
Theorem (spectrum of H_N).

1. HVZ theorem (Hunziger '66, van Winten '60, Zhislin '60)

$\sigma_c(H_N) = [\Sigma_N, +\infty)$ **with** $\Sigma_N = \min \sigma(H_{N-1}) \leq 0$ **and** $\Sigma_N < 0$ **iff** $N \geq 2$.

2. Bound states of neutral molecules and positive ions (Zhislin '61)

If $N \leq Z := \sum_{k=1}^{M} z_k$, **then** H_N **has an infinite number of bound states**.



3. Bound states of negative ions (Yafaev '72)

If $N \geq Z + 1$, **then** H_N **has at most a finite number of bound states.**

Assumptions

1. Non-degeneracy of the N-particle ground state

E_N^0 **is a simple eigenvalue of** $H_N, \quad H_N \Psi_N^0 = E_N^0 \Psi_N^0, \quad \|\Psi_N^0\| = 1.$

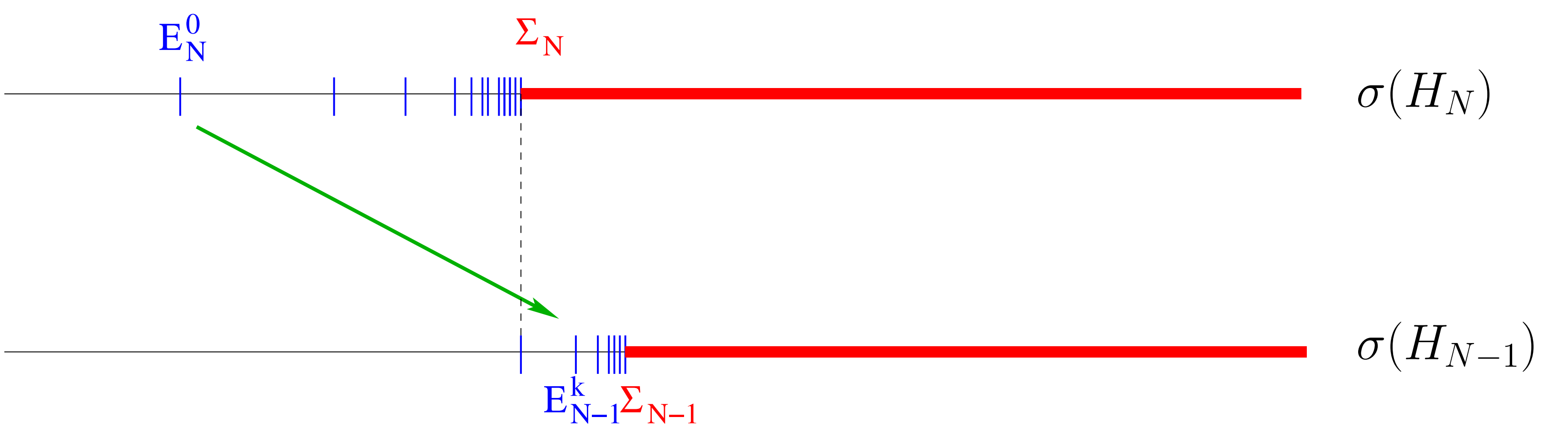
2. Stability of the N-particle system

$$2E_N^0 < E_{N+1}^0 + E_{N-1}^0.$$

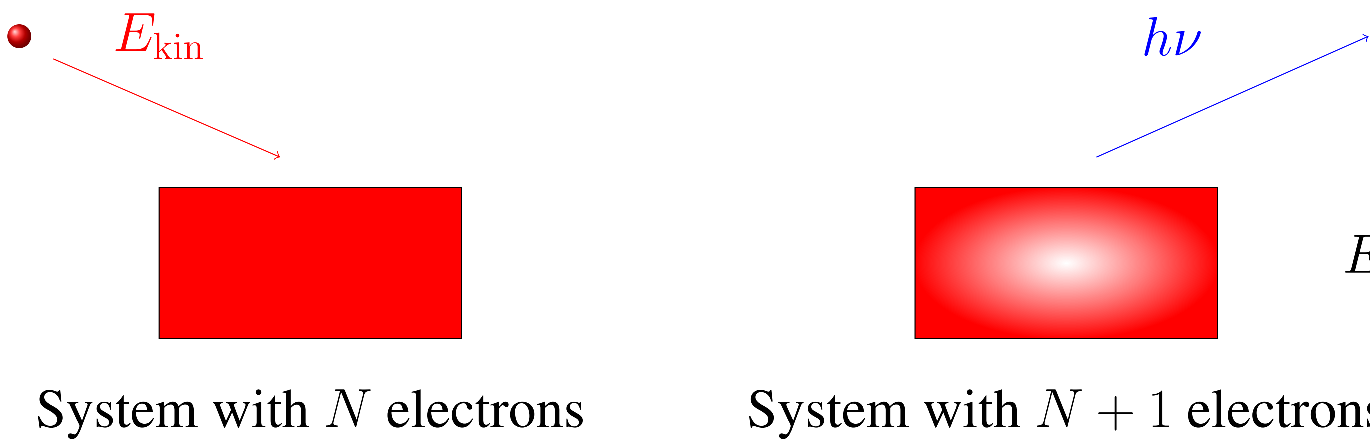
Photoemission spectroscopy (PES)

$$E_{N-1}^k - E_N^0 = h\nu - E_{\mathrm{kin}}$$

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



Inverse photoemission spectroscopy (IPES)



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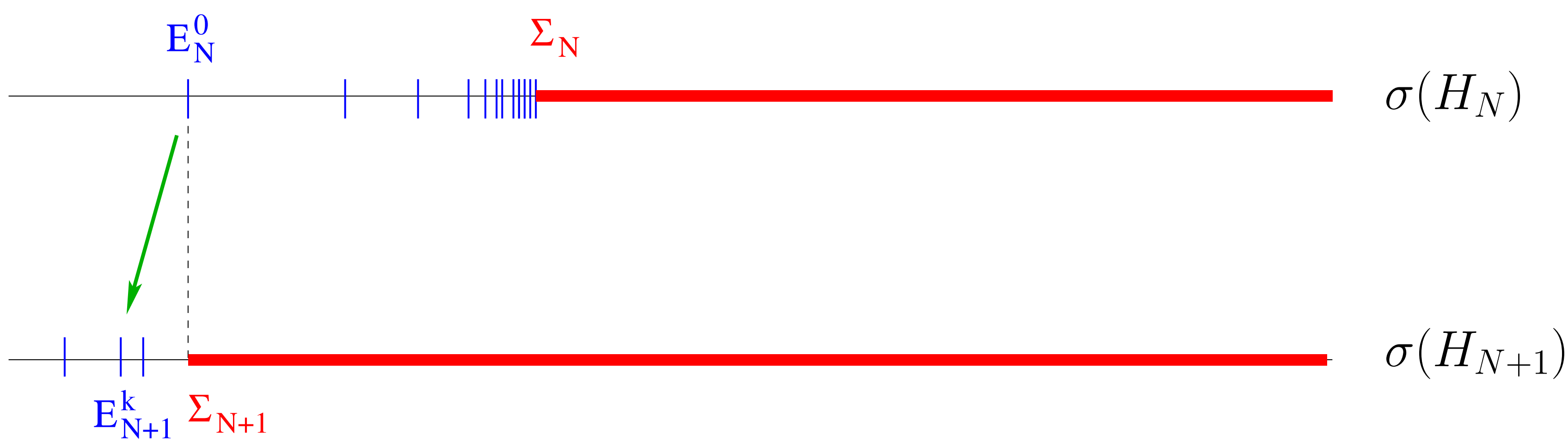

Goal: compute the excitation energies $E^k_{N+1} - E^0_N$ and $E^k_{N-1} - E^0_N$

