Mathematical and numerical analysis of embedding methods in quantum mechanics

PhD defense - November 18 2024

Alfred Kirsch
CERMICS (ENPC) & MATHERIALS (INRIA)
supervision: É. Cancès (CERMICS) & D. Gontier (CEREMADE)

Experiment in pictures

(a) Pouring liquid nitrogen (white fumes).

(b) Magnet (gray) flies over the (black) pastil.

Figure: Levitation experiment (students: A. Barthélemy (exp.), K. Chikhaoui (pictures)).

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures.

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C})\\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally ``hot''}$$

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally ``hot''}$$

"High T_c superconductor": yttrium, barium, copper, oxygen (YBCO).

(a) Discovery: 1986 by J. G. Bednorz & K. A. Müller.

(b) Nobel: 1987 (1 year after!)

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).
Embedding methods: *approximate* **computations** for materials with strong correlations.

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K\ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K\ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).
Embedding methods: *approximate* **computations** for materials with strong correlations.
Subject of this thesis: **mathematical** *and numerical* properties of two of these methods.

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).
Embedding methods: *approximate* **computations** for materials with strong correlations.
Subject of this thesis: **mathematical** *and numerical* properties of two of these methods.

- Quantum chemistry: **Density Matrix Embedding Theory** (DMET, since $2010'$s) [Knizia, Chan 2012 & 2013], [Wouters, al. 2016], [Wu, al. 2020], [Faulstich, al. 2022].

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^\circ\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^\circ\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).
Embedding methods: *approximate* **computations** for materials with strong correlations.
Subject of this thesis: **mathematical** *and numerical* properties of two of these methods.

- Quantum chemistry: **Density Matrix Embedding Theory** (DMET, since $2010'$s) [Knizia, Chan 2012 & 2013], [Wouters, al. 2016], [Wu, al. 2020], [Faulstich, al. 2022].
- Condensed matter physics: **Dynamical Mean-Field Theory** (DMFT, since $1990'$s) [Metzner, Vollhardt 1989], [Georges, Kotliar 1992], [Georges, al. 1996], [Kotliar, al. 2001].

From superconductivity to embedding methods and mathematics

Fact: the magnet levitates above the black knob at low temperatures. *Why?*

- **Levitation**: due to *Meissner-Ochsenfeld effect*, consequence of **superconductivity**.
- Superconductivity: exists for temperature $T \leq T_c$ (*critical temperature* of the material).

$$\left.\begin{array}{l}\text{Conventional theory (BCS) predicts } T_c \leq 20K \ (\approx -250^{\circ}\text{C}) \\ \text{Experiment: boiling liquid nitrogen } T = 77K \ (\approx -200^{\circ}\text{C})\end{array}\right\} \textbf{Abnormally “hot”}$$

“High T_c superconductor”: yttrium, barium, copper, oxygen (YBCO).

Actual paradigm: *unconventional* mechanism, due to electron *correlation* (hard problem).
Embedding methods: *approximate* **computations** for materials with strong correlations.
Subject of this thesis: **mathematical** *and numerical* properties of two of these methods.

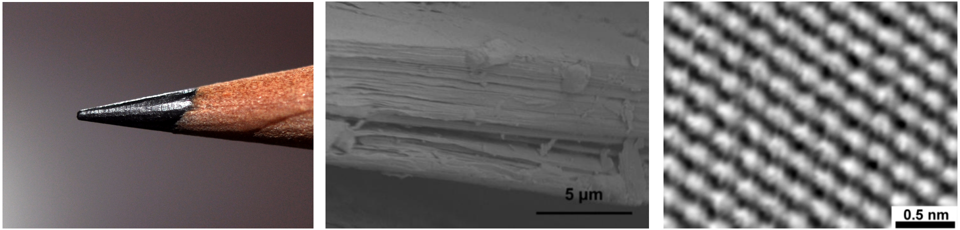
- Quantum chemistry: **Density Matrix Embedding Theory** (DMET, since $2010'$s) [Knizia, Chan 2012 & 2013], [Wouters, al. 2016], [Wu, al. 2020], [Faulstich, al. 2022].
- Condensed matter physics: **Dynamical Mean-Field Theory** (DMFT, since $1990'$s) [Metzner, Vollhardt 1989], [Georges, Kotliar 1992], [Georges, al. 1996], [Kotliar, al. 2001].

In short: Mathematics of two methods that could explain levitation at $T = 77K$.

Outline

Outline

Matter under microscope



(a) Graphite in a pencil. (b) Graphene in graphite. (c) Atoms in graphene.

Figure: A pencil under microscope: atoms are the building blocks of matter.

- **Matter**: arrangement (molecules, crystals, etc.) of **atoms** (carbon, oxygen, etc.).
- Any phenomenon: consequence of the properties of (many) atoms (statistical physics).
- **Properties** of atoms: **counterintuitive**, described by **quantum mechanics**.

Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy.
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light.

Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Problem: **we can't see** electrons, we can only **measure** them (energy, position).

Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Problem: **we can't see** electrons, we can only **measure** them (energy, position).

- Results can be **random**: one experiment $\rightarrow$ many results! **Probabilistic**.

Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Problem: **we can't see** electrons, we can only **measure** them (energy, position).

- Results can be **random**: one experiment $\rightarrow$ many results! **Probabilistic**.
- Results can be **quantized**: **discrete** values, "0 or 1, not 0.5" (**energy**, measured by light).

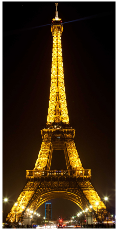
Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Problem: **we can't see** electrons, we can only **measure** them (energy, position).

- Results can be **random**: one experiment $\rightarrow$ many results! **Probabilistic**.
- Results can be **quantized**: **discrete** values, "0 or 1, not 0.5" (**energy**, measured by light).



(a) Some tower at night.

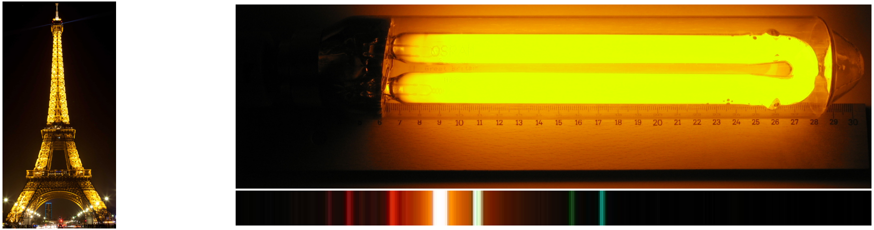
Properties of atoms

All atoms are made of smaller particles, bound by electric forces ($\oplus \rightarrow\leftarrow \ominus, \ominus \leftrightsquigarrow \ominus$)

- A **nucleus**, $\oplus$ charged, very heavy. **Fixed** (Born-Oppenheimer approximation).
- Many identical **electrons** (6 for carbon, 8 for oxygen), $\ominus$ charged, light. **Moving**.

Problem: **we can't see** electrons, we can only **measure** them (energy, position).

- Results can be **random**: one experiment $\rightarrow$ many results! **Probabilistic**.
- Results can be **quantized**: **discrete** values, "0 or 1, not 0.5" (**energy**, measured by light).

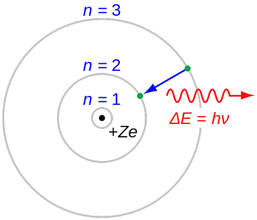


(a) Some tower at night.

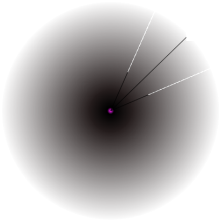
(b) Orange lightning: sodium lamp and its spectrum.

Figure: Quantization of energy in cities lightning system.

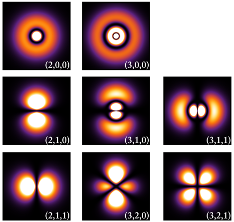
Quantum mechanics in (small) atoms



(a) Bohr model



(b) Probabilistic approach

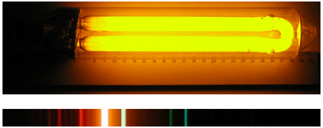


(c) Easy: 1 e^- solutions (H)

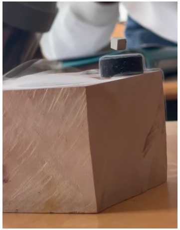
Quantum mechanics gives an explanation, using a precise **mathematical theory**:

- **Probabilistic** aspects: modeled by the **wavefunction** $\Psi : x \mapsto \Psi(x)$.
  $x \mapsto |\Psi(x)|^2$: probability to find the electron near x.
- **Quantized** aspects: modeled by the **Hamiltonian** $\hat{H} : \Psi \mapsto \hat{H}\Psi$.
  E can be measured $\Rightarrow$ exists a solution to the *Schrödinger equation*.

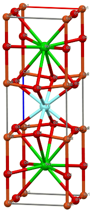
$$\boxed{\hat{H}\Psi = E\Psi, \quad E \in \mathbb{R}} \tag{1}$$



(a) Sodium emission spectrum: an 11-interacting-electron problem.



(b) Levitation with YBCO.

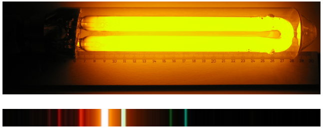


(c) Unit cell of YBCO

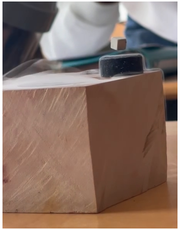
Problem: Schrödinger equation is *very hard* to solve explicitly for **large** & **interacting** systems.

- Analytically: general properties of the solution (e.g. spectral theory).

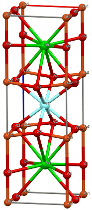
Approximations in quantum mechanics



(a) Sodium emission spectrum: an 11-interacting-electron problem.



(b) Levitation with YBCO.

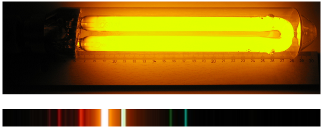


(c) Unit cell of YBCO

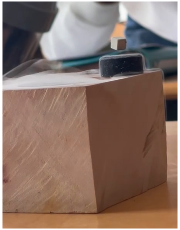
Problem: Schrödinger equation is *very hard* to solve explicitly for **large** & **interacting** systems.

- Analytically: general properties of the solution (e.g. spectral theory).
- Numerically: high dimensional ($3N$) partial differential equation (e.g. too large for FEM).

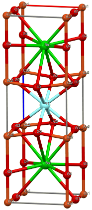
Approximations in quantum mechanics



(a) Sodium emission spectrum: an 11-interacting-electron problem.



(b) Levitation with YBCO.



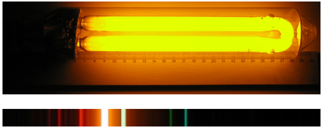
(c) Unit cell of YBCO

Problem: Schrödinger equation is *very hard* to solve explicitly for **large** & **interacting** systems.

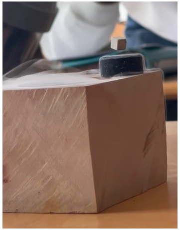
- Analytically: general properties of the solution (e.g. spectral theory).
- Numerically: high dimensional ($3N$) partial differential equation (e.g. too large for FEM).

Solution: find a "good" approximation ("good": problem dependent ⇒ many of them).

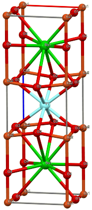
Approximations in quantum mechanics



(a) Sodium emission spectrum: an 11-interacting-electron problem.



(b) Levitation with YBCO.



(c) Unit cell of YBCO

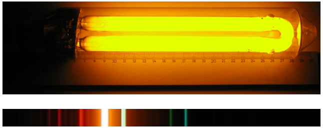
Problem: Schrödinger equation is *very hard* to solve explicitly for **large** & **interacting** systems.

- Analytically: general properties of the solution (e.g. spectral theory).
- Numerically: high dimensional ($3N$) partial differential equation (e.g. too large for FEM).

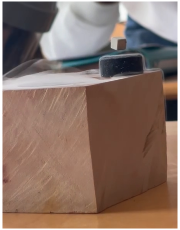
Solution: find a "good" approximation ("good": problem dependent $\Rightarrow$ many of them).

