Mathematical and numerical analysis of embedding methods in quantum mechanics

PhD defense - November 18 2024

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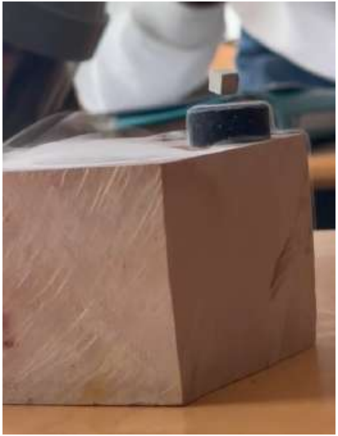
Experiment in pictures

(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

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

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

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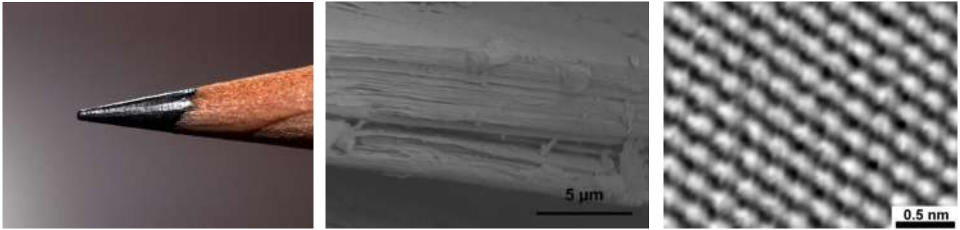
In short: Mathematics of two methods that could explain levitation at $T = 77K$.

Outline

1. Embedding methods in quantum mechanics
   - Why (not) quantum mechanics ?
   - Overview of embedding methods
2. Density Matrix Embedding Theory (DMET)
   - Reduced density matrices and DMET setting
   - Main results and numerical evidences
3. Dynamical Mean-Field Theory (DMFT)
   - Green's functions, Hubbard and Anderson Impurity Model
   - Mathematical (and numerical) results
4. Conclusion and perspectives

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.
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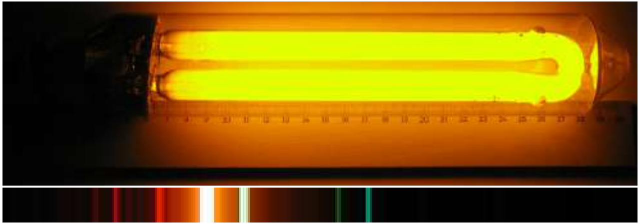
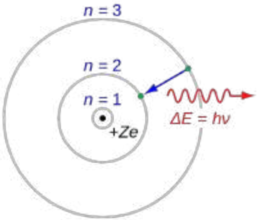


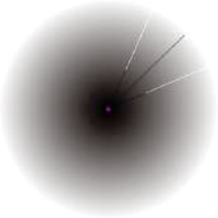
(b) Orange lightning: sodium lamp and its spectrum.

Figure: Quantization of energy in cities lightning system.

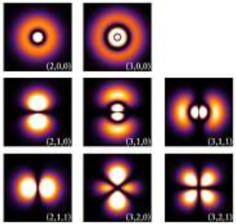
Quantum mechanics in (small) atoms



(a) Bohr model



(b) Probabilistic approach



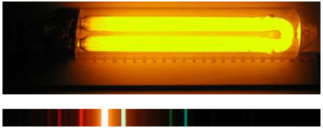
(c) Easy: 1 e^- solutions (H)

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*.

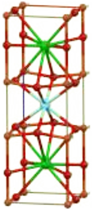
$$\boxed{\hat{H}\Psi = E\Psi, \quad E \in \mathbb{R}} \tag{1}$$

Approximations in quantum mechanics



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

(b) Levitation with YBCO.