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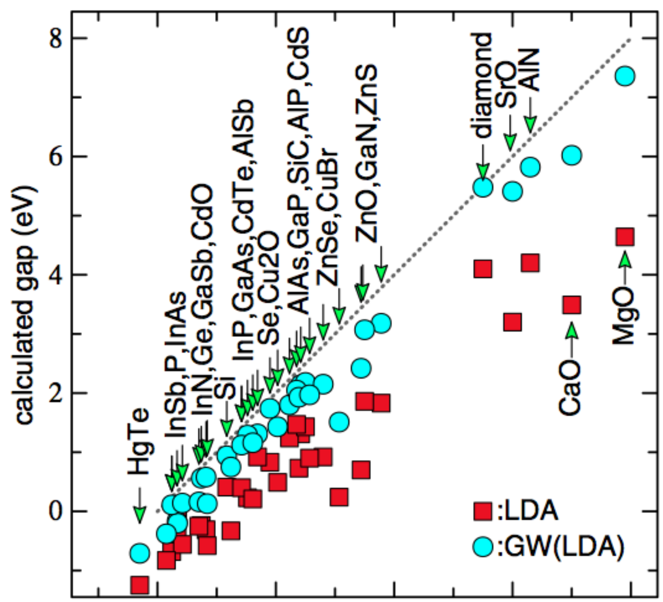
- **GW: decent to very good results (especially for extended systems).**

Electronic excitations for perfect crystals ($N \to +\infty$)



Electronic ground state density

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

One-body electronic ground state density matrix

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

One-body Green's function

$$G(\mathbf{r}, \mathbf{r}', t - t') = -i \langle \Psi_0^N | T(\Psi_{\mathrm{H}}(\mathbf{r}, t) \Psi_{\mathrm{H}}^\dagger(\mathbf{r}', t')) | \Psi_0^N \rangle$$

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

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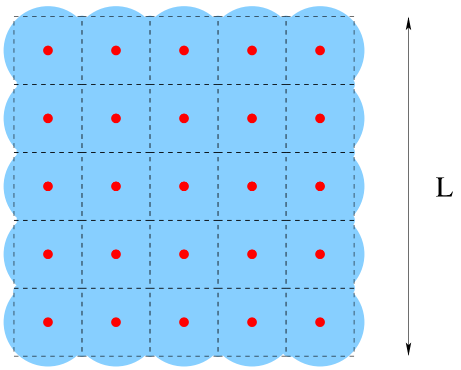
Thermodynamic limit problem (for periodic crystals):



$$\frac{E^0_{ZL^3}}{L^3} \overset{?}{\underset{L\to\infty}{\longrightarrow}} E^0_{\mathrm{per}}, \qquad \rho^0_{ZL^3}(\mathbf{r}) \overset{?}{\underset{L\to\infty}{\longrightarrow}} \rho^0_{\mathrm{per}}(\mathbf{r})$$

$$\gamma^0_{ZL^3}(\mathbf{r}, \mathbf{r}') \overset{?}{\underset{L\to\infty}{\longrightarrow}} \gamma^0_{\mathrm{per}}(\mathbf{r}, \mathbf{r}'), \qquad G(\mathbf{r}, \mathbf{r}', t) \overset{?}{\underset{L\to\infty}{\longrightarrow}} G_{\mathrm{per}}(\mathbf{r}, \mathbf{r}', t).$$

3 - One-body Green's function and self-energy

Let X be a Banach space (typically $X = \mathcal{B}(\mathcal{H}_1)$).

Fourier transform: let $f \in L^1(\mathbb{R}_t, X)$

$$\forall \omega \in \mathbb{R}, \quad [\mathcal{F} f](\omega) = \widehat{f}(\omega) = \int_{-\infty}^{+\infty} f(t)\, e^{i\omega t}\, dt.$$

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The Fourier and Laplace transforms can be extended to some distribution spaces. (extension of the Fourier transform to the space of tempered distributions).

Second quantization formalism (for fermions)

- **Fock space**

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

- **Creation and annihilation operators**

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

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

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

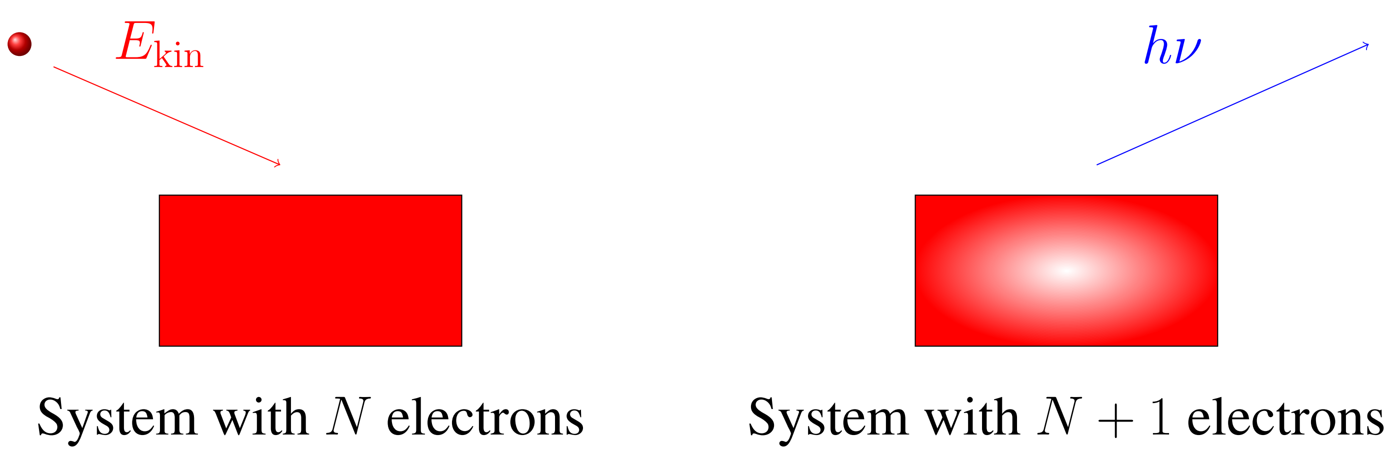
- **Canonical commutation relations (CCR)**

$$\forall \phi, \psi \in \mathcal{H}_1, \quad a(\phi)a(\psi)^\dagger + a(\psi)^\dagger a(\phi) = \langle \phi | \psi \rangle \, \mathrm{Id}_{\mathbb{F}}.$$

Particle Green's function

- **Time representation:** $G_{\rm p} \in L^\infty(\mathbb{R}_t, \mathcal{B}(\mathcal{H}_1))$ **defined by**

$$\forall t \in \mathbb{R}, \quad \forall (f,g) \in \mathcal{H}_1 \times \mathcal{H}_1, \quad \langle g|G_{\rm p}(t)|f\rangle = -i\Theta(t)\langle \Psi_0^N|a(g)e^{-it(H_{N+1}-E_0^N)}a^\dagger(f)|\Psi_0^N\rangle.$$



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

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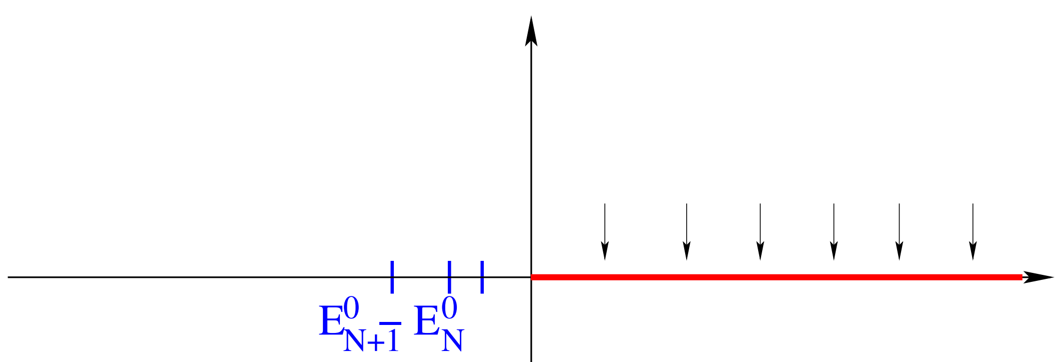
- **Complex plane representation (analytic continuation of the Laplace transform)**

$$\widetilde{G}_{\rm p}(z) = A_+(z-(H_{N+1}-E_N^0))^{-1} A_+^* \qquad \textbf{where} \qquad \begin{array}{rccl} A_+^* : & \mathcal{H}_1 & \to & \mathcal{H}_{N+1} \\ & f & \mapsto & a^\dagger(f)|\Psi_N^0\rangle \end{array}$$

The singularities of $z \mapsto \widetilde{G}_{\rm p}(z)$ are contained in $\sigma(H_{N+1} - E_N^0)$.