- Reduce to one-electron models: mean-field Hamiltonians, Hartree-Fock, (TD)DFT etc.

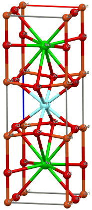
Approximations in quantum mechanics



(a) Sodium emission spectrum: an 11-interacting-electron problem.



(b) Levitation with YBCO.



(c) Unit cell of YBCO

Problem: Schrödinger equation is *very hard* to solve explicitly for **large** & **interacting** systems.

- Analytically: general properties of the solution (e.g. spectral theory).
- Numerically: high dimensional ($3N$) partial differential equation (e.g. too large for FEM).

Solution: find a "good" approximation ("good": problem dependent $\Rightarrow$ many of them).

- Reduce to one-electron models: mean-field Hamiltonians, Hartree-Fock, (TD)DFT etc.
- **Reduce to smaller but interacting** systems: **embedding methods**, e.g. DMFT, DMET.

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Principle: quantum counterpart of *mean-field* approach to Ising models. ($\approx$ **Domain dec.**)

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Principle: quantum counterpart of *mean-field* approach to Ising models. ($\approx$ **Domain dec.**)

Fixed Decomposition: one-particle Hilbert space (DMET), partition a graph (DMFT).
Given $X_{\mathrm{DM?T}}$ a trial solution,

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Principle: quantum counterpart of *mean-field* approach to Ising models. ($\approx$ **Domain dec.**)

Fixed Decomposition: one-particle Hilbert space (DMET), partition a graph (DMFT).
Given $X_{\text{DM?T}}$ a trial solution,

1. Reduce: exponential law and partial trace (DMET), Anderson Impurity Model (DMFT).

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Principle: quantum counterpart of *mean-field* approach to Ising models. ($\approx$ **Domain dec.**)

Fixed Decomposition: one-particle Hilbert space (DMET), partition a graph (DMFT).
Given $X_{\mathrm{DM?T}}$ a trial solution,

1. Reduce: exponential law and partial trace (DMET), Anderson Impurity Model (DMFT).
2. Solve (easier): finite dimensional problems (DMET), self-energy sparsity pattern (DMFT).

Embedding methods: approximate computation of correlations

Goal: compute **directly** an approx. of **correlations** $\langle XY \rangle$ ~~wave-function~~ (DMFT&DMET).

- DMET: **static** correlations (one-particle reduced density matrix *blocks*) of ground-states.
- DMFT: **dynamical** correlations (Green's functions *blocks*) of Hubbard model Gibbs states.

Principle: quantum counterpart of *mean-field* approach to Ising models. ($\approx$ **Domain dec.**)

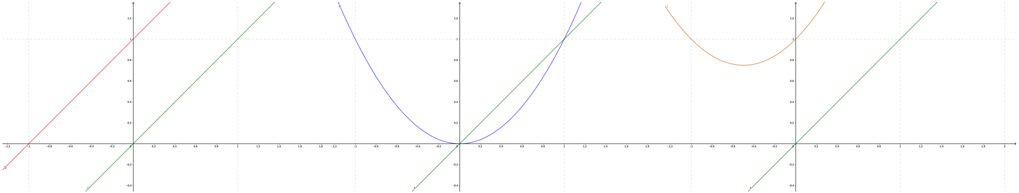
Fixed Decomposition: one-particle Hilbert space (DMET), partition a graph (DMFT).
Given $X_{\text{DM?T}}$ a trial solution,

1. Reduce: exponential law and partial trace (DMET), Anderson Impurity Model (DMFT).
2. Solve (easier): finite dimensional problems (DMET), self-energy sparsity pattern (DMFT).
3. Update: low-level map (DMET), bath update map (DMFT).

Self-consistently! $\iff$ *fixed-point equation*.

$$\boxed{F^{\text{DM?T}}(X_{\text{DM?T}}) = X_{\text{DM?T}}, \qquad \begin{array}{ll} X_{\text{DMET}} = D \in \mathcal{D} & \text{(1-RDM)} \\ X_{\text{DMFT}} = \Delta \in \mathfrak{D} & \text{(Hybridization function)} \end{array}} \tag{2}$$

Mathematical challenges with $f(x) = x, \quad x \in X$



(a) No solution: $f_1 : x \mapsto x + 1$
x goes to $+\infty$.

(b) Many solutions: $f_2 : x \mapsto x^2$
Solutions are $x = 0$ and $x = 1$.

(c) Bad solutions: $f_3 : x \mapsto x^2 + x + 1$
Solutions are $x = \pm i$ (complex!)

Figure: Numerical fixed point problems: $f_i(x) = x, \quad x \in \mathbb{R}$.

For each of the methods, we address the following mathematical questions:

- How many "*physical*" solutions are there? In which *space* (**completeness**)?
- What are their properties? How *good* is the approximation?

Outline

Second quantization formalism: DMET & DMFT background

Second quantization: C^*-algebra of **bounded** operators on fermionic Fock space of $(\mathcal{H}, \langle\cdot,\cdot\rangle)$.

$$\mathcal{F} = P_-\left(\tilde{\mathcal{F}}\right), \quad \tilde{\mathcal{F}} = \bigoplus_{n=0}^{+\infty} \mathcal{H}^{\otimes n}, \quad \mathcal{H}^{\otimes n} = \bigotimes^{n} \mathcal{H}, \quad \mathcal{H}^{\otimes 0} = \mathbb{C}, \quad (\text{Fock space, “}\mathcal{F} = e^{\mathcal{H}}\text{”})$$

$$P_-(\phi_1 \otimes \ldots \otimes \phi_n) = \frac{1}{n!}\sum \epsilon(\sigma)\phi_{\sigma(1)} \otimes \ldots \otimes \phi_{\sigma(n)}, \sigma \in \mathfrak{S}_n \ (\text{Fermions: antisymmetric})$$

$$\forall \phi' \in \mathcal{H}, \quad \tilde{a}_{\phi'}{}^{\dagger}(\phi_1 \otimes \ldots \otimes \phi_n) = (\sqrt{n+1})\phi' \otimes \phi_1 \ldots \otimes \phi_n, \quad (\textbf{Linear} \text{ in } \phi' \text{ (creation)})$$

$$\hat{a}^{\dagger}_{\phi'} = P_- \tilde{a}_{\phi'}{}^{\dagger} P_-, \quad \hat{a}_{\phi} = \left(\hat{a}^{\dagger}_{\phi}\right)^{\dagger}, \quad \|\hat{a}^{\dagger}_{\phi}\| = \|\hat{a}_{\phi}\| = \|\phi\| \quad (\textbf{Antilin.} \text{ in } \phi, \text{ bounded})$$

$$\forall \phi, \phi' \in \mathcal{H}, \quad \{\hat{a}_{\phi}, \hat{a}_{\phi'}\} = \{\hat{a}^{\dagger}_{\phi}, \hat{a}^{\dagger}_{\phi'}\} = 0, \quad \{\hat{a}_{\phi}, \hat{a}^{\dagger}_{\phi'}\} = \langle \phi, \phi' \rangle \qquad (\{A, B\} = AB + BA)$$

Definition (Equilibrium state: average value of observables $\langle O \rangle = \Omega(\hat{O})$)

Given $\hat{H} \in \mathcal{S}(\mathcal{F})$, an equilibrium **state**, with *density matrix* $\hat{\rho}$, is a ≥ 0 bounded **linear form** on bounded operators $\Omega : B(\mathcal{F}) \ni \hat{O} \mapsto \mathrm{Tr}(\hat{\rho}\hat{O})$, with $\hat{\rho} \in \mathcal{S}(\mathcal{F})$, $\quad \mathrm{Tr}(\hat{\rho}) = 1, \quad [\hat{\rho}, e^{it\hat{H}}] = 0$.

One-particle reduced density matrices (1-RDM); DMET goal

Includes: ground-states ($\Omega : \hat{O} \mapsto \langle \Psi_N, \hat{O}\Psi_N \rangle$, DMET), Gibbs states ($\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$, DMFT).

One-particle reduced density matrices (1-RDM); DMET goal

Includes: ground-states ($\Omega : \hat{O} \mapsto \langle \Psi_N, \hat{O}\Psi_N \rangle$, DMET), Gibbs states ($\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$, DMFT).

Definition (One-particle reduced density matrix γ_Ω: correlation of creation/annihilation pairs)

The one-particle reduced density matrix (1-RDM) γ_Ω associated to Ω is the unique **self-adjoint operator** in $B(\mathcal{H})$ represented by the sesquilinear **form** defined by for all $\phi, \phi' \in \mathcal{H}$,

$$\langle \phi, \gamma_\Omega \phi' \rangle = \Omega\left(\hat{a}^\dagger_{\phi'} \hat{a}_\phi\right). \qquad \text{It satisfies } 0 \leq \gamma_\Omega \leq 1.$$

One-particle reduced density matrices (1-RDM); DMET goal

Includes: ground-states ($\Omega : \hat{O} \mapsto \langle \Psi_N, \hat{O}\Psi_N \rangle$, DMET), Gibbs states ($\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$, DMFT).

Definition (One-particle reduced density matrix γ_Ω: correlation of creation/annihilation pairs)

The one-particle reduced density matrix (1-RDM) γ_Ω associated to Ω is the unique **self-adjoint operator** in $B(\mathcal{H})$ represented by the sesquilinear **form** defined by for all $\phi, \phi' \in \mathcal{H}$,

$$\langle \phi, \gamma_\Omega \phi' \rangle = \Omega\left(\hat{a}^\dagger_{\phi'} \hat{a}_\phi\right). \qquad \text{It satisfies } 0 \leq \gamma_\Omega \leq 1.$$

Remark: $\gamma_\Omega^2 = \gamma_\Omega \iff \Omega(\hat{O}) = \langle \Psi_N, \hat{O}\Psi_N \rangle \quad \& \quad \Psi_N = \hat{a}^\dagger_{\phi_1} \dots \hat{a}^\dagger_{\phi_N} |\emptyset\rangle$ (**Slater** state),

In such case, $\mathrm{Ran}(\gamma_{\Psi_N}) = \mathrm{Span}(\phi_i)_{i \in [\![1,N]\!]}$ and $\mathrm{Tr}(\gamma_{\Psi_N}) = N$.

One-particle reduced density matrices (1-RDM); DMET goal

Includes: ground-states ($\Omega : \hat{O} \mapsto \langle \Psi_N, \hat{O}\Psi_N \rangle$, DMET), Gibbs states ($\hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z}$, DMFT).

Definition (One-particle reduced density matrix γ_Ω: correlation of creation/annihilation pairs)

The one-particle reduced density matrix (1-RDM) γ_Ω associated to Ω is the unique **self-adjoint operator** in $B(\mathcal{H})$ represented by the sesquilinear **form** defined by for all $\phi, \phi' \in \mathcal{H}$,

$$\langle \phi, \gamma_\Omega \phi' \rangle = \Omega\left(\hat{a}^\dagger_{\phi'} \hat{a}_\phi\right). \qquad \text{It satisfies } 0 \leq \gamma_\Omega \leq 1.$$

Remark: $\gamma_\Omega^2 = \gamma_\Omega \iff \Omega(\hat{O}) = \langle \Psi_N, \hat{O}\Psi_N \rangle \quad \& \quad \Psi_N = \hat{a}^\dagger_{\phi_1} \ldots \hat{a}^\dagger_{\phi_N} |\emptyset\rangle$ (**Slater** state),

In such case, $\mathrm{Ran}(\gamma_{\Psi_N}) = \mathrm{Span}(\phi_i)_{i \in [\![1,N]\!]}$ and $\mathrm{Tr}(\gamma_{\Psi_N}) = N$.

DMET goal: approximate γ_{Ψ_N} ground-state 1-RDM by D Slater 1-RDM (like Hartree-Fock).

$$\gamma_{\Psi_N} \in \mathrm{CH}(\mathcal{D}) = \left\{D^\dagger = D, \quad 0 \leq D \leq 1, \quad \mathrm{Tr}(D) = N\right\} \qquad \text{(N-particle 1-RDM)}$$

$$\approx_{\text{DMET}} D \in \mathcal{D} = \left\{D^\dagger = D, \quad D^2 = D, \quad \mathrm{Tr}(D) = N\right\} \qquad \text{(**Slater** like 1-RDM)}$$

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**
Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**

Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1-D)(X_x)$.