(c) Unit cell of YBCO

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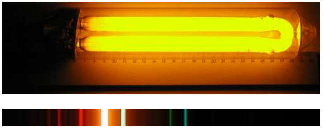

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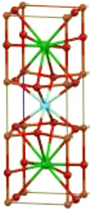

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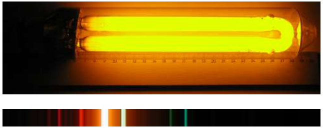

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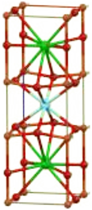

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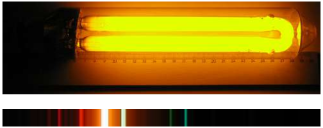

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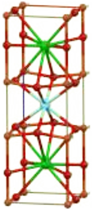

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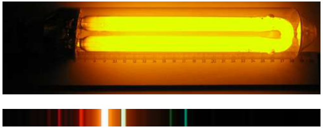

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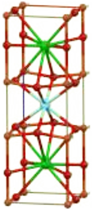

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- **Reduce to smaller but interacting** systems: **embedding methods**, e.g. DMFT, DMET.

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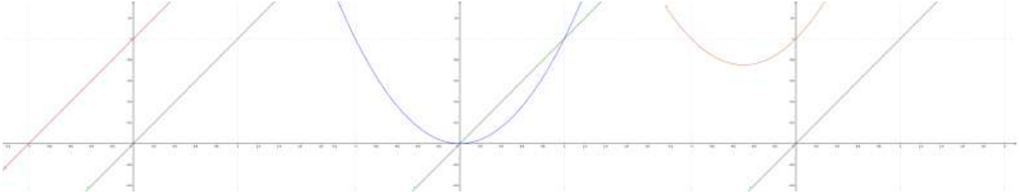
3. Update: low-level map (DMET), bath update map (DMFT).

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

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

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 $(\mathcal{H}, \langle\cdot,\cdot\rangle)$.

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

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

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

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

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

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).

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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 $\phi, \phi' \in \mathcal{H}$,

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

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

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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**
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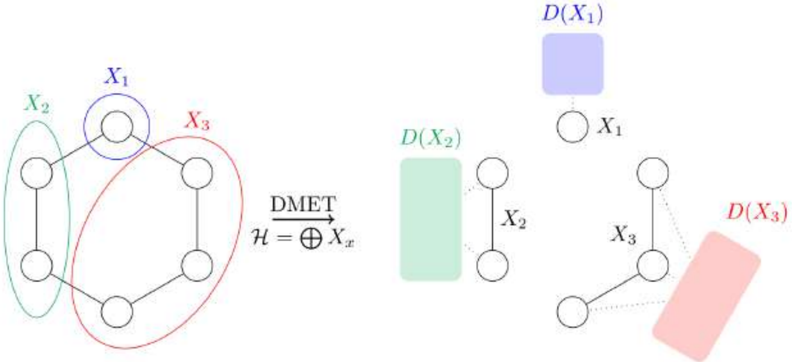

Figure: DMET mapping principle. **Assumption:** $\dim(W_{x,D}) = 2L_x$ **(maximal)**.

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

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

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

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

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

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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** !).

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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 $\mathcal{T}_{F_0^{\text{LL}}(D_0)}\mathcal{P}$,

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

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

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

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.

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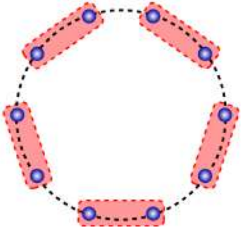
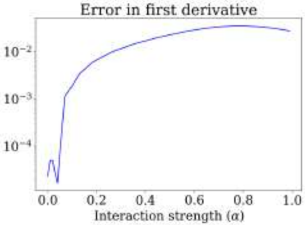


(a) H_{10} molecule and its fragmentation (ST0-6G)



(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: $\langle O\rangle(t) = \Omega(\mathbb{H}(\hat{O})(t))$).