Hole Green's function

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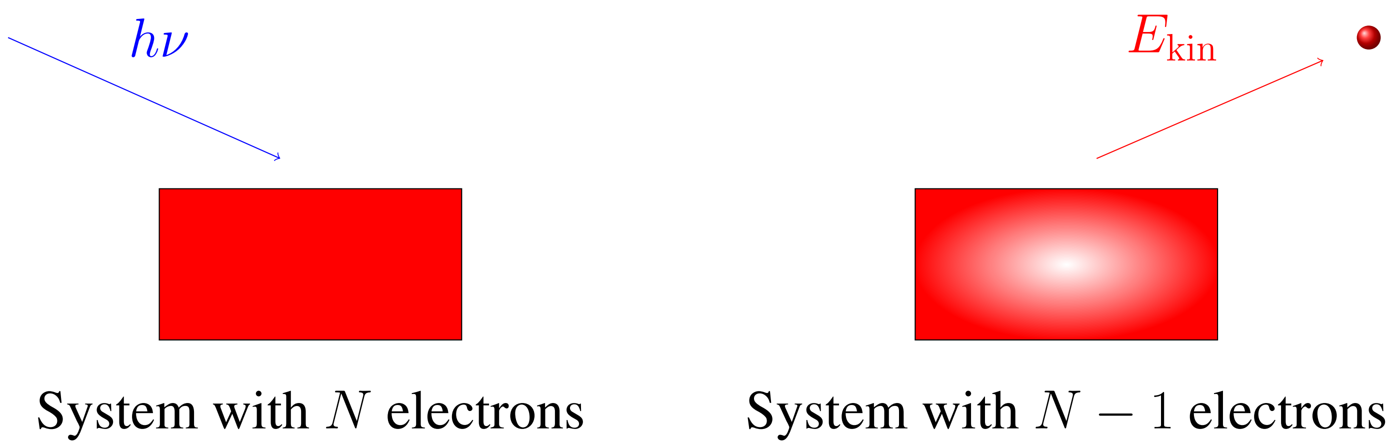

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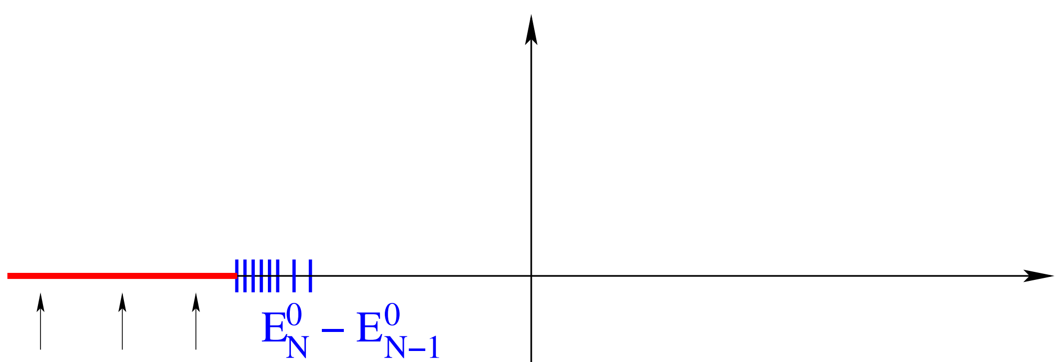

Properties of the particle and hole Green's functions

- **Spectral functions (operator-valued measures on $\mathbb{R}_\omega$)**

$$\forall b \in \mathscr{B}(\mathbb{R}_\omega), \quad \begin{aligned} \mathcal{A}_{\mathrm{p}}(b) &= -\pi^{-1}\Im\widehat{G_{\mathrm{p}}}(b) \\ \mathcal{A}_{\mathrm{h}}(b) &= +\pi^{-1}\Im\widehat{G_{\mathrm{h}}}(b) \\ \mathcal{A}(b) &= \mathcal{A}_{\mathrm{p}}(b) + \mathcal{A}_{\mathrm{h}}(b) \end{aligned}$$

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- **Galitskii-Migdal formula**

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

Green's functions of non-interacting systems

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

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

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(resolvent of h_1 at z)

Dynamical Hamiltonian

Non-interacting systems: $\widetilde{G}_0(z) = (z - h_1)^{-1}$
Interacting systems: $\widetilde{G}(z) = (z - \widetilde{H}(z))^{-1}, \quad \widetilde{H}(z):$ **dynamical Hamiltonian**

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(Dyson equation)

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

Proposition. **Let $z \in \mathbb{C} \setminus \mathbb{R}$. The dynamical Hamiltonian is a well-defined closed unbounded operator on $\mathcal{H}_1$ with dense domain $\widetilde{D}(z) \subset H^2(\mathbb{R}^3)$.**

Self-energy operator

$$\forall z \in \mathbb{C}\setminus\mathbb{R}, \quad \widetilde{\Sigma}(z) := (\widetilde{G}_0(z))^{-1} - (\widetilde{G}(z))^{-1} \quad \Leftrightarrow \quad \widetilde{H}(z) = h_1 + \widetilde{\Sigma}(z).$$

Road map:

1. **construct a non-interacting Green's function $\widetilde{G}_0$ (using e.g. the Kohn-Sham LDA Hamiltonian);**
2. **construct an approximation $\widetilde{\Sigma}^{\rm app}(z)$ of the self-energy operator;**
3. **seek the singularities of $\widetilde{G}^{\rm app}(z) := (z - (h_1 + \widetilde{\Sigma}^{\rm app}(z)))^{-1}$.**

4 - The dynamically screened Coulomb operator W

The (bare) Coulomb operator v_c

In the vacuum and neglecting relativistic effects, the electrostatic potential created by a time-dependent charge distribution ρ at point $\mathbf{r}$ and time t is

$$[V\rho](\mathbf{r},t) = \int_{\mathbb{R}^3} \frac{1}{|\mathbf{r}-\mathbf{r}'|} \, \rho(\mathbf{r}',t) \, d\mathbf{r}'$$

$$V(\tau) = v_c \delta_0(\tau), \qquad \widehat{v_c \rho}(\mathbf{k}) = \frac{4\pi}{|\mathbf{k}|^2} \widehat{\rho}(\mathbf{k}).$$

The (bare) Coulomb operator $v_{\rm c}$

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Screening: **in the presence of the molecular system, the perturbation of the electrostatic potential created at point r and time t by a time-dependent external charge distribution $\delta\rho$, is given, in the linear response regime, by**

$$\delta V(\mathbf{r},t) = \int_{-\infty}^{t} W_+(\mathbf{r},\mathbf{r}',t-t')\;\delta\rho(\mathbf{r}',t')\,dt'.$$

The (bare) Coulomb operator $v_{\rm c}$

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The dynamically screened Coulomb operator is defined by

$$\forall \tau \in \mathbb{R}, \quad W(\tau) = \Theta(\tau)W_+(\tau) + \Theta(-\tau)W_+(-\tau) = v_{\rm c}^{1/2}(\delta(\tau) - \chi_{\rm sym}(\tau))v_{\rm c}^{1/2}.$$

The (bare) Coulomb operator v_c

In the vacuum and neglecting relativistic effects, the electrostatic potential created by a time-dependent charge distribution ρ at point $\mathbf{r}$ and time t is

$$[V\rho](\mathbf{r},t) = \int_{\mathbb{R}^3} \frac{1}{|\mathbf{r}-\mathbf{r}'|}\,\rho(\mathbf{r}',t)\,d\mathbf{r}'$$

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The dynamically screened Coulomb operator is defined by

$$\forall\tau\in\mathbb{R},\quad W(\tau) = \Theta(\tau)W_+(\tau)+\Theta(-\tau)W_+(-\tau) = v_c^{1/2}(\delta(\tau)-\underbrace{\chi_{\rm sym}}_{\in L^\infty(\mathbb{R},\mathcal{B}(L^2(\mathbb{R}^3)))}(\tau))v_c^{1/2}.$$