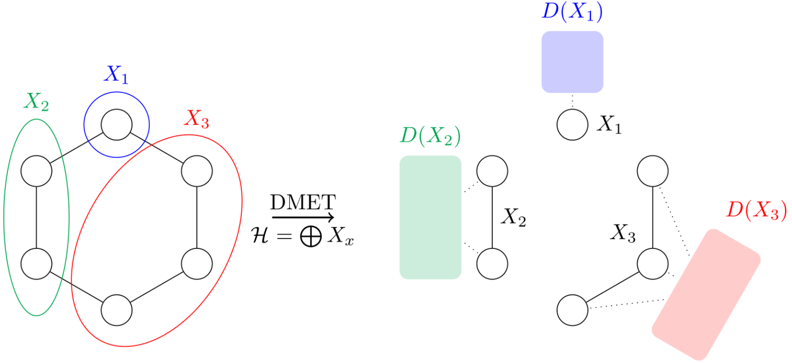


Figure: DMET mapping principle. **Assumption:** $\dim(W_{x,D}) = 2L_x$ **(maximal)**.

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**
Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1-D)(X_x)$.
2. $\mathcal{H} = W_{x,D} \oplus \mathcal{H}^{\mathrm{env}}_{x,D} \implies \boxed{\hat{\rho} = \hat{\rho}_{\Psi_{W_{x,D}}} \otimes \hat{\rho}_{\Psi_{\mathcal{H}^{\mathrm{env}}_{x,D}}}}$ in $\mathcal{F} \simeq \mathcal{F}(W_{x,D}) \otimes \mathcal{F}(\mathcal{H}^{\mathrm{env}}_{x,D})$, "$\mathcal{F} = e^{\mathcal{H}}$"

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**
Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1-D)(X_x)$.
2. $\mathcal{H} = W_{x,D} \oplus \mathcal{H}^{\mathsf{env}}_{x,D} \implies \boxed{\hat{\rho} = \hat{\rho}_{\Psi_{W_{x,D}}} \otimes \hat{\rho}_{\Psi_{\mathcal{H}^{\mathsf{env}}_{x,D}}}}$ in $\mathcal{F} \simeq \mathcal{F}(W_{x,D}) \otimes \mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})$, "$\mathcal{F} = e^{\mathcal{H}}$"
3. **Partial trace**,

$$\hat{H}^{\mathsf{imp}}_{x,D} = \mathrm{Tr}_{\mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})}((\mathbf{1} \otimes \hat{\rho}_{\mathcal{H}^{\mathsf{env}}_{x,D}})\hat{H})$$

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**
Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1-D)(X_x)$.
2. $\mathcal{H} = W_{x,D} \oplus \mathcal{H}^{\mathsf{env}}_{x,D} \implies \boxed{\hat{\rho} = \hat{\rho}_{\Psi_{W_{x,D}}} \otimes \hat{\rho}_{\Psi_{\mathcal{H}^{\mathsf{env}}_{x,D}}}}$ in $\mathcal{F} \simeq \mathcal{F}(W_{x,D}) \otimes \mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})$, "$\mathcal{F} = e^{\mathcal{H}}$"
3. **Partial trace**, solve (accurately) "grand-canonical" ground-state problem

$$\hat{H}^{\mathsf{imp}}_{x,D} = \mathrm{Tr}_{\mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})}((\mathbf{1} \otimes \hat{\rho}_{\mathcal{H}^{\mathsf{env}}_{x,D}})\hat{H}) \Rightarrow \inf_{\Psi^{\mathsf{imp}}_x \in \mathcal{F}(W_{x,D})} \langle \Psi^{\mathsf{imp}}_x, \left(\hat{H}^{\mathsf{imp}}_{x,D} - \mu \hat{N}_x\right) \Psi^{\mathsf{imp}}_x \rangle,$$

($\hat{N}_x = d\Gamma(\Pi_{X_x})$: **fragment** number operator, Π_x: orthogonal projector on X_x.)

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**

Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1-D)(X_x)$.
2. $\mathcal{H} = W_{x,D} \oplus \mathcal{H}^{\mathsf{env}}_{x,D} \implies \boxed{\hat{\rho} = \hat{\rho}_{\Psi_{W_{x,D}}} \otimes \hat{\rho}_{\Psi_{\mathcal{H}^{\mathsf{env}}_{x,D}}}}$ in $\mathcal{F} \simeq \mathcal{F}(W_{x,D}) \otimes \mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})$, "$\mathcal{F} = e^{\mathcal{H}}$"
3. **Partial trace**, solve (accurately) "grand-canonical" ground-state problem $\Rightarrow$ 1-RDM: $P_{\mu,x}$

$$\hat{H}^{\mathsf{imp}}_{x,D} = \mathrm{Tr}_{\mathcal{F}(\mathcal{H}^{\mathsf{env}}_{x,D})}((\mathbf{1} \otimes \hat{\rho}_{\mathcal{H}^{\mathsf{env}}_{x,D}})\hat{H}) \Rightarrow \inf_{\Psi^{\mathsf{imp}}_x \in \mathcal{F}(W_{x,D})} \langle \Psi^{\mathsf{imp}}_x, \left(\hat{H}^{\mathsf{imp}}_{x,D} - \mu \hat{N}_x\right) \Psi^{\mathsf{imp}}_x \rangle,$$

($\hat{N}_x = d\Gamma(\Pi_{X_x})$: **fragment** number operator, Π_x: orthogonal projector on X_x.)

Decomposition and high-level map F^{HL} (with accurate solver)

Fixed: *orthogonal* decomposition of $\mathcal{H}$ into "fragments" $\mathcal{H} = \bigoplus_{x=1}^{N_f} X_x$, $\dim(X_x) = L_x$ **finite**
Given $D \in \mathcal{D}$ **matrix**, define for **each** fragment X_x:

1. **"Impurity space"**: $W_{x,D} = D(X_x) + X_x = D(X_x) \oplus (1 - D)(X_x)$.
2. $\mathcal{H} = W_{x,D} \oplus \mathcal{H}_{x,D}^{\mathsf{env}} \implies \boxed{\hat{\rho} = \hat{\rho}_{\Psi_{W_{x,D}}} \otimes \hat{\rho}_{\Psi_{\mathcal{H}_{x,D}^{\mathsf{env}}}}}$ in $\mathcal{F} \simeq \mathcal{F}(W_{x,D}) \otimes \mathcal{F}(\mathcal{H}_{x,D}^{\mathsf{env}})$, "$\mathcal{F} = e^{\mathcal{H}}$"
3. **Partial trace**, solve (accurately) "grand-canonical" ground-state problem $\Rightarrow$ 1-RDM: $P_{\mu,x}$

$$\hat{H}_{x,D}^{\mathsf{imp}} = \mathrm{Tr}_{\mathcal{F}(\mathcal{H}_{x,D}^{\mathsf{env}})}((\mathbf{1} \otimes \hat{\rho}_{\mathcal{H}_{x,D}^{\mathsf{env}}})\hat{H}) \Rightarrow \inf_{\Psi_x^{\mathsf{imp}} \in \mathcal{F}(W_{x,D})} \langle \Psi_x^{\mathsf{imp}}, \left(\hat{H}_{x,D}^{\mathsf{imp}} - \mu \hat{N}_x\right) \Psi_x^{\mathsf{imp}} \rangle,$$

($\hat{N}_x = d\Gamma(\Pi_{X_x})$: **fragment** number operator, Π_x: orthogonal projector on X_x.)

$$\Rightarrow \boxed{F^{\mathsf{HL}}(D) = \sum_{x=1}^{N_f} \Pi_x P_{\mu,x} \Pi_x} = \begin{pmatrix} \Pi_1 P_{\mu,1} \Pi_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \Pi_{N_f} P_{\mu,N_f} \Pi_{N_f} \end{pmatrix}, \quad \mu \text{ s.t. } \mathrm{Tr}(F^{\mathsf{HL}}(D)) = N$$

Low level map F^{LL} (feedback) and DMET equations

By definition, $F^{\mathsf{HL}}(D) \in \mathcal{P} = \mathsf{Bd}(\mathsf{CH}(\mathcal{D}))$, with $\mathsf{Bd}(\hat{O}) = \sum_{x=1}^{N_f} \Pi_x \hat{O} \Pi_x$.
Feedback: given $P \in \mathcal{P}$, find a $D \in \mathcal{D}$ s.t. $\mathsf{Bd}(D) = P$ (representability issues [Lemma 2.8]).

For instance, $F^{\mathsf{LL}}(P) = \underset{D \in \mathcal{D}, \mathsf{Bd}(D) = P}{\operatorname{argmin}} \mathcal{E}^{\mathrm{HF}}(D)$, $\quad \mathcal{E}^{\mathsf{HF}}(D)$: $\hat{H}$ Hartree-Fock energy functional.

DMET equations: impose self-consistency (define $F^{\mathsf{DMET}} = F^{\mathsf{LL}} \circ F^{\mathsf{HL}}$), i.e.

$$\begin{cases} D = F^{\mathsf{LL}}(P) \in \mathcal{D} \\ P = F^{\mathsf{HL}}(D) \in \mathcal{P} \end{cases} \iff \begin{cases} \boxed{D = F^{\mathsf{DMET}}(D), D \in \mathcal{D}} \\ P = F^{\mathsf{HL}}(D) \in \mathcal{P}. \end{cases}$$

Mathematical starting point: DMET "is exact in the non-interacting [...] limit" [Knizia, 2012].

Consider $\hat{H} = d\Gamma(H^0) + \hat{H}^I, \quad \hat{H}^I$: **interactions** e.g. two-body.

Low level map F^{LL} (feedback) and DMET equations

By definition, $F^{\mathsf{HL}}(D) \in \mathcal{P} = \mathsf{Bd}(\mathsf{CH}(\mathcal{D}))$, with $\mathsf{Bd}(\hat{O}) = \sum_{x=1}^{N_f} \Pi_x \hat{O} \Pi_x$.
Feedback: given $P \in \mathcal{P}$, find a $D \in \mathcal{D}$ s.t. $\mathsf{Bd}(D) = P$ (representability issues [Lemma 2.8]).

For instance, $F^{\mathsf{LL}}(P) = \underset{D \in \mathcal{D}, \mathsf{Bd}(D) = P}{\operatorname{argmin}} \mathcal{E}^{\mathrm{HF}}(D)$, $\mathcal{E}^{\mathsf{HF}}(D)$: $\hat{H}$ Hartree-Fock energy functional.

DMET equations: impose self-consistency (define $F^{\mathsf{DMET}} = F^{\mathsf{LL}} \circ F^{\mathsf{HL}}$), i.e.

$$\begin{cases} D = F^{\mathsf{LL}}(P) \in \mathcal{D} \\ P = F^{\mathsf{HL}}(D) \in \mathcal{P} \end{cases} \iff \begin{cases} \boxed{D = F^{\mathsf{DMET}}(D), D \in \mathcal{D}} \\ P = F^{\mathsf{HL}}(D) \in \mathcal{P}. \end{cases}$$

Mathematical starting point: DMET "is exact in the non-interacting [...] limit" [Knizia, 2012].

Consider $\hat{H}_{\alpha} = d\Gamma(H^0) + \alpha \hat{H}^I$, with $\alpha \in [0, 1]$.

Low level map F^{LL} (feedback) and DMET equations

By definition, $F_\alpha^{\mathsf{HL}}(D) \in \mathcal{P} = \mathsf{Bd}(\mathsf{CH}(\mathcal{D}))$, with $\mathsf{Bd}(\hat{O}) = \sum_{x=1}^{N_f} \Pi_x \hat{O} \Pi_x$.
Feedback: given $P \in \mathcal{P}$, find a $D \in \mathcal{D}$ s.t. $\mathsf{Bd}(D) = P$ (representability issues [Lemma 2.8]).

For instance, $F_\alpha^{\mathsf{LL}}(P) = \underset{D \in \mathcal{D}, \mathsf{Bd}(D) = P}{\operatorname{argmin}} \mathcal{E}_\alpha^{\mathrm{HF}}(D)$, $\mathcal{E}_\alpha^{\mathrm{HF}}(D)$: $\hat{H}_\alpha$ Hartree-Fock energy functional.