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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, $\forall t \in \mathbb{R}, \forall \phi, \phi' \in \mathcal{H}$,

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

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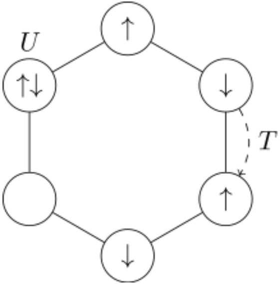
- $\dim(\mathcal{H}) < +\infty$: Källen-Lehmann, **spectral measure** A describes **one-body excitations**,

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

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

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

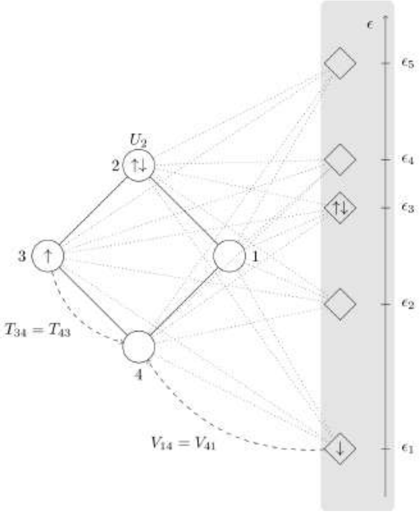
- Given a hopping matrix $T : E \to \mathbb{R}$ and an on-site repulsion $U : \Lambda \to \mathbb{R}$, the Hamiltonian is

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

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

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

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 $V : [\![1, B]\!] \times \Lambda \to \mathbb{R}$,

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

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

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

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** $(\mathcal{G}_H = (\Lambda, E), T, U)$

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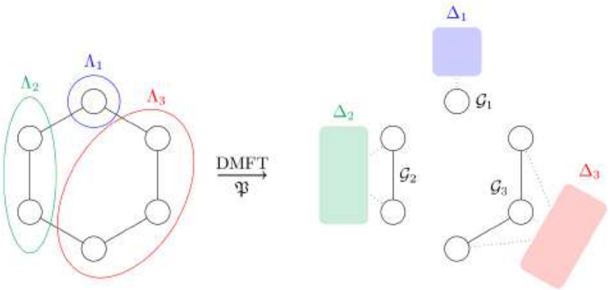

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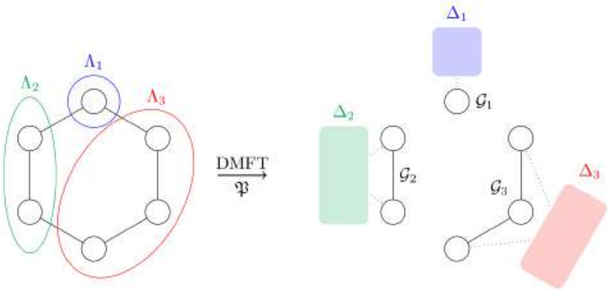

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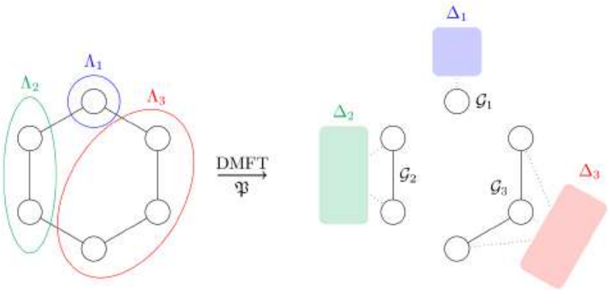

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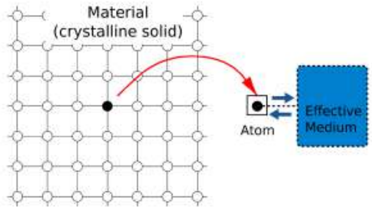
The Iterated Perturbation Theory (IPT) impurity solver (vanilla)



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

Non-existence of finite dimensional solution

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

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

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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

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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)