5 - Hedin's equations and the GW approximation

5 - Hedin's equations and the GW approximation

Notation

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

$$A((\mathbf{r}_1,t_1),(\mathbf{r}_2,t_2)) \qquad \leftrightarrow \qquad A(12)$$

- **If A is a time-translation invariant space-time operator**

$$A(12^+) = A((\mathbf{r}_1,t_1),(\mathbf{r}_2,t_2^+)) = \lim_{t\to t_2^+} A((\mathbf{r}_1,t_1),(\mathbf{r}_2,t)) = [A((t_1-t_2)^-)](\mathbf{r}_1,\mathbf{r}_2).$$

Hedin's equations (Hedin '65)

- **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**

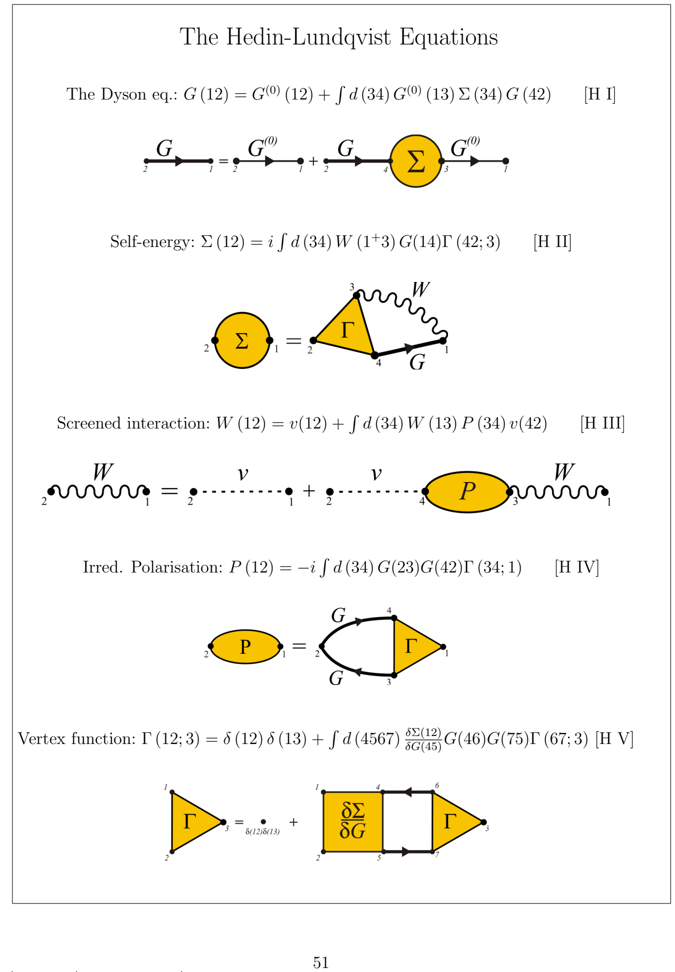
$$W(12) = v_c(12) + \int d(34) v_c(13) P(34) W(42)$$

- **Irreducible polarization**

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

- **Vertex function**

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



GW approximation (Hedin ’65)

- **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**

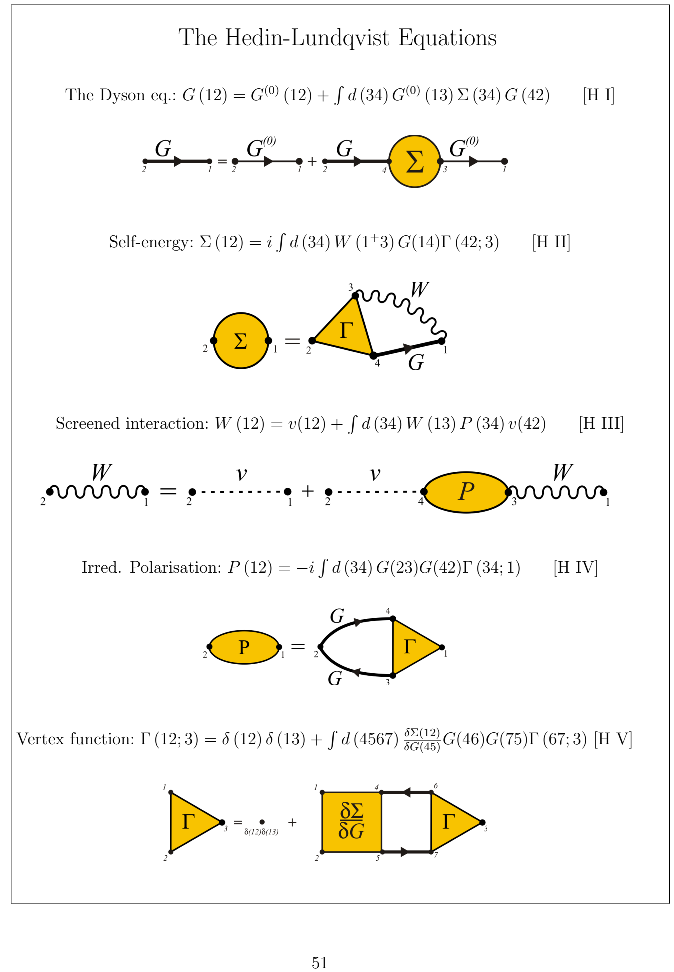
$$W(12) = v_c(12) + \int d(34) v_c(13) P(34) W(42)$$

- **Irreducible polarization**

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

- **Vertex function**

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



Neglect this term

GW equations (Hedin '65)

- **Dyson equation**

$$G^{\mathrm{app}}(12) = G_0(12) + \int d(34) G_0(13) \Sigma^{\mathrm{app}}(34) G^{\mathrm{app}}(42)$$

- **Self-energy**

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

- **Screened interaction**

$$W^{\mathrm{app}}(12) = v_{\mathrm{c}}(12) + \int d(34) v_{\mathrm{c}}(13) P^{\mathrm{app}}(34) W^{\mathrm{app}}(42)$$

- **Irreducible polarization**

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

GW equations in a mixed time-frequency representation

- **Dyson equation**

$$\widehat{G}^{\mathrm{app}}(\omega) = \widehat{G}_0(\omega) + \widehat{G}_0(\omega)\widehat{\Sigma}^{\mathrm{app}}(\omega)\widehat{G}^{\mathrm{app}}(\omega)$$

- **Self-energy**

$$\Sigma^{\mathrm{app}}(\tau) = iG^{\mathrm{app}}(0^-) \odot v_{\mathrm{c}}\delta_0(\tau) + G^{\mathrm{app}}(\tau) \odot W_{\mathrm{c}}^{\mathrm{app}}(-\tau)$$

- **Screened interaction**

$$\widehat{W}_{\mathrm{c}}^{\mathrm{app}}(\omega) = \left[\left(1 - v_{\mathrm{c}}\widehat{P}^{\mathrm{app}}(\omega)\right)^{-1} - 1\right] v_{\mathrm{c}}$$

- **Irreducible polarization**

$$P^{\mathrm{app}}(\tau) = -iG^{\mathrm{app}}(\tau) \odot G^{\mathrm{app}}(-\tau)$$

Hadamard product of two operators: $(A \odot B)(\mathbf{r}_1, \mathbf{r}_2) = A(\mathbf{r}_1, \mathbf{r}_2)B(\mathbf{r}_2, \mathbf{r}_1).$

GW equations on imaginary axes

- **Dyson equation**

$$\widetilde{G}^{\rm app}(\mu+i\omega)=\widetilde{G}_0(\mu+i\omega)+\widetilde{G}_0(\mu+i\omega)\widetilde{\Sigma}^{\rm app}(\mu+i\omega)\widetilde{G}^{\rm app}(\mu+i\omega)$$