DMET equations: impose self-consistency (define $F_\alpha^{\mathsf{DMET}} = F_\alpha^{\mathsf{LL}} \circ F_\alpha^{\mathsf{HL}}$), i.e.

$$\begin{cases} D = F_\alpha^{\mathsf{LL}}(P) \in \mathcal{D} \\ P = F_\alpha^{\mathsf{HL}}(D) \in \mathcal{P} \end{cases} \iff \begin{cases} \boxed{D = F_\alpha^{\mathsf{DMET}}(D), D \in \mathcal{D}} \\ P = F_\alpha^{\mathsf{HL}}(D) \in \mathcal{P}. \end{cases}$$

Mathematical starting point: DMET "is exact in the non-interacting [...] limit" [Knizia, 2012].

Consider $\hat{H}_\alpha = d\Gamma(H^0) + \alpha \hat{H}^I$, with $\alpha \in [0,1]$.

Low level map F^{LL} (feedback) and DMET equations

By definition, $F^{\mathsf{HL}}_\alpha(D) \in \mathcal{P} = \mathsf{Bd}(\mathsf{CH}(\mathcal{D}))$, with $\mathsf{Bd}(\hat{O}) = \sum_{x=1}^{N_f} \Pi_x \hat{O} \Pi_x$.
Feedback: given $P \in \mathcal{P}$, find a $D \in \mathcal{D}$ s.t. $\mathsf{Bd}(D) = P$ (representability issues [Lemma 2.8]).

For instance, $F^{\mathsf{LL}}_\alpha(P) = \underset{D\in\mathcal{D}, \mathsf{Bd}(D)=P}{\operatorname{argmin}} \mathcal{E}^{\mathrm{HF}}_\alpha(D)$, $\quad \mathcal{E}^{\mathrm{HF}}_\alpha(D)$: $\hat{H}_\alpha$ Hartree-Fock energy functional.

DMET equations: impose self-consistency (define $F^{\mathsf{DMET}}_\alpha = F^{\mathsf{LL}}_\alpha \circ F^{\mathsf{HL}}_\alpha$), i.e.

$$\left\{ \begin{array}{l} D = F^{\mathsf{LL}}_\alpha(P) \in \mathcal{D} \\ P = F^{\mathsf{HL}}_\alpha(D) \in \mathcal{P} \end{array} \right. \iff \left\{ \begin{array}{l} \boxed{D = F^{\mathsf{DMET}}_\alpha(D), D \in \mathcal{D}} \\ P = F^{\mathsf{HL}}_\alpha(D) \in \mathcal{P}. \end{array} \right.$$

Mathematical starting point: DMET "is exact in the non-interacting [...] limit" [Knizia, 2012].

Consider $\hat{H}_\alpha = d\Gamma(H^0) + \alpha \hat{H}^I$, with $\alpha \in [0,1]$ **small**.

Weakly interacting uniqueness

Proposition 2.1: DMET non-interacting exactness, $\alpha = 0$

Under the following assumptions on H^0 and $(X_x)_{x\in[\![1,N]\!]}$:

A1) The one-particle Hamiltonian H^0 has an energy gap: $\epsilon_N < 0 < \epsilon_{N+1}$,

A2) The associated unique ground-state 1-RDM $D_0 = \chi_{\mathbb{R}_-}(H^0)$ satisfies $\dim(W_{x,D_0}) = 2L_x$,

the 1-RDM D_0 is **a** fixed point of the non-interacting F_0^{DMET} (**nothing ensures it is unique** !).

Weakly interacting uniqueness

Proposition 2.1: DMET non-interacting exactness, $\alpha = 0$

Under the following assumptions on H^0 and $(X_x)_{x\in[\![1,N]\!]}$:

A1) The one-particle Hamiltonian H^0 has an energy gap: $\epsilon_N < 0 < \epsilon_{N+1}$,

A2) The associated unique ground-state 1-RDM $D_0 = \chi_{\mathbb{R}_-}(H^0)$ satisfies $\dim(W_{x,D_0}) = 2L_x$,

the 1-RDM D_0 is **a** fixed point of the non-interacting F_0^{DMET} (**nothing ensures it is unique** !).

Theorem 2.4: DMET weakly interacting locally unique solution, α small

Under the following extra assumptions on H^0 and $(X_x)_{x\in[\![1,N_f]\!]}$:

A3) The block-diagonal map Bd is surjective from $\mathcal{T}_{D_0}\mathcal{D}$ to $\mathcal{T}_{F_0^{\mathrm{LL}}(D_0)}\mathcal{P}$,

A4) The response function $R : \mathcal{T}_{F_0^{\mathrm{LL}}(D_0)}\mathcal{P} \to \mathcal{T}_{F_0^{\mathrm{LL}}(D_0)}\mathcal{P}$ is invertible [Eq. 2.26],

there exists $\alpha_+ > 0$ and a **neighborhood** ω of D_0 in D s.t. for all $\alpha \in [0, \alpha_+)$,

$$D = F_\alpha^{\mathrm{DMET}}(D), \quad D \in \omega \quad \text{has a } \textbf{unique} \text{ solution } D_\alpha^{\mathrm{DMET}}.$$

Weakly interacting exactness

Theorem 2.4 (bis): the solution is analytic and exact at 0th order

Moreover, $\alpha \mapsto D_\alpha^{\mathsf{DMET}}$ is real-analytic on $[0, \alpha_+)$ and such that $D_0^{\mathsf{DMET}} = D_0 = \chi_{\mathbb{R}_-}(H^0)$.

Proof's idea: implicit function theorem. "Physical": shares properties of the *exact* solution.

Weakly interacting exactness

Theorem 2.4 (bis): the solution is analytic and exact at 0th order

Moreover, $\alpha \mapsto D_\alpha^{\mathrm{DMET}}$ is real-analytic on $[0, \alpha_+)$ and such that $D_0^{\mathrm{DMET}} = D_0 = \chi_{\mathbb{R}_-}(H^0)$.

Proof's idea: implicit function theorem. "Physical": shares properties of the *exact* solution.

Theorem 2.5: DMET is exact up to $O(\alpha^2)$

Under the same assumptions (A1)-(A4), it holds $D_\alpha^{\mathrm{DMET}} = D_\alpha^{\mathrm{exact}} + O(\alpha^2)$.

Weakly interacting exactness

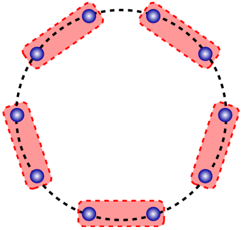
Theorem 2.4 (bis): the solution is analytic and exact at 0th order

Moreover, $\alpha \mapsto D_\alpha^{\mathrm{DMET}}$ is real-analytic on $[0, \alpha_+)$ and such that $D_0^{\mathrm{DMET}} = D_0 = \chi_{\mathbb{R}_-}(H^0)$.

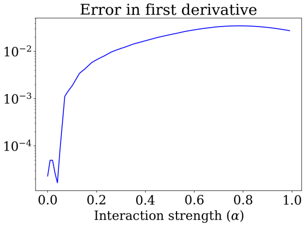
Proof's idea: implicit function theorem. "Physical": shares properties of the *exact* solution.

Theorem 2.5: DMET is exact up to $O(\alpha^2)$

Under the same assumptions (A1)-(A4), it holds $D_\alpha^{\mathrm{DMET}} = D_\alpha^{\mathrm{exact}} + O(\alpha^2)$.



(a) H_{10} molecule and its fragmentation (ST0-6G)



(b) First derivative error, w.r.t. α.

Outline

Green's functions: dynamic correlations ...

Hamiltonian dynamics on a C*-algebra: strongly continuous one-parameter unitary semigroup.
Heisenberg picture $\mathbb{H} : \hat{O} \mapsto (\mathbb{H}(\hat{O}) : t \mapsto e^{it\hat{H}} \hat{O} e^{-it\hat{H}})$ (useful: $\langle O \rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

Green's functions: dynamic correlations ...

Hamiltonian dynamics on a C*-algebra: strongly continuous one-parameter unitary semigroup. **Heisenberg picture** $\mathbb{H} : \hat{O} \mapsto (\mathbb{H}(\hat{O}) : t \mapsto e^{it\hat{H}}\hat{O}e^{-it\hat{H}})$ (useful: $\langle O\rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

Definition (One-body time-ordered Green's function: linear comb. of dynamic correlations)

Given an associated equilibrium state Ω, the one-body time-ordered Green's function is the unique **bounded-operator**-valued map $\tilde{G} : \mathbb{R} \to B(\mathcal{H})$ defined by, $\forall t \in \mathbb{R}, \forall \phi, \phi' \in \mathcal{H}$,

$$\langle \phi, (i\tilde{G}(t))\phi'\rangle = \underbrace{\chi_{\mathbb{R}_+}(t)\Omega\left(\mathbb{H}(\hat{a}_\phi)(t)\hat{a}^\dagger_{\phi'}\right)}_{\text{added particle}} - \underbrace{\chi_{\mathbb{R}_-}(t)\Omega\left(\hat{a}^\dagger_{\phi'}\mathbb{H}(\hat{a}_\phi)(t)\right)}_{\text{added hole}}.$$

Green's functions: dynamic correlations ...

Hamiltonian dynamics on a C*-algebra: strongly continuous one-parameter unitary semigroup.
Heisenberg picture $\mathbb{H} : \hat{O} \mapsto (\mathbb{H}(\hat{O}) : t \mapsto e^{it\hat{H}}\hat{O}e^{-it\hat{H}})$ (useful: $\langle O\rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

Definition (One-body time-ordered Green's function: linear comb. of dynamic correlations)

Given an associated equilibrium state Ω, the one-body time-ordered Green's function is the unique **bounded-operator**-valued map $\tilde{G} : \mathbb{R} \to B(\mathcal{H})$ defined by, $\forall t \in \mathbb{R}, \forall \phi, \phi' \in \mathcal{H}$,

$$\langle \phi, (i\tilde{G}(t))\phi'\rangle = \underbrace{\chi_{\mathbb{R}_+}(t)\Omega\left(\mathbb{H}(\hat{a}_\phi)(t)\hat{a}^\dagger_{\phi'}\right)}_{\text{added particle}} - \underbrace{\chi_{\mathbb{R}_-}(t)\Omega\left(\hat{a}^\dagger_{\phi'}\mathbb{H}(\hat{a}_\phi)(t)\right)}_{\text{added hole}}.$$

- Quantum Green's functions are **explicitly defined** as **dynamic correlations**.

Green's functions: dynamic correlations ...

Hamiltonian dynamics on a C*-algebra: strongly continuous one-parameter unitary semigroup.
Heisenberg picture $\mathbb{H} : \hat{O} \mapsto (\mathbb{H}(\hat{O}) : t \mapsto e^{it\hat{H}}\hat{O}e^{-it\hat{H}})$ (useful: $\langle O\rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

Definition (One-body time-ordered Green's function: linear comb. of dynamic correlations)

Given an associated equilibrium state Ω, the one-body time-ordered Green's function is the unique **bounded-operator**-valued map $\tilde{G} : \mathbb{R} \to B(\mathcal{H})$ defined by, $\forall t \in \mathbb{R}, \forall \phi, \phi' \in \mathcal{H}$,

$$\langle \phi, (i\tilde{G}(t))\phi'\rangle = \underbrace{\chi_{\mathbb{R}_+}(t)\Omega\left(\mathbb{H}(\hat{a}_\phi)(t)\hat{a}^\dagger_{\phi'}\right)}_{\text{added particle}} - \underbrace{\chi_{\mathbb{R}_-}(t)\Omega\left(\hat{a}^\dagger_{\phi'}\mathbb{H}(\hat{a}_\phi)(t)\right)}_{\text{added hole}}.$$

- Quantum Green's functions are **explicitly defined** as **dynamic correlations**.
- **Enough for**: average energy (Galitskii-Migdal, $\hat{H}^I$ two-body), **metal/ins.** (numerics).

Green's functions: dynamic correlations ...