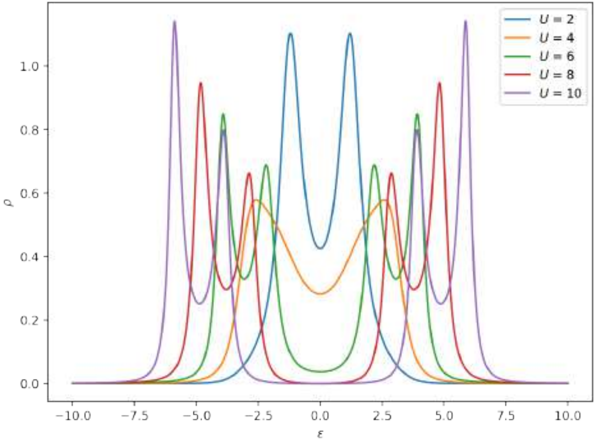

Figure: Spectral function ρ (a.k.a. A): analytic continuation results for the Hubbard dimer ($\beta = 1$). Metallic criteria: $\rho(0) > 0$ (TRIQS simulations).

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 $(W_{x,D}, \hat{H}^{\mathrm{imp}}_{x,D})$
Bath dimension	Infinite (non-interacting)	$\dim(W_{x,D}) = 2\dim(X_x)$
Impurity step	Impurity solver $\Delta \mapsto \Sigma$ (IPT here)	High-level $F^{\mathrm{HL}} : D \mapsto P$
Self-consistency	Bath Update map $\Sigma \mapsto \Delta$	Low-level $F^{\mathrm{LL}} : P \mapsto D$
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

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

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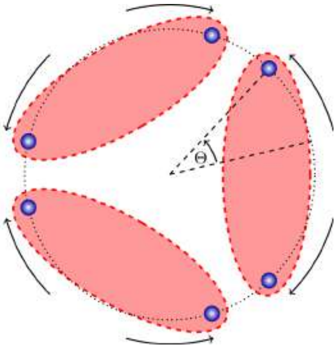
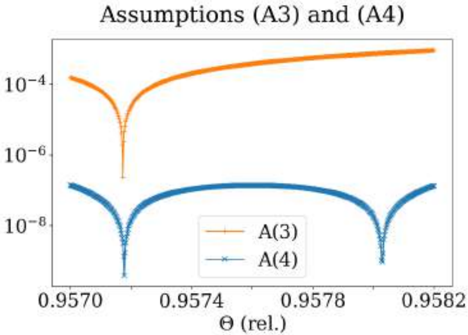
- Later: **thermodynamic limits**, "$d = \infty$" exactness [Metzner, Vollhardt 1989].

Numerical results: DMET assumptions' test on H_6.



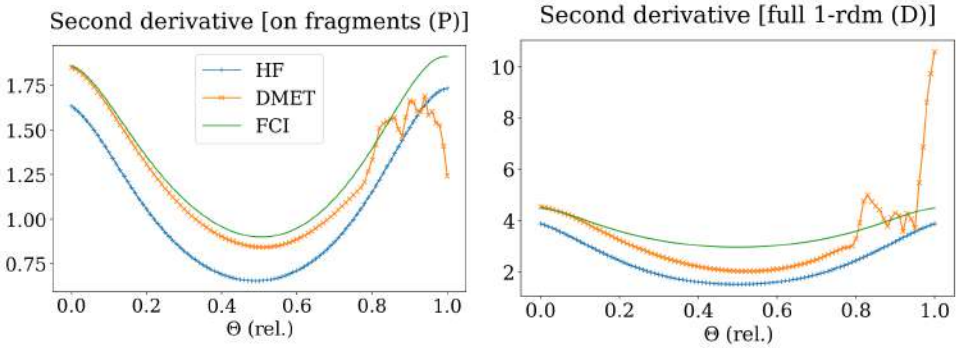
(a) H_6 molecule, with Θ varying.



(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

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

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.