- **Self-energy**

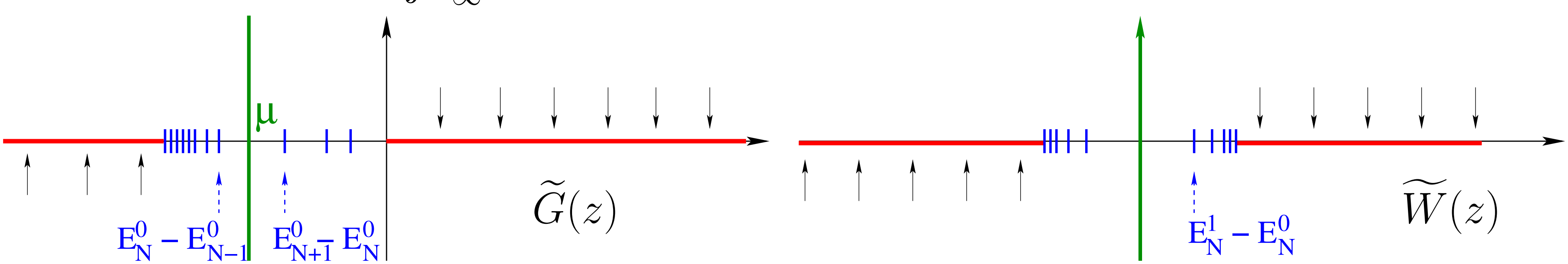
$$\widetilde{\Sigma}^{\rm app}(\mu+i\omega)=-\gamma_N^{0,{\rm LDA}}\odot v_{\rm c}-\frac{1}{2\pi}\int_{-\infty}^{+\infty}\widetilde{G}^{\rm app}(\mu+i(\omega-\omega'))\odot\widetilde{W}_{\rm c}^{\rm app}(i\omega')\,d\omega'$$

- **Screened interaction**

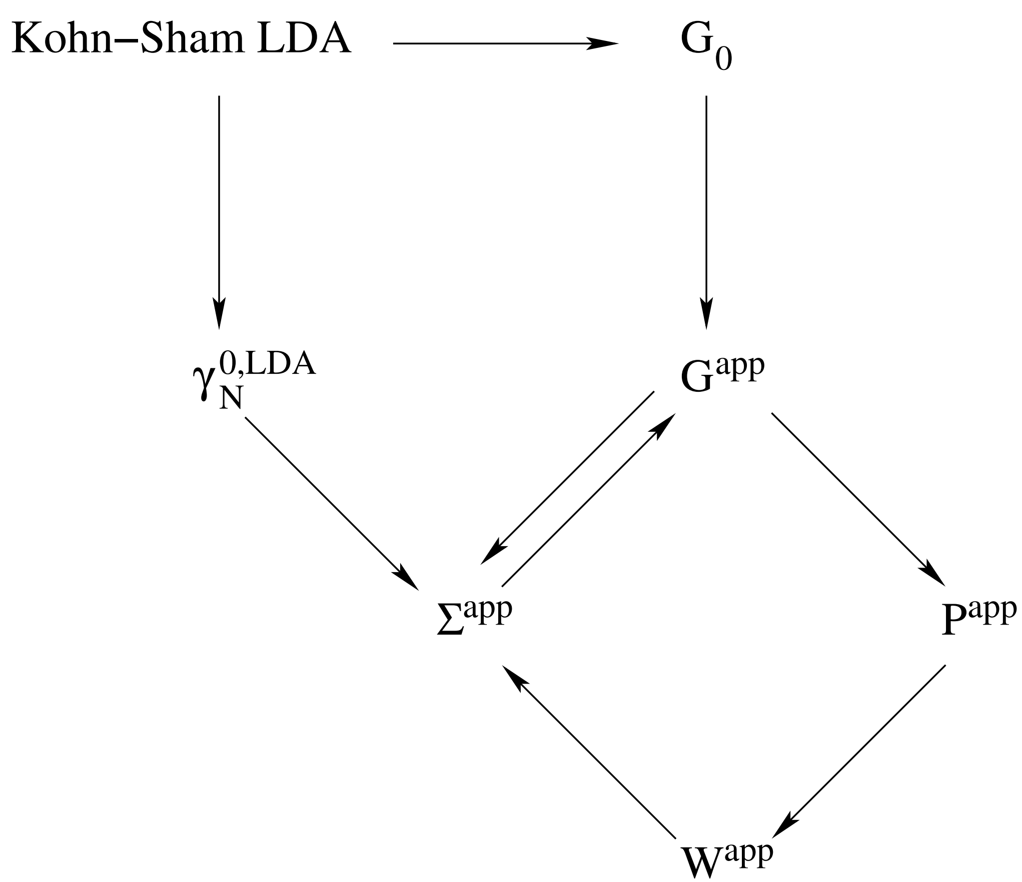
$$\widetilde{W}_{\rm c}^{\rm app}(i\omega)=\left[\left(1-v_{\rm c}\widetilde{P}^{\rm app}(i\omega)\right)^{-1}-1\right]v_{\rm c}$$

- **Irreducible polarization**

$$\widetilde{P}^{\rm app}(i\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\widetilde{G}^{\rm app}(\mu+i\omega')\odot\widetilde{G}^{\rm app}(\mu+i(\omega'-\omega))\,d\omega'$$