Hamiltonian dynamics on a C*-algebra: strongly continuous one-parameter unitary semigroup.
Heisenberg picture $\mathbb{H} : \hat{O} \mapsto (\mathbb{H}(\hat{O}) : t \mapsto e^{it\hat{H}}\hat{O}e^{-it\hat{H}})$ (useful: $\langle O\rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

Definition (One-body time-ordered Green's function: linear comb. of dynamic correlations)

Given an associated equilibrium state Ω, the one-body time-ordered Green's function is the unique **bounded-operator**-valued map $\tilde{G} : \mathbb{R} \to B(\mathcal{H})$ defined by, $\forall t \in \mathbb{R}, \forall \phi, \phi' \in \mathcal{H}$,

$$\langle \phi, (i\tilde{G}(t))\phi'\rangle = \underbrace{\chi_{\mathbb{R}_+}(t)\Omega\left(\mathbb{H}(\hat{a}_\phi)(t)\hat{a}^\dagger_{\phi'}\right)}_{\text{added particle}} - \underbrace{\chi_{\mathbb{R}_-}(t)\Omega\left(\hat{a}^\dagger_{\phi'}\mathbb{H}(\hat{a}_\phi)(t)\right)}_{\text{added hole}}.$$

- Quantum Green's functions are **explicitly defined** as **dynamic correlations**.
- **Enough for**: average energy (Galitskii-Migdal, $\hat{H}^I$ two-body), **metal/ins.** (numerics).
- Experimentally "**measurable**": in Angle Resolved PhotoEmission Spectroscopy (ARPES).

Green's functions: ... are Green's functions if **non-interacting**.

Non-interacting electrons: $\hat{H} = d\Gamma(H^0)$ with $H^0 \in \mathcal{S}(\mathcal{H}) \Rightarrow \mathbb{H}(\hat{a}_\phi)(t) = \hat{a}_{e^{itH^0}\phi}$.

Green's functions: ... are Green's functions if **non-interacting**.

Non-interacting electrons: $\hat{H} = d\Gamma(H^0)$ with $H^0 \in \mathcal{S}(\mathcal{H}) \Rightarrow \mathbb{H}(\hat{a}_\phi)(t) = \hat{a}_{e^{itH^0}\phi}$.

When Green is Green: non-interacting electrons.

In this case, $\tilde{G}$ satisfies in the distribution sense, for all $\phi \in D(H^0)$ $\left(i\frac{d}{dt} - H^0\right)\tilde{G}\phi = \delta_0\phi$.
Its Generalized Fourier Transform $G : \mathbb{C}_+ \to B(\mathcal{H})$, defined by $(\mathbb{C}_+ = \{\Im(z) > 0\})$

$$G(z) = G_+(z) + G_-(\overline{z})^\dagger, \quad G_+(z) = \int_{\mathbb{R}_+} e^{izt}\tilde{G}(t)dt, \quad G_-(z) = \int_{\mathbb{R}_-} e^{izt}\tilde{G}(t)dt.$$

is well-defined and is the **resolvent** of H^0: for all $z \in \mathbb{C}_+$, $\boxed{G(z) = \left(z - H^0\right)^{-1}}$.

Green's functions: ... are Green's functions if **non-interacting**.

Non-interacting electrons: $\hat{H} = d\Gamma(H^0)$ with $H^0 \in \mathcal{S}(\mathcal{H}) \Rightarrow \mathbb{H}(\hat{a}_\phi)(t) = \hat{a}_{e^{itH^0}\phi}$.

When Green is Green: non-interacting electrons.

In this case, $\tilde{G}$ satisfies in the distribution sense, for all $\phi \in D(H^0)$ $\left(i\frac{d}{dt} - H^0\right)\tilde{G}\phi = \delta_0\phi$.
Its Generalized Fourier Transform $G : \mathbb{C}_+ \to B(\mathcal{H})$, defined by ($\mathbb{C}_+ = \{\Im(z) > 0\}$)

$$G(z) = G_+(z) + G_-(\overline{z})^\dagger, \quad G_+(z) = \int_{\mathbb{R}_+} e^{izt}\tilde{G}(t)dt, \quad G_-(z) = \int_{\mathbb{R}_-} e^{izt}\tilde{G}(t)dt.$$

is well-defined and is the **resolvent** of H^0: for all $z \in \mathbb{C}_+$, $\boxed{G(z) = \left(z - H^0\right)^{-1}}$.

- In general, $-G$ is **Nevanlinna-Pick funct.**: $G(z) = \int_{\mathbb{R}} \frac{1}{z-\varepsilon}dA(\varepsilon)$, $\quad A \geq 0$ ($B(\mathcal{H})$-valued)

Green's functions: ... are Green's functions if **non-interacting**.

Non-interacting electrons: $\hat{H} = d\Gamma(H^0)$ with $H^0 \in \mathcal{S}(\mathcal{H}) \Rightarrow \mathbb{H}(\hat{a}_\phi)(t) = \hat{a}_{e^{itH^0}\phi}$.

When Green is Green: non-interacting electrons.

In this case, $\tilde{G}$ satisfies in the distribution sense, for all $\phi \in D(H^0)$ $\left(i\frac{d}{dt} - H^0\right)\tilde{G}\phi = \delta_0\phi$.
Its Generalized Fourier Transform $G : \mathbb{C}_+ \to B(\mathcal{H})$, defined by ($\mathbb{C}_+ = \{\Im(z) > 0\}$)

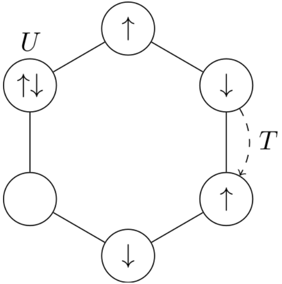
$$G(z) = G_+(z) + G_-(\overline{z})^\dagger, \quad G_+(z) = \int_{\mathbb{R}_+} e^{izt}\tilde{G}(t)dt, \quad G_-(z) = \int_{\mathbb{R}_-} e^{izt}\tilde{G}(t)dt.$$

is well-defined and is the **resolvent** of H^0: for all $z \in \mathbb{C}_+$, $\boxed{G(z) = \left(z - H^0\right)^{-1}}$.

- In general, $-G$ is **Nevanlinna-Pick funct.**: $G(z) = \int_{\mathbb{R}} \frac{1}{z-\varepsilon}dA(\varepsilon)$, $\quad A \geq 0$ ($B(\mathcal{H})$-valued)
- $\dim(\mathcal{H}) < +\infty$: Källen-Lehmann, **spectral measure** A describes **one-body excitations**,

$$\langle \phi, G(z)\phi' \rangle = \sum_{\psi,\psi' \in \mathcal{B}} \frac{\rho_\psi + \rho_{\psi'}}{z + (E_\psi - E_{\psi'})} \langle \psi, \hat{a}_\phi \psi' \rangle \langle \psi', \hat{a}^\dagger_{\phi'} \psi \rangle, \quad \hat{H}\psi = E_\psi \psi, \quad \hat{\rho}\psi = \rho_\psi \psi.$$

Hubbard model: interacting electrons on a graph



(a) Hubbard model on C_6.

Analytic solutions: [Lieb 2001].

- Given a **finite graph** $\mathcal{G}_H = (\Lambda, E)$, the Fock space is

$$\mathcal{F}_H = \bigotimes_{i\in\Lambda} \mathcal{F}_1, \quad \mathcal{F}_1 = \mathrm{Span}(|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle).$$

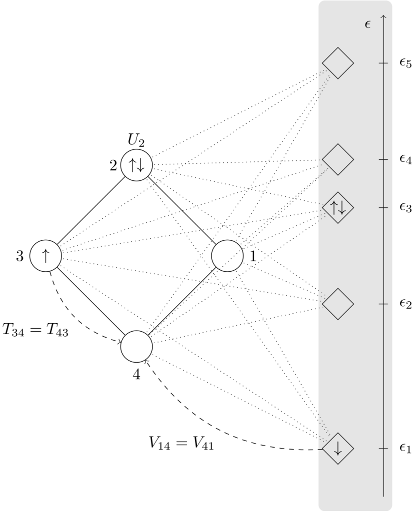
- Given a hopping matrix $T : E \to \mathbb{R}$ and an on-site repulsion $U : \Lambda \to \mathbb{R}$, the Hamiltonian is

$$\hat{H}_H = \hat{H}^0 + \hat{H}^I \in \mathcal{S}(\mathcal{F}_H), \text{ with}$$

$$\hat{H}^0 = \sum_{\substack{\{i,j\}\in E \\ \sigma=\uparrow,\downarrow}} T_{i,j} \left(\hat{a}^\dagger_{i,\sigma}\hat{a}_{j,\sigma} + \hat{a}^\dagger_{j,\sigma}\hat{a}_{i,\sigma}\right),$$

$$\hat{H}^I = \sum_{i\in\Lambda} U_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}, \quad \hat{n}_{i,\sigma} = \hat{a}^\dagger_{i,\sigma}\hat{a}_{i,\sigma}.$$

Anderson Impurity Model (AIM): an embedded Hubbard model



(a) AIM with $\mathcal{G}_H = C_4$ and $B = 5$.

- Given $B \in \mathbb{N}$ a bath dimension,

$$\mathcal{F}_{\mathrm{AIM}} = \mathcal{F}_H \otimes \mathcal{F}_{\mathrm{bath}}, \quad \mathcal{F}_{\mathrm{bath}} = \bigotimes_{i=1}^{B} \mathcal{F}_1$$

- Given bath levels $\epsilon : [\![1, B]\!] \to \mathbb{R}$ and a coupling $V : [\![1, B]\!] \times \Lambda \to \mathbb{R}$,

$$\hat{H}_{\mathrm{AIM}} = \hat{H}_H + \hat{H}^0_{\mathrm{bath}} + \hat{H}^0_{\mathrm{int}}, \text{ with}$$

$$\hat{H}^0_{\mathrm{bath}} = \sum_{k \in [\![1,B]\!]} \epsilon_k \left(\hat{n}_{k,\uparrow} + \hat{n}_{k,\downarrow} \right),$$

$$\hat{H}^0_{\mathrm{int}} = \sum_{\substack{k \in [\![1,B]\!] \\ i \in \Lambda, \sigma = \uparrow,\downarrow}} V_{k,i} \left(\hat{a}^\dagger_{k,\sigma} \hat{a}_{i,\sigma} + \hat{a}^\dagger_{i,\sigma} \hat{a}_{k,\sigma} \right).$$

Self-energy and hybridization functions

For finite dimensional systems, assuming $\hat{H} = d\Gamma(H^0) + \hat{H}^I$, (Hubbard and AIM),

Self-energy and hybridization functions

For finite dimensional systems, assuming $\hat{H} = d\Gamma(H^0) + \hat{H}^I$, (Hubbard and AIM),

Definition (Self-energy: Σ s.t. $G(z) = \left(z - (H^0 + \Sigma(z))\right)^{-1}$ (local *non-interacting* picture))

Given Ω, the self-energy is the unique bounded operators $\Sigma : \mathbb{C}_+ \to B(\mathcal{H})$ defined by, $\forall z \in \mathbb{C}_+$,

$$\Sigma(z) = \left(G^0(z)\right)^{-1} - G(z)^{-1} = z - H^0 - G(z)^{-1} \qquad (-\Sigma \text{ is } \textbf{Nevanlinna-Pick}.)$$

Self-energy and hybridization functions

For finite dimensional systems, assuming $\hat{H} = d\Gamma(H^0) + \hat{H}^I$, (Hubbard and AIM),

Definition (Self-energy: Σ s.t. $G(z) = \left(z - (H^0 + \Sigma(z))\right)^{-1}$ (local *non-interacting* picture))

Given Ω, the self-energy is the unique bounded operators $\Sigma : \mathbb{C}_+ \to B(\mathcal{H})$ defined by, $\forall z \in \mathbb{C}_+$,

$$\Sigma(z) = \left(G^0(z)\right)^{-1} - G(z)^{-1} = z - H^0 - G(z)^{-1}$$

($-\Sigma$ is **Nevanlinna-Pick**.)