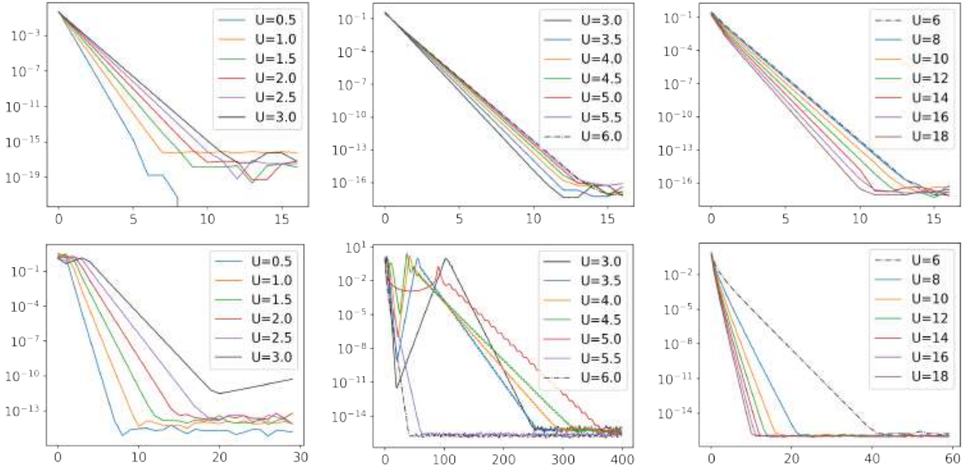
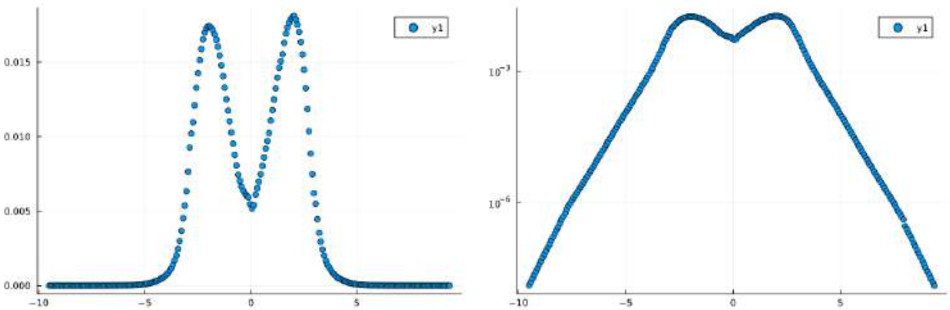


Figure: Residual $\|\Delta^{(n+1)} - \Delta^{(n)}\|_2$ in log scale, for $n \in [\![0, N_{\text{iter}}]\!]$, $\beta = 1$ (top), $\beta = 10$ (bottom).

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**.



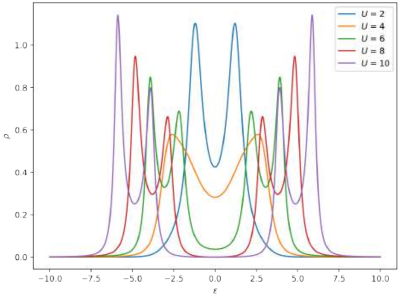
(a) Nevanlinna-Pick measure of Δ (b) Nevanlinna-Pick measure of Δ (log scale)

Figure: New ED-truncation scheme results, $U = 4$, $\beta = 0$, Hubbard dimer.

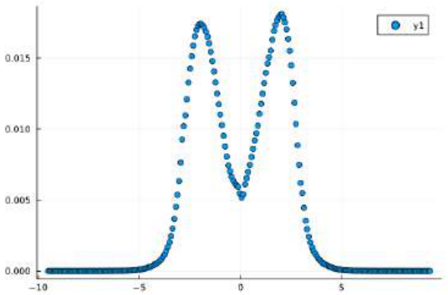
Suggests measure is **exponentially decreasing**: would prove **uniqueness** of the solution!

Preliminary results: particle-hole symmetry (Coulson Rushbrooke)

Hubbard: particle-hole **symmetry** $\Longleftrightarrow$ $\mathcal{G}_H$ 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** $\Longleftrightarrow$ $\mathcal{G}_H$ *is* **bipartite**.

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