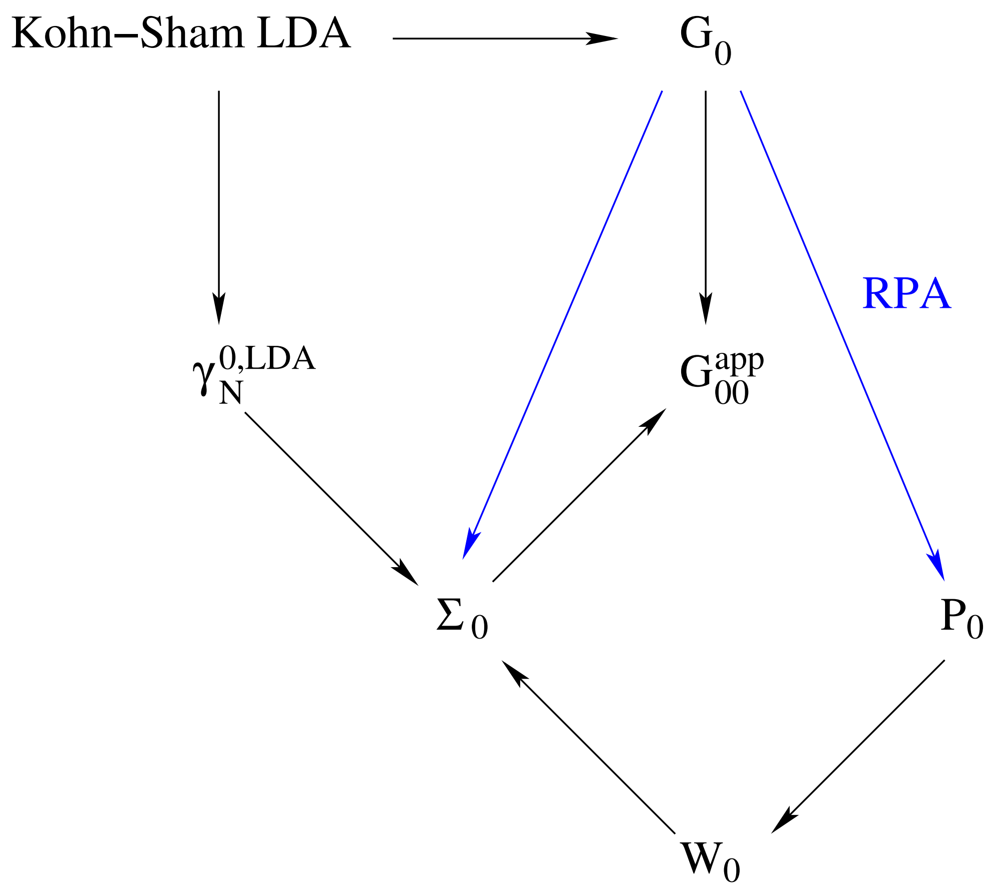


GW flowchart



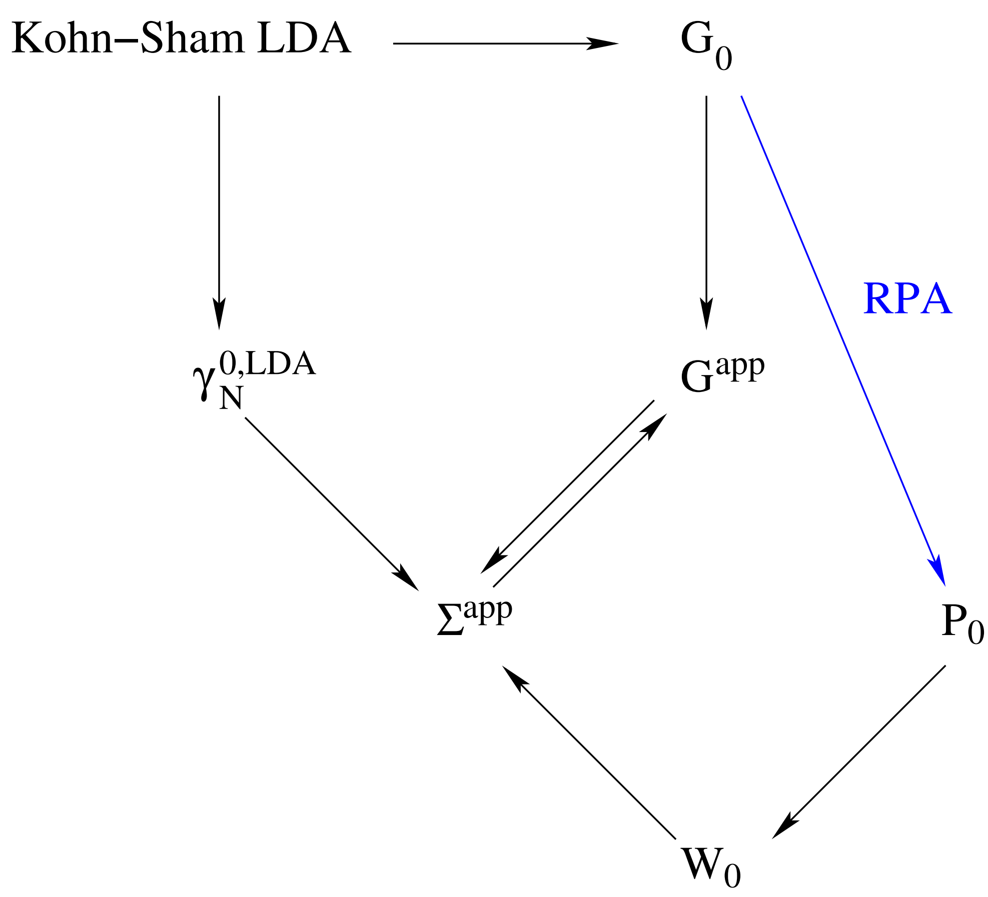
The existence of a solution to these equations is an open problem.

G_0W_0 method

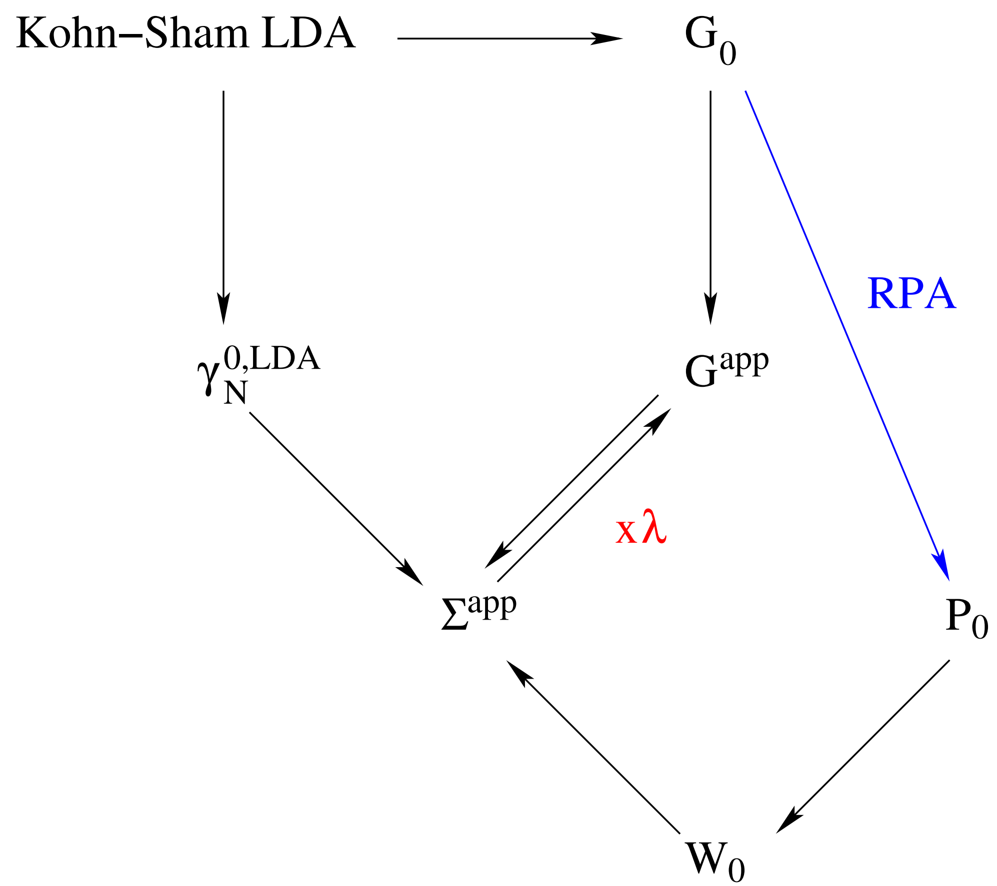


Theorem (EC, Gontier, Stoltz '15). The G_0W_0 method is well defined.

Self-consistent GW$_0$ method



Self-consistent GW_0 method



Theorem (EC, Gontier, Stoltz '15). **The self-consistent GW_0 method is well defined in the perturbative regime (λ small enough).**

Summary of the current mathematical results

EC, D. Gontier and G. Stoltz, ***A mathematical analysis of the GW method for computing electronic excited state energies of molecules*****, arXiv 1506.01737.**

- **The fundamental objects (G, G_0, Σ, P, W) involved in the GW formalism are mathematically well-defined.**
- **Some of their properties (sum rules, signs, Galitskii-Migdal formula) have been rigorously established.**
- **The G_0W_0 version of the GW approach is well defined.**
- **The self-consistent GW_0 method is well-defined in the perturbation regime.**

Work in progress

- **Analysis of the partially self-consistent GW method (self-consistency on the eigenvalues only).**
- **Analysis of the fully self-consistent GW method.**
- **Infinite systems (periodic crystals, disordered materials).**
- **Numerical algorithms.**

A1 - Fourier transform

Definition (Schwartz space). A function $\phi : \mathbb{R} \to \mathbb{C}$ of class C^∞ is called rapidly decreasing if for all $p \in \mathbb{N}$,

$$\mathcal{N}_p(\phi) := \max_{0\leq k\leq p} \max_{0\leq l\leq p} \sup_{t\in\mathbb{R}} \left| t^k \frac{d^l\phi}{dt^l}(t) \right| < \infty.$$

The vector space of all C^∞ rapidly decreasing functions from $\mathbb{R}$ to $\mathbb{C}$ is denoted by $\mathcal{S}(\mathbb{R})$ and is called the Schwartz space.

Gaussian functions and gaussian-polynomial functions are in $\mathcal{S}(\mathbb{R})$.

Definition (convergence in $\mathcal{S}(\mathbb{R})$). A sequence $(\phi_n)_{n\in\mathbb{N}}$ of functions of $\mathcal{S}(\mathbb{R})$ converges in $\mathcal{S}(\mathbb{R})$ to $\phi \in \mathcal{S}(\mathbb{R})$ if

$$\forall p \in \mathbb{N}, \quad \mathcal{N}_p(\phi_n - \phi) \underset{n\to+\infty}{\longrightarrow} 0.$$

Definition (Fourier transform in $\mathcal{S}(\mathbb{R})$). The Fourier transform of a function $\phi \in \mathcal{S}(\mathbb{R})$ is the function denoted by $\widehat{\phi}$ or $\mathcal{F}\phi$ and defined by

$$\boxed{\forall \omega \in \mathbb{R}, \quad \widehat{\phi}(\omega) = \mathcal{F}\phi(\omega) := \int_{-\infty}^{+\infty} \phi(t)\, e^{i\omega t}\, dt.}$$

Remark. Other sign and normalization conventions are also commonly used in the physics and mathematical literatures.