Definition (Hybridization: Δ s.t. $G^0(z)_{\text{imp}} = \left(z - (H^0_{\text{imp}} + \Delta(z))\right)^{-1}$ (local *isolated* picture))

For an AIM, $\mathcal{H} = \mathcal{H}_{\text{imp}} \oplus \mathcal{H}_{\text{imp}}^\perp$, the hybridization function $\Delta : \mathbb{C}_+ \to B(\mathcal{H}_{\text{imp}}$ is defined by

$$\Delta(z) = z - H^0_{\text{imp}} - \left(G^0(z)_{\text{imp}}\right)^{-1}$$

(Schur complement). ($-\Delta$ is **Nevanlinna-Pick**)

Self-energy and hybridization functions

For finite dimensional systems, assuming $\hat{H} = d\Gamma(H^0) + \hat{H}^I$, (Hubbard and AIM),

Definition (Self-energy: Σ s.t. $G(z) = \left(z - (H^0 + \Sigma(z))\right)^{-1}$ (local *non-interacting* picture))

Given Ω, the self-energy is the unique bounded operators $\Sigma : \mathbb{C}_+ \to B(\mathcal{H})$ defined by, $\forall z \in \mathbb{C}_+$,

$$\Sigma(z) = \left(G^0(z)\right)^{-1} - G(z)^{-1} = z - H^0 - G(z)^{-1}$$

($-\Sigma$ is **Nevanlinna-Pick**.)

Definition (Hybridization: Δ s.t. $G^0(z)_{\text{imp}} = \left(z - (H^0_{\text{imp}} + \Delta(z))\right)^{-1}$ (local *isolated* picture))

For an AIM, $\mathcal{H} = \mathcal{H}_{\text{imp}} \oplus \mathcal{H}_{\text{imp}}^{\perp}$, the hybridization function $\Delta : \mathbb{C}_+ \to B(\mathcal{H}_{\text{imp}}$ is defined by

$$\Delta(z) = z - H^0_{\text{imp}} - \left(G^0(z)_{\text{imp}}\right)^{-1} \quad \text{(Schur complement).}$$

($-\Delta$ is **Nevanlinna-Pick**)

DMFT foundation: sparsity pattern and impurity solver [Lin, Lindsey 2019], [Proposition 3.2.8]

Given an AIM $(\mathcal{G}_H, T, U, B, \epsilon, V)$, $\Sigma_{\text{AIM}} = \Sigma_{\text{imp}} \oplus 0$ and $\Sigma_{\text{imp}} = \text{ImpSolv}_{\mathcal{G}_H,T,U,\Omega}(\Delta)$.

Dynamical Mean-Field Theory (DMFT) equations

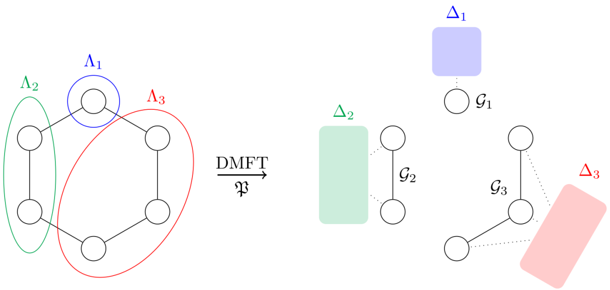
DMFT **goal**: G associated to Gibb's states $\hat{\rho} = \frac{1}{Z} e^{-\beta\left(\hat{H} - \mu \hat{N}\right)}$ of **Hubbard** $(\mathcal{G}_H = (\Lambda, E), T, U)$

Dynamical Mean-Field Theory (DMFT) equations

DMFT **goal**: G associated to Gibb's states $\hat{\rho} = \frac{1}{Z} e^{-\beta\left(\hat{H} - \mu \hat{N}\right)}$ of **Hubbard** $(\mathcal{G}_H = (\Lambda, E), T, U)$
DMFT **principle**: approximate using **many but simpler** $(G_i)_{i \in [\![1, |\mathfrak{P}|]\!]}$ of Gibb's states of **AIM**.

Dynamical Mean-Field Theory (DMFT) equations

DMFT **goal**: G associated to Gibb's states $\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu \hat{N})}$ of **Hubbard** $(\mathcal{G}_H = (\Lambda, E), T, U)$
DMFT **principle**: approximate using **many but simpler** $(G_i)_{i \in [\![1, |\mathfrak{P}|]\!]}$ of Gibb's states of **AIM**.



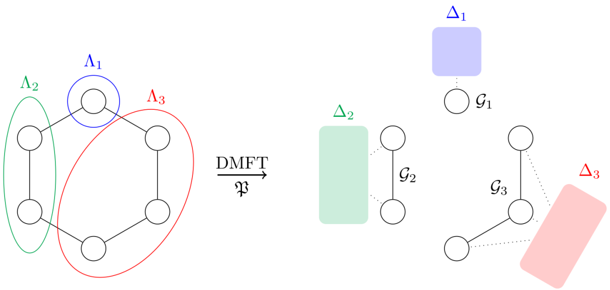
DMFT equations:

$$G_{i,\mathrm{imp}}(\Delta_i) = G_{\mathrm{DMFT},i}$$
$$G_{\mathrm{DMFT}}^{-1} = G_H^{0,-1} - \Sigma_{\mathrm{DMFT}}$$
$$\Sigma_{\mathrm{DMFT}} = \bigoplus_{i=1}^{|\mathfrak{P}|} \Sigma_{i,\mathrm{imp}}$$
$$\Sigma_{i,\mathrm{imp}} = \mathrm{ImpSolv}_i(\Delta_i)$$

DMFT **parameters (fixed)**:

Dynamical Mean-Field Theory (DMFT) equations

DMFT **goal**: G associated to Gibb's states $\hat{\rho} = \frac{1}{Z} e^{-\beta(\hat{H} - \mu \hat{N})}$ of **Hubbard** $(\mathcal{G}_H = (\Lambda, E), T, U)$
DMFT **principle**: approximate using **many but simpler** $(G_i)_{i \in [\![1, |\mathfrak{P}|]\!]}$ of Gibb's states of **AIM**.



DMFT equations:

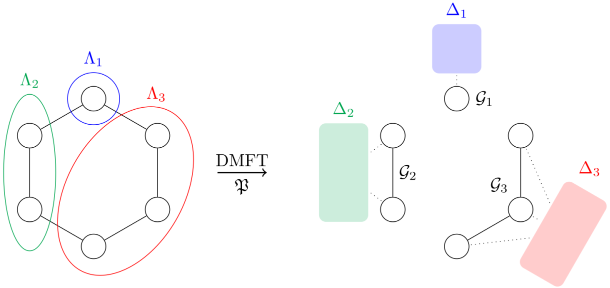
$$
\begin{aligned}
G_{i,\mathrm{imp}}(\Delta_i) &= G_{\mathrm{DMFT},i} \\
G_{\mathrm{DMFT}}^{-1} &= G_H^{0,-1} - \Sigma_{\mathrm{DMFT}} \\
\Sigma_{\mathrm{DMFT}} &= \bigoplus_{i=1}^{|\mathfrak{P}|} \Sigma_{i,\mathrm{imp}} \\
\Sigma_{i,\mathrm{imp}} &= \mathrm{ImpSolv}_i(\Delta_i)
\end{aligned}
$$

DMFT **parameters (fixed)**:

1. **Partition** $\mathfrak{P} = (\Lambda_i)_{i \in [\![1, |\Lambda|]\!]}$ of Λ. **Our work: singletons.**

Dynamical Mean-Field Theory (DMFT) equations

DMFT **goal**: G associated to Gibb's states $\hat\rho = \frac{1}{Z} e^{-\beta(\hat H - \mu \hat N)}$ of **Hubbard** $(\mathcal{G}_H = (\Lambda, E), T, U)$
DMFT **principle**: approximate using **many but simpler** $(G_i)_{i \in [\![1, |\mathfrak{P}|]\!]}$ of Gibb's states of **AIM**.



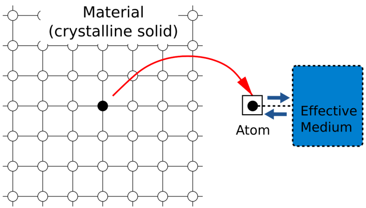
DMFT equations:

$$\begin{aligned} G_{i,\mathrm{imp}}(\Delta_i) &= G_{\mathrm{DMFT},i} \\ G_{\mathrm{DMFT}}^{-1} &= G_H^{0,-1} - \Sigma_{\mathrm{DMFT}} \\ \Sigma_{\mathrm{DMFT}} &= \bigoplus_{i=1}^{|\mathfrak{P}|} \Sigma_{i,\mathrm{imp}} \\ \Sigma_{i,\mathrm{imp}} &= \mathrm{ImpSolv}_i(\Delta_i) \end{aligned}$$

DMFT **parameters (fixed)**:

1. **Partition** $\mathfrak{P} = (\Lambda_i)_{i \in [\![1, |\Lambda|]\!]}$ of Λ. **Our work: singletons**.
2. **Approximation** of $\mathrm{ImpSolv}$ ($\simeq$ DFT universal functional). **Our work: IPT** approximation.

The Iterated Perturbation Theory (IPT) impurity solver (vanilla)



- Freq. used in physics.
- 2nd order pert. in U.
- Figure: [Georges 2016].

Assumptions: single-site translation-invariant paramagnetic DMFT (half-filling)

Assume that $|\mathfrak{P}| = |\Lambda|$ and $(\mathcal{G}_H, T, U)$ is a (weighted) **vertex-transitive** graph.
Restrict to solutions $\forall i \in \mathfrak{P}, \quad -\Delta_i = -\Delta : \mathbb{C}_+ \to \overline{\mathbb{C}_+}, \quad -\Sigma_{i,\mathrm{imp}} = -\Sigma : \mathbb{C}_+ \to \overline{\mathbb{C}_+}$.

$\mathrm{IPT}_\beta(U \in \mathbb{R}, \Delta)$: defined in Matsubara's formalism, temperature $1/\beta$, **analytic continuation**:

Find Σ analytic s.t. $\Im(-\Sigma) \geq 0$ **(Nevanlinna-Pick function)** and $\forall n \in \mathbb{N}, \quad \Sigma(i\omega_n) = \Sigma_n^{\mathrm{IPT}}$,

with $\omega_n = \dfrac{(2n+1)\pi}{\beta}, \quad \Sigma_n^{\mathrm{IPT}} = U^2 \displaystyle\int_0^\beta e^{i\omega_n\tau}\Big(\frac{1}{\beta}\sum_{n' \in \mathbb{Z}} e^{-i\omega_{n'}\tau}\,(i\omega_{n'} - \Delta(i\omega_{n'}))^{-1}\Big)^3 d\tau.$

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_{\perp}^{0} - \Sigma(z)\right)^{-1} W^{\dagger}$$
$$\Sigma = \mathrm{IPT}_{\beta}(U, \Delta)$$

Non-existence of finite dimensional solution

$$\begin{aligned}\Delta(z) &= W\left(z - H^0_\perp - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \\ \Sigma &= \mathrm{IPT}_\beta(U,\Delta)\end{aligned}$$

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_\perp^0 - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \iff \Delta = F^{\mathrm{DMFT}}(\Delta), \Delta \in \mathfrak{D}?$$
$$\Sigma = \mathrm{IPT}_\beta(U, \Delta)$$

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_\perp^0 - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \iff \Delta = F^{\mathrm{DMFT}}(\Delta), \Delta \in \mathfrak{D}?$$
$$\Sigma = \mathrm{IPT}_\beta(U, \Delta)$$

Fact (Functional spaces for finite dimensional bath: mathematical starting point)

For an AIM, $\Delta(z) = \sum_{k=1}^{B} \frac{|V_k|^2}{z - \epsilon_k}$. *For* $\Delta \in \mathrm{Ran}(\mathrm{BU}_{\mathcal{G}_H,T})$, $\sum_{k=1}^{B} |V_k|^2 = WW^\dagger \in \mathbb{R}$.

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_\perp^0 - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \iff \Delta = F^{\mathrm{DMFT}}(\Delta), \Delta \in \mathfrak{D}?$$
$$\Sigma = \mathrm{IPT}_\beta(U,\Delta)$$

Fact (Functional spaces for finite dimensional bath: mathematical starting point)

For an AIM, $\Delta(z) = \sum_{k=1}^{B} \frac{|V_k|^2}{z - \epsilon_k}$. *For* $\Delta \in \mathrm{Ran}(\mathrm{BU}_{\mathcal{G}_H,T}), \sum_{k=1}^{B} |V_k|^2 = WW^\dagger \in \mathbb{R}$.