Theorem (some properties of $\mathcal{S}(\mathbb{R})$). The Schwartz space $\mathcal{S}(\mathcal{R})$ is stable by

1. **translation, scaling, complex conjugation;**
2. **derivation and multiplication by polynomials;**
3. **Fourier transform ($\forall p \in \mathbb{N},\ \exists C_p \in \mathbb{R}_+$ s.t.$\forall \phi \in \mathcal{S}(\mathbb{R}),\ \mathcal{N}_p(\widehat{\phi}) \leq C_p\, \mathcal{N}_{p+2}(\phi)$).**

   Besides, the Fourier transform defines a sequentially bicontinuous linear map from $\mathcal{S}(\mathcal{R})$ onto itself, with inverse $\mathcal{F}^{-1}$ defined by

$$\boxed{\forall \psi \in \mathcal{S}(\mathbb{R}), \quad \forall t \in \mathbb{R}, \quad [\mathcal{F}^{-1}\psi](t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \psi(\omega)\, e^{-i\omega t}\, d\omega.}$$

Definition (tempered distributions). We denote by $\mathcal{S}'(\mathbb{R})$ the vector space of the linear forms $u : \mathcal{S}(\mathbb{R}) \to \mathbb{C}$ satisfying the following continuity property : there exists $p \in \mathbb{N}$ and $C \in \mathbb{R}_+$ such that

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \qquad |\langle u, \phi \rangle| \leq C\mathcal{N}_p(\phi). \tag{1}$$

Theorem (canonical embedding of $L^p(\mathbb{R})$ in $\mathcal{S}'(\mathbb{R})$). Let $1 \leq p \leq +\infty$ and $f \in L^p(\mathbb{R})$. Then, the linear form $u_f : \mathcal{S}(\mathbb{R}) \to \mathbb{C}$ defined by

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle u_f, \phi \rangle := \int_{-\infty}^{+\infty} f(t)\phi(t)\, dt$$

is a tempered distribution, and if f_1 and f_2 are both in $L^p(\mathbb{R})$ and such that $u_{f_1} = u_{f_2}$, then $f_1 = f_2$.

We can therefore, with no ambiguity, denote f instead of u_f:

$$f \in L^p(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R}) \quad \text{and} \quad \forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle f, \phi \rangle := \int_{-\infty}^{+\infty} f(t)\phi(t)\, dt.$$

Definition-Theorem (basic operations on $\mathcal{S}'(\mathbb{R})$)

1. **Let $u \in \mathcal{S}'(\mathbb{R})$. The derivative of u is the element of $\mathcal{S}'(\mathbb{R})$ denote by $\frac{du}{dt}$ and defined by**

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle \frac{du}{dt}, \phi \rangle = -\langle u, \frac{d\phi}{dt} \rangle.$$

2. **Let $u \in \mathcal{S}'(\mathbb{R})$ and $p : \mathbb{R} \to \mathbb{C}$ a polynomial function. The product pu is the element of $\mathcal{S}'(\mathbb{R})$ defined by**

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle pu, \phi \rangle = \langle u, p\phi \rangle.$$

3. **Let $u \in \mathcal{S}'(\mathbb{R})$. The Fourier transform of u is the element of $\mathcal{S}'(\mathbb{R})$ denoted by $\widehat{u}$ or $\mathcal{F}u$ and defined by**

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle \widehat{u}, \phi \rangle = \langle u, \widehat{\phi} \rangle.$$

Crucial point: the above definitions are consistent with the usual definitions for "nice" functions (ex: $\hat{u}(\omega) = \displaystyle\int_{-\infty}^{+\infty} u(t) e^{i\omega t}\, dt$ for all $u \in L^1(\mathbb{R})$).

Exercise: define the translation, scaling, and complex conjugation operations on $\mathcal{S}'(\mathbb{R})$.

Definition (convergence in $\mathcal{S}'(\mathbb{R})$). A sequence $(u_n)_{n\in\mathbb{N}}$ of elements of $\mathcal{S}'(\mathbb{R})$ converges in $\mathcal{S}'(\mathbb{R})$ to $u \in \mathcal{S}'(\mathbb{R})$ if and only if

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle u_n, \phi \rangle \underset{n\to+\infty}{\longrightarrow} \langle u, \phi \rangle.$$

Theorem (some properties of the Fourier transform on $\mathcal{S}'(\mathbb{R})$).

1. **Let $u \in \mathcal{S}'(\mathbb{R})$. Then**

$$\boxed{\mathcal{F}\left(\frac{du}{dt}\right) = i\omega\widehat{u}(\omega) \qquad \textbf{and} \qquad \mathcal{F}\left(tu(t)\right) = i\frac{d\widehat{u}}{d\omega}(\omega).}$$

2. **The Fourier transform is a sequentially bicontinuous linear map from $\mathcal{S}'(\mathbb{R})$ onto itself, with inverse $\mathcal{F}^{-1}$ defined by**

$$\boxed{\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle \mathcal{F}^{-1}u, \phi \rangle_{\mathcal{S}',\mathcal{S}} = \langle u, \mathcal{F}^{-1}\phi \rangle_{\mathcal{S}',\mathcal{S}}.}$$

Exercise: compute the Fourier transform of a translated tempered distribution, of a scaled tempered distribution, and of the complex conjugate of a tempered distribution.

Two important cases

1. **The Dirac distribution at $t_0 \in \mathbb{R}$ is the tempered distribution denoted by δ_{t_0} and defined by**

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle \delta_{t_0}, \phi \rangle = \phi(t_0).$$

Computation of the Fourier transform δ_{t_0}:

$$\forall \phi \in \mathcal{S}(\mathbb{R}), \quad \langle \widehat{\delta_{t_0}}, \phi \rangle = \langle \delta_{t_0}, \widehat{\phi} \rangle = \widehat{\phi}(t_0) = \int_{-\infty}^{+\infty} \phi(\omega) e^{i\omega t_0} \, d\omega = \langle e^{i\omega t_0}, \phi \rangle.$$

Thus, the Fourier transform of δ_{t_0} is the smooth function $\boxed{\widehat{\delta_{t_0}}(\omega) = e^{i\omega t_0}.}$

2. **The Heaviside function is the function of $L^\infty(\mathbb{R}) \hookrightarrow \mathcal{S}'(\mathbb{R})$ defined by**

$$\Theta(t) = 1 \text{ if } t > 0 \quad \text{and} \quad \Theta(t) = 0 \text{ if } t < 0.$$

Fourier transform of the Heaviside function $\Theta(t)$:

$$\boxed{\widehat{\Theta}(\omega) = \pi \delta_0(\omega) + i \text{ p.v.} \left(\frac{1}{\omega} \right)} \tag{2}$$

where $\forall \phi \in \mathcal{S}(\mathbb{R}), \ \langle \text{p.v.} \left(\frac{1}{\cdot} \right), \phi \rangle := \lim_{\varepsilon \to 0^+} \int_{\mathbb{R} \setminus [-\varepsilon, \varepsilon]} \frac{\phi(\omega)}{\omega} d\omega = \lim_{\eta \to 0^+} \int_{-\infty}^{+\infty} \frac{\omega}{\eta^2 + \omega^2} \phi(\omega) \, d\omega.$

Proof of (2). **For all** $\eta > 0$**, we set** $\Theta_\eta(t) = \Theta(t)e^{-\eta t}$**.**

- **Since for all** $\eta > 0$**,** $\Theta_\eta \in L^1(\mathbb{R})$**, we have**

$$\widehat{\Theta}_\eta(\omega) = \int_{-\infty}^{+\infty} \Theta_\eta(t)e^{i\omega t}\,dt = \int_0^{+\infty} e^{-(\eta - i\omega)t}\,dt = \frac{1}{\eta - i\omega} = \frac{\eta}{\eta^2+\omega^2} + i\frac{\omega}{\eta^2+\omega^2}.$$

- **We have** $\Theta_\eta \xrightarrow[\eta\to 0^+]{\mathcal{S}'(\mathbb{R})} \Theta$**. Indeed, for all** $\phi \in \mathcal{S}(\mathbb{R})$**,**

$$\langle \Theta_\eta, \phi\rangle = \int_{-\infty}^{+\infty} \Theta_\eta(t)\phi(t)\,dt = \int_0^{+\infty} e^{-\eta t}\phi(t)\,dt \xrightarrow[\eta\to 0^+]{\text{DCT}} \int_0^{+\infty} \phi(t)\,dt = \langle \Theta, \phi\rangle.$$

- **We have** $\widehat{\Theta}_\eta \xrightarrow[\eta\to 0^+]{\mathcal{S}'(\mathbb{R})} \pi\delta_0 + i\ \text{p.v.}\left(\frac{1}{\cdot}\right)$**. Indeed, for all** $\phi \in \mathcal{S}(\mathbb{R})$**,**

$$\langle \widehat{\Theta}_\eta, \phi\rangle = \int_{-\infty}^{+\infty} \frac{\eta}{\eta^2+\omega^2}\phi(\omega)\,d\omega + i\int_{-\infty}^{+\infty} \frac{\omega}{\eta^2+\omega^2}\phi(\omega)\,d\omega \xrightarrow[\eta\to 0^+]{} \pi\phi(0) + i\langle \text{p.v.}\left(\frac{1}{\cdot}\right), \phi\rangle.$$

- **By sequential continuity of the Fourier transform in** $\mathcal{S}'(\mathbb{R})$**, we have**

$$\Theta_\eta \xrightarrow[\eta\to 0^+]{\mathcal{S}'(\mathbb{R})} \Theta \quad \Rightarrow \quad \widehat{\Theta}_\eta \xrightarrow[\eta\to 0^+]{\mathcal{S}'(\mathbb{R})} \widehat{\Theta}.$$

We obtain (2) by uniqueness of the limit in $\mathcal{S}'(\mathbb{R})$**.**

Remark. **The space $\mathcal{S}'(\mathbb{R})$ contains**

- **all the functions of the form $p(t)f(t)$, where p is a polynomial function and $f \in L^p(\mathbb{R})$ for some $1 \leq p \leq \infty$;**
- **all the compactly supported distributions on $\mathbb{R}$;**
- **all the periodic distributions on $\mathbb{R}$. In addition,**

$$u \ T\text{-periodic distribution} \quad \Rightarrow \quad \widehat{u} = \sum_{k \in \mathbb{Z}} c_k(u)\, \delta_{k\omega}, \quad \text{with } \omega = \frac{2\pi}{T}$$

where the $c_k(u)$ are the Fourier coefficients of u. If u is a locally integrable function, then

$$c_k(u) = \int_0^T u(t) e^{ik\omega t}\, dt = \int_0^T u(t) e^{2i\pi kt/T}\, dt.$$

The space $\mathcal{S}'(\mathbb{R})$ does not contain the distributions which rapidly grow at infinity, such as the exponential function.

Theorem (Fourier transform on $L^2(\mathbb{R})$). Up to a normalization constant, the Fourier transform is a unitary operator on $L^2(\mathbb{R})$: for all $u \in L^2(\mathbb{R})$, $\widehat{u} \in L^2(\mathbb{R})$ and $\|\widehat{u}\|_{L^2} = (2\pi)^{1/2}\|u\|_{L^2}$.

Theorem (Convolution and Fourier transform).

1. **The convolution product of two functions f and g of $L^1(\mathbb{R})$ is the function of $L^1(\mathbb{R})$ denoted by $f \star g$ and defined (almost everywhere) by**

$$\boxed{(f \star g)(t) := \int_{-\infty}^{+\infty} f(t-t')\, g(t')\, dt'.} \quad (3)$$

   We have for all f and g in $L^1(\mathbb{R})$,

$$\boxed{\widehat{f \star g}(\omega) = \widehat{f}(\omega)\, \widehat{g}(\omega).} \quad (4)$$

2. **We have for all f and g in $L^1(\mathbb{R})$ such that $\widehat{f}$ and $\widehat{g}$ also are in $L^1(\mathbb{R})$,**

$$\boxed{\widehat{fg}(\omega) = \frac{1}{2\pi}(\widehat{f} \star \widehat{g})(\omega).} \quad (5)$$

The definition (3) and the equalities (4)- (5) can be extended to wider classes of tempered distributions. In particular, $\boxed{\delta_0 \star u = u}$ for all $u \in \mathcal{S}'(\mathbb{R})$.

A2 - Causal functions, Hilbert transform and Kramers-Kronig relations

Definition (causal function). **A function $f \in \mathbb{R}_t \to \mathbb{C}$ is called causal if $f = 0$ a.e. on $(-\infty, 0)$.**

Definition (Hilbert transform on $\mathcal{S}(\mathbb{R}_\omega)$). The Hilbert transform of a function $\widehat{\phi} \in \mathcal{S}(\mathbb{R}_\omega)$ is the function of $C^\infty(\mathbb{R}_\omega)$ denoted by $\mathfrak{h}\widehat{\phi}$ and defined as

$$\boxed{\mathfrak{h}\widehat{\phi} = \frac{1}{\pi}\,\text{p.v.}\left(\frac{1}{\cdot}\right) \star \widehat{\phi} \quad \textbf{or equivalently as} \quad \mathfrak{h}\widehat{\phi} = \mathcal{F}\left(-i\ \text{sgn}(\cdot)\mathcal{F}^{-1}\widehat{\phi}\right).}$$

Proposition (Hilbert transform on $L^2(\mathbb{R}_\omega)$). The Hilbert transform $\mathfrak{h}$ defines a unitary operator on $L^2(\mathbb{R}_\omega)$, with inverse $-\mathfrak{h}$, which commutes with the translations and the positive dilations, and anticommutes with the reflexions.

The Hilbert transform can be extended by continuity to a large class of tempered distributions. In particular, it is well defined on the set of Fourier transforms of bounded functions.

Theorem (Karmers-Kronig relations). Let $f \in L^\infty(\mathbb{R}_t)$ be a causal function and let $\widehat{f}$ be its Fourier transform. Then,

$$\boxed{\Re\widehat{f} = -\mathfrak{h}\left(\Im\widehat{f}\right) \quad \textbf{and} \quad \Im\widehat{f} = \mathfrak{h}\left(\Re\widehat{f}\right).} \tag{6}$$

Elements of proof. Since f is causal, we have $f = \Theta f$. Hence,

$$\widehat{f} = \frac{1}{2\pi}\left(\widehat{\Theta} \star \widehat{f}\right) = \frac{1}{2\pi}\left(\pi\delta_0 + i \text{ p.v.}\left(\frac{1}{\cdot}\right)\right) \star \widehat{f} = \frac{1}{2}\left(\widehat{f} + i\,\mathfrak{h}\widehat{f}\right).$$

Therefore,

$$\widehat{f} = i\mathfrak{h}\widehat{f}.$$

Inserting the identity $\widehat{f} = \Re\widehat{f} + i\Im\widehat{f}$, and identifying the real and imaginary parts, we get

$$\Re\widehat{f} = -\mathfrak{h}\left(\Im\widehat{f}\right) \quad \textbf{and} \quad \Im\widehat{f} = \mathfrak{h}\left(\Re\widehat{f}\right).$$

Definition **(Laplace transform of a causal function). Let**

$$\mathbb{U} = \{z \in \mathbb{C} \mid \Im(z) > 0\}$$

be the upper-half plane, and $f : \mathbb{R} \to \mathbb{C}$ be a causal function of $L^p(\mathbb{R})$ for some $1 \leq p \leq \infty$. The Laplace transform of f is the $\mathbb{C}$-valued function on the upper-half plane $\mathbb{U}$ denoted by $\widetilde{f}$ or $\mathcal{L}f$ and defined by

$$\forall z \in \mathbb{U}, \quad \widetilde{f}(z) = \mathcal{L}f(z) = \int_{-\infty}^{+\infty} f(t)e^{izt}\,dt.$$

Remark. **The Laplace transform can in fact be defined for any causal tempered distribution.**

Remark. **Other (equivalent) definitions can be found in the mathematics and physics literatures.**