Try: $\mathfrak{D} = \mathfrak{D}_f = WW^\dagger \mathcal{S}\left(\mathcal{P}(\mathbb{R}) \cap \{\mathrm{supp}(\mu) \text{ fin.}\}\right)$, $\boxed{\mathcal{S}_\mu(z) = \int \frac{d\mu(\epsilon)}{z-\epsilon}}$ (Stieljes transform).

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_\perp^0 - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \iff \Delta = F^{\mathrm{DMFT}}(\Delta), \Delta \in \mathfrak{D}?$$
$$\Sigma = \mathrm{IPT}_\beta(U, \Delta)$$

Fact (Functional spaces for finite dimensional bath: mathematical starting point)

For an AIM, $\Delta(z) = \sum_{k=1}^{B} \frac{|V_k|^2}{z - \epsilon_k}$. *For* $\Delta \in \mathrm{Ran}(\mathrm{BU}_{\mathcal{G}_H,T})$, $\sum_{k=1}^{B} |V_k|^2 = WW^\dagger \in \mathbb{R}$.

Try: $\mathfrak{D} = \mathfrak{D}_f = WW^\dagger \mathcal{S}\left(\mathcal{P}(\mathbb{R}) \cap \{\mathrm{supp}(\mu) \text{ fin.}\}\right)$, $\boxed{\mathcal{S}_\mu(z) = \int \frac{d\mu(\epsilon)}{z - \epsilon}}$ (Stieljes transform).

Proposition (Well-def.: BU[Lindsey 2019], IPT[Prop. 3.2.18]; non-$\exists$ of solution [Prop. 3.3.5])

$\mathrm{BU} : \mathfrak{S}_f \to \mathfrak{D}_f$, $\mathrm{IPT} : \mathfrak{D}_f \to \mathfrak{S}_f$ are well-defined w. $\mathfrak{S}_f = \mathcal{S}(\mathcal{M}_+(\mathbb{R}) \cap \{\mathrm{supp}(\mu) \text{ fin}\})$
Apart from strictly/non interacting cases, $\mathrm{DMFT} = \mathrm{BU} \circ \mathrm{IPT}$ has **no fixed point in** $\mathfrak{D}_f$.

Non-existence of finite dimensional solution

$$\Delta(z) = W\left(z - H_\perp^0 - \Sigma(z)\right)^{-1} W^\dagger = \mathrm{BU}_{\mathcal{G}_H,T}(\Sigma(z)) \iff \Delta = F^{\mathrm{DMFT}}(\Delta), \Delta \in \mathfrak{D}?$$
$$\Sigma = \mathrm{IPT}_\beta(U, \Delta)$$

Fact (Functional spaces for finite dimensional bath: mathematical starting point)

For an AIM, $\Delta(z) = \sum_{k=1}^{\mathbf{B}\to\infty} \frac{|V_k|^2}{z-\epsilon_k}$. *For* $\Delta \in \mathrm{Ran}(\mathrm{BU}_{\mathcal{G}_H,T})$, $\sum_{k=1}^{B} |V_k|^2 = WW^\dagger \in \mathbb{R}$.

Try: $\mathfrak{D} = \mathfrak{D}_f = WW^\dagger \mathcal{S}\left(\mathcal{P}(\mathbb{R}) \cap \{\mathrm{supp}(\mu) \text{ fin.}\}\right)$, $\boxed{\mathcal{S}_\mu(z) = \int \frac{d\mu(\epsilon)}{z-\epsilon}}$ (Stieljes transform).

Proposition (Well-def.: BU[Lindsey 2019], IPT[Prop. 3.2.18]; non-∃ of solution [Prop. 3.3.5])

$\mathrm{BU} : \mathfrak{S}_f \to \mathfrak{D}_f$, $\mathrm{IPT} : \mathfrak{D}_f \to \mathfrak{S}_f$ are well-defined w. $\mathfrak{S}_f = \mathcal{S}(\mathcal{M}_+(\mathbb{R}) \cap \{\mathrm{supp}(\mu) \text{ fin}\})$
Apart from strictly/non interacting cases, $\mathrm{DMFT} = \mathrm{BU} \circ \mathrm{IPT}$ has **no fixed point in** $\mathfrak{D}_f$.

Extension of domain and existence

Extension: $\boxed{\mathfrak{D} = WW^\dagger \mathcal{S}(\mathcal{P}(\mathbb{R})), \quad \mathfrak{S} = \mathcal{S}(\mathcal{M}_+(\mathbb{R}))}$

Extension of domain and existence

Extension: $\boxed{\mathfrak{D} = WW^{\dagger}\mathcal{S}(\mathcal{P}(\mathbb{R})), \quad \mathfrak{S} = \mathcal{S}(\mathcal{M}_{+}(\mathbb{R}))}$

Physics: "**Infinite**" dimensional **bath**. **Mathematics**: **measure analysis** (up to $\mathcal{S}, \mathcal{S}^{-1}$).

Extension of domain and existence

Extension: $\boxed{\mathfrak{D} = WW^\dagger \mathcal{S}(\mathcal{P}(\mathbb{R})), \quad \mathfrak{S} = \mathcal{S}(\mathcal{M}_+(\mathbb{R}))}$

Physics: "**Infinite**" dimensional **bath**. **Mathematics**: **measure analysis** (up to $\mathcal{S}, \mathcal{S}^{-1}$).

[Propositions 3.3.6-3.3.8], BU and IPT for infinite dimensional bath

$\mathrm{BU} : \mathfrak{D} \to \mathfrak{S}$ is well-defined. IPT admits a unique continuous extension $\mathfrak{D} \to \mathfrak{S}$ for the Kantorovich-Rubinstein distance.

Extension of domain and existence

Extension: $\boxed{\mathfrak{D} = WW^\dagger \mathcal{S}(\mathcal{P}(\mathbb{R})), \quad \mathfrak{G} = \mathcal{S}(\mathcal{M}_+(\mathbb{R}))}$

Physics: "**Infinite**" dimensional **bath**. **Mathematics**: **measure analysis** (up to $\mathcal{S}, \mathcal{S}^{-1}$).

[Propositions 3.3.6-3.3.8], BU and IPT for infinite dimensional bath

$\mathrm{BU} : \mathfrak{D} \to \mathfrak{G}$ is well-defined. IPT admits a unique continuous extension $\mathfrak{D} \to \mathfrak{G}$ for the Kantorovich-Rubinstein distance.

Main theorem ([Theorem 3.3.9], [Proposition 3.3.10])

DMFT **admits a fixed point** in $\mathfrak{D}$. Any fixed point admits **fin. moments up to any order**.

Extension of domain and existence

Extension: $\boxed{\mathfrak{D} = WW^\dagger \mathcal{S}(\mathcal{P}(\mathbb{R})), \quad \mathfrak{G} = \mathcal{S}(\mathcal{M}_+(\mathbb{R}))}$

Physics: "**Infinite**" dimensional **bath**. **Mathematics**: **measure analysis** (up to $\mathcal{S}, \mathcal{S}^{-1}$).

[Propositions 3.3.6-3.3.8], BU and IPT for infinite dimensional bath

$\mathrm{BU} : \mathfrak{D} \to \mathfrak{G}$ is well-defined. IPT admits a unique continuous extension $\mathfrak{D} \to \mathfrak{G}$ for the Kantorovich-Rubinstein distance.

Main theorem ([Theorem 3.3.9], [Proposition 3.3.10])

DMFT **admits a fixed point** in $\mathfrak{D}$. Any fixed point admits **fin. moments up to any order**.

Proof (with measures).

DMFT : μ with k-moments $\mapsto k+4$ moments (compactness) and weakly continuous. Schauder(-Singbal) fixed-point theorem on $\mathcal{P}(\mathbb{R})$ (**completeness**). $\square$

Numerical results: Mott transition (Matsubara discretized)

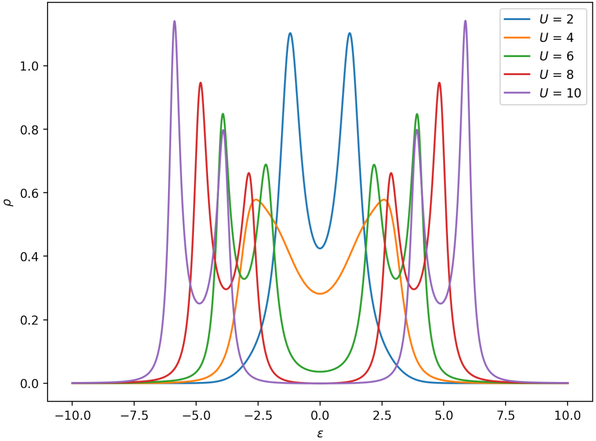


Figure: Spectral function ρ (a.k.a. A): analytic continuation results for the Hubbard dimer ($\beta = 1$). Metallic criteria: $\rho(0) > 0$ (TRIQS simulations).

Outline

Concluding table

	DMFT	DMET
General framework		
Equilibrium state	Gibbs state, $\hat{\rho} = e^{-\beta(\hat{H}-\mu\hat{N})}/Z$	Ground state, $\hat{\rho}$ proj. onto Ψ
Reduced quantity	Green's function G (Pick function)	1-RDM D (self-adjoint)
Model of interest	Hubbard model $(\mathcal{G}_H = (\Lambda, E), T, U)$	Any finite dimensional
Decomposition of $\mathcal{H}$	DMFT partition $\mathfrak{P}$ of Λ	$\perp$ decomposition $\oplus_x X_x$
Mean-field model	Collection of AIMs	Collection of $(W_{x,D}, \hat{H}^{\text{imp}}_{x,D})$
Bath dimension	Infinite (non-interacting)	$\dim(W_{x,D}) = 2\dim(X_x)$
Impurity step	Impurity solver $\Delta \mapsto \Sigma$ (IPT here)	High-level $F^{\text{HL}} : D \mapsto P$
Self-consistency	Bath Update map $\Sigma \mapsto \Delta$	Low-level $F^{\text{LL}} : P \mapsto D$
Mathematical results on self-consistent equations in this thesis		
Existence	Global , conditional Chapter 4	Near $\alpha = 0$, under (A1)-(A4)
Uniqueness	Trivial limits , locally Chapter 4	Near $\alpha = 0$, locally
Exactness	Trivial limits	First order in α, near $\alpha = 0$

Table: Overview table of the main features of DMFT and DMET from the perspective of this thesis.

Perspectives

Regarding **DMET**:

Regarding **DMFT**:

Perspectives

Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).

Regarding **DMFT**:

Perspectives

Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).
- Mathematics of the **finite-temperature** extension
  Physics: [Sun, Ray, Cui, Stoudenmire, Ferrero, Chan 2020].

Regarding **DMFT**:

Perspectives

Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).
- Mathematics of the **finite-temperature** extension
  Physics: [Sun, Ray, Cui, Stoudenmire, Ferrero, Chan 2020].

Regarding **DMFT**:

- Preliminary results: **numerical analysis** Matsubara discretized scheme, new **numerical scheme** and particle-hole **symmetry** condition.

Perspectives

Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).
- Mathematics of the **finite-temperature** extension
  Physics: [Sun, Ray, Cui, Stoudenmire, Ferrero, Chan 2020].

Regarding **DMFT**:

- Preliminary results: **numerical analysis** Matsubara discretized scheme, new **numerical scheme** and particle-hole **symmetry** condition.
- **Uniqueness** to the IPT-DMFT equations.

Perspectives

Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).
- Mathematics of the **finite-temperature** extension
  Physics: [Sun, Ray, Cui, Stoudenmire, Ferrero, Chan 2020].

Regarding **DMFT**:

- Preliminary results: **numerical analysis** Matsubara discretized scheme, new **numerical scheme** and particle-hole **symmetry** condition.
- **Uniqueness** to the IPT-DMFT equations.
- Soon: **Impurity solver** well-posedness (easier setting to study **quantum Luttinger-Ward** functional formalism [Lin, Lindsey 2021]) and higher order solvers (**CTQMC**).

Perspectives

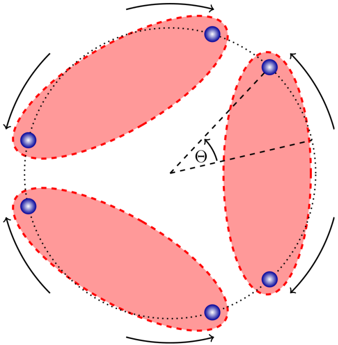
Regarding **DMET**:

- **Strictly** interacting setting (already started by Cancès, Faulstich et al.).
- Mathematics of the **finite-temperature** extension
  Physics: [Sun, Ray, Cui, Stoudenmire, Ferrero, Chan 2020].

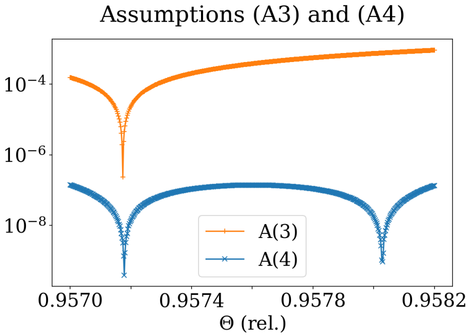
Regarding **DMFT**:

- Preliminary results: **numerical analysis** Matsubara discretized scheme, new **numerical scheme** and particle-hole **symmetry** condition.
- **Uniqueness** to the IPT-DMFT equations.
- Soon: **Impurity solver** well-posedness (easier setting to study **quantum Luttinger-Ward** functional formalism [Lin, Lindsey 2021]) and higher order solvers (**CTQMC**).
- Later: **thermodynamic limits**, "$d = \infty$" exactness [Metzner, Vollhardt 1989].

Numerical results: DMET assumptions' test on H_6.



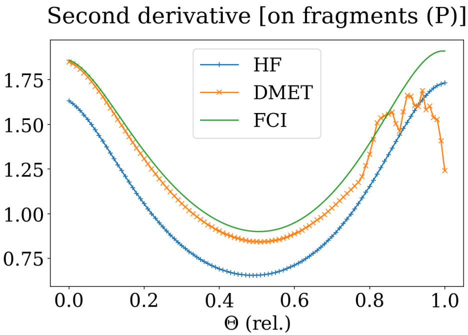
(a) H_6 molecule, with Θ varying.



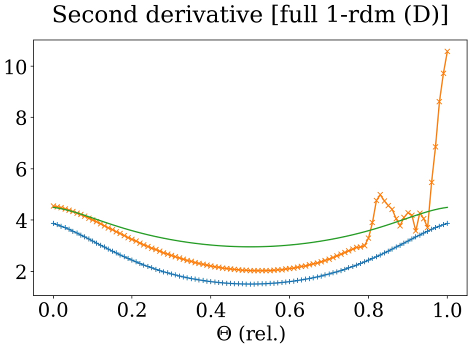
(b) A3 & A4 assumptions, with Θ varying.

Figure: Numerical test of assumptions A3 & A4 on H_6 molecule.

Numerical results: DMET VS Hartree-Fock



(a) $\|\partial_\alpha^2 P_\alpha|_{\alpha=0}\|_F$ for HF, DMET and FCI



(b) $\|\partial_\alpha^2 D_\alpha|_{\alpha=0}\|_F$ for HF, DMET and FCI

Figure: Numerical tests for H_6 molecule, with varying Θ.

Matsubara's frequencies discretized IPT-DMFT equations

Definition (Matsubara discretized scheme)

Given $N_\omega \in \mathbb{N}$ a Matsubara's frequencies cutoff, solve for all $n \in [\![0, N_\omega]\!]$,

$$\Delta_n = W \left(i\omega_n - H_\perp^0 - \Sigma_n\right)^{-1} W^\dagger \tag{3}$$

$$\Sigma_n = U^2 \int_0^\beta e^{i\omega_n \tau} \left(\frac{1}{\beta} \sum_{n'=-(N_\omega+1)}^{N_\omega} e^{-i\omega_{n'}\tau} \left(i\omega_{n'} - \Delta_{n'}\right)^{-1} \right)^3 d\tau \tag{4}$$

with $-\Delta = (-\Delta_n)_{n\in[\![0,N_\omega]\!]}, -\Sigma = (-\Sigma_n)_{n\in[\![0,N_\omega]\!]} \subset \overline{\mathbb{C}_+}^{N_\omega+1}$.

Looks similar: *completely different strategy* (and results !), no Nevanlinna-Pick functions.
$\rightarrow$ Non-physical solutions exist (and are exhibited !).
Only *conditional* existence, *but* uniqueness result (also conditional, finite dimensional).

Theoretical results: conditional existence

$$R_{N_\omega} = \sup\left\{R \in \mathbb{R}_+ \text{ s.t. } \forall z \in B(0,R) \cap \overline{\mathbb{C}_+}^{N_\omega+1}, \forall n \in [\![0, N_\omega]\!], \quad \Im\left(F_{n,N_\omega}(z)\right) \leq 0\right\}, \quad (5)$$

$$\text{where } F_{n,N_\omega}(z) = \sum_{\substack{n_1,n_2,n_3=-(N_\omega+1) \\ n_1+n_2+n_3=n-1}}^{N_\omega} \prod_{i=1}^{3} \left(i(2n_i+1)/\pi + z_{n_i}\right)^{-1}. \quad (6)$$

Theorem 4.2.1: Existence of solution

The critical radius R_{N_ω} is well-defined and > 0. Moreover, $\forall \beta \in \mathbb{R}_+^*$, $W^\dagger \in \mathbb{R}_{L-1}$ satisfying

$$\beta \|W\|_2 \leq \sqrt{2\sqrt{2} R_{N_\omega}}, \quad (7)$$

and $\forall U \in \mathbb{R}$, (3) & (4) admit a solution $(\Delta, \Sigma) \in \mathfrak{D}_{\beta,N_\omega} \times \mathfrak{S}_{\beta,N_\omega,U}$ where

$$\mathfrak{D}_{\beta,N_\omega} = B(0, R_{N_\omega}/\beta) \cap \left(-\overline{\mathbb{C}_+}^{N_\omega+1}\right), \quad \mathfrak{S}_{\beta,N_\omega,U} = \mathrm{IPT}_{N_\omega}(\mathfrak{D}_{\beta,N_\omega}).$$

Theoretical results: conditional uniqueness

$$L_{N_\omega} = \max_{n \in [\![0, N_\omega]\!]} \mathrm{Lip}_{\mathbb{C}_+}(F_{n,N_\omega}). \tag{8}$$

Theorem 4.2.2: Uniqueness of solution

For all $N_\omega \in \mathbb{N}$, $\beta \in \mathbb{R}_+^*$, $W^\dagger \in \mathbb{R}_{L-1}$, $U \in \mathbb{R}$ satisfying with the previous assumption and

$$\left(\frac{\beta^2 \|W\|_2 U}{\pi}\right)^2 L_{N_\omega} < 1,$$

the discretized IPT-DMFT equations (3) (4) admits a unique solution in $\mathfrak{D}_\beta \times \mathfrak{S}_{\beta,N_\omega,U}$. Moreover, the fixed point algorithm sequence $\left(\Delta^{(n)}\right)_{n\in\mathbb{N}}$

$$\Delta^{(0)} \in \mathfrak{D}_\beta, \quad \forall n \in \mathbb{N}, \quad \Delta^{(n+1)} = \mathrm{DMFT}_{N_\omega}(\Delta^{(n)})$$

converges linearly toward this solution.

Numerical results: Matsubara discretized, Hubbard dimer.

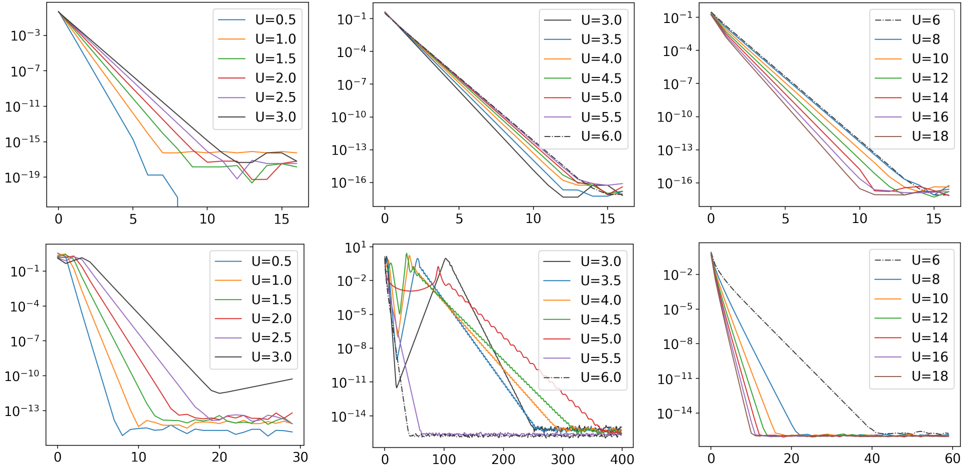
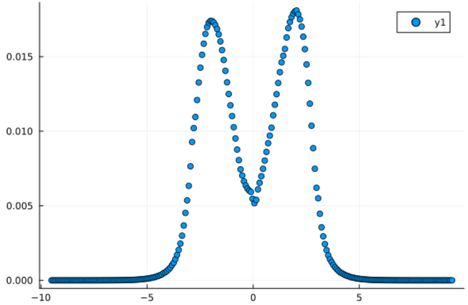


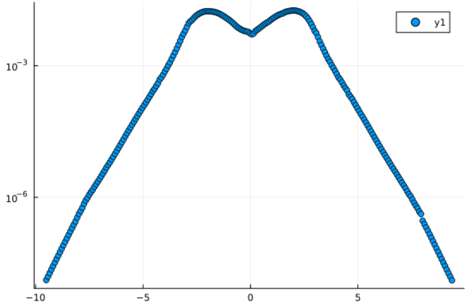
Figure: Residual $\|\Delta^{(n+1)} - \Delta^{(n)}\|_2$ in log scale, for $n \in [\![0, N_{\text{iter}}]\!]$, $\beta = 1$ (top), $\beta = 10$ (bottom).

Preliminary results: new numerical scheme for IPT-DMFT

Solutions: measures with **finite moments** up to any order: show it **numerically**?
New “exact diagonalization”-truncation num. scheme. **without num. analytic continuation**.



(a) Nevanlinna-Pick measure of Δ

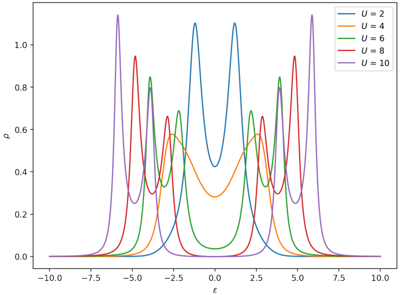


(b) Nevanlinna-Pick measure of Δ (log scale)

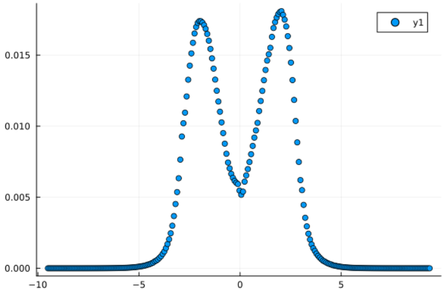
Figure: New ED-truncation scheme results, $U = 4$, $\beta = 0$, Hubbard dimer.
Suggests measure is **exponentially decreasing**: would prove **uniqueness** of the solution!

Preliminary results: particle-hole symmetry (Coulson Rushbrooke)

Hubbard: particle-hole **symmetry** $\iff$ $\mathcal{G}_H$ is **bipartite** [Bach, Solovej, Lieb 1994] (**76** "sym")



(a) Matsubara discretized



(b) New ED-truncation scheme

Theorem (translation invariant IPT-DMFT particle-hole symmetry condition)

Given ν an IPT-DMFT fixed point: ν is **symmetric** $\iff$ $\mathcal{G}_H$ *is* **bipartite**.

Proof: for now, $\beta = 0$ only.