Some mathematical insights on DMFT applied to the Hubbard model

Well-posedness (pedagogically)

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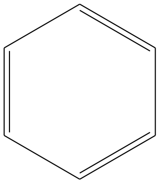
[2]MATHERIALS, INRIA

MSQM workshop, January 12

Overview

The finite Hubbard model in one slide



Interacting model for the π-electrons

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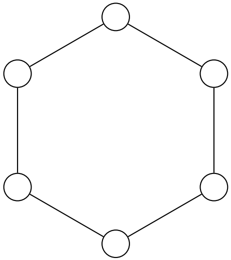

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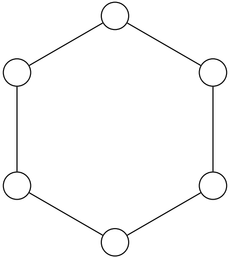

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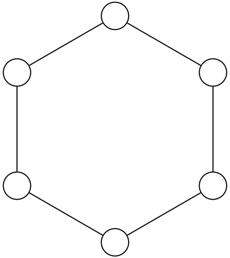

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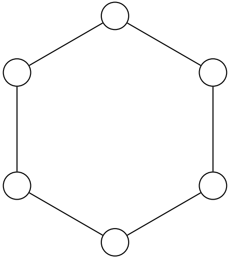

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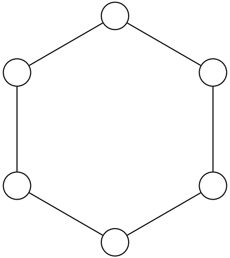

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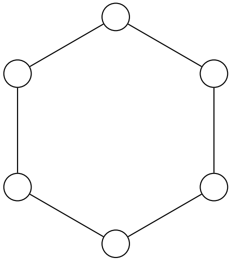

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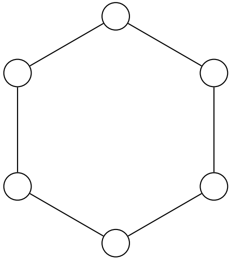

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Analytic solutions : [Lieb, 2001]

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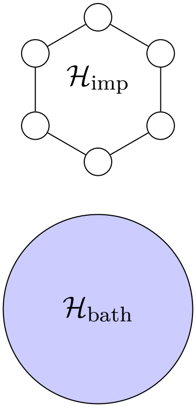

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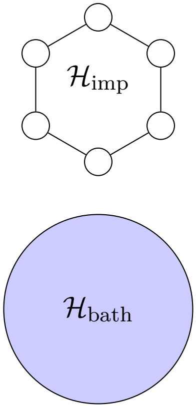

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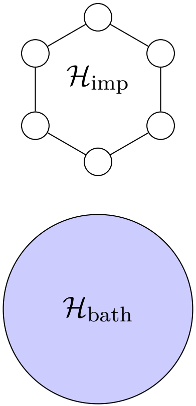

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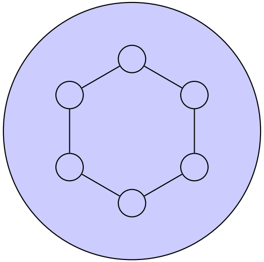

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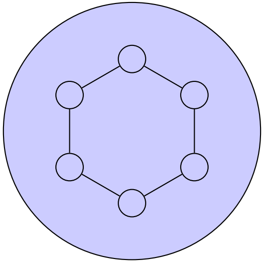

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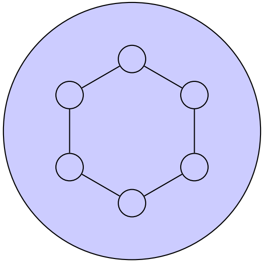

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Quantum physics Green's functions (Propagators) are not always *mathematical Green's functions* (Fundamental solution associated to a Linear Differential Operator).

Quantum physics Green's functions

Heisenberg picture : $\mathbb{H}(\mathcal{O})(t) = e^{-it\hat{H}}\mathcal{O}e^{-it\hat{H}}$.
State is a linear form on operators $\Gamma(\mathcal{O}) = \mathrm{Tr}(\rho\mathcal{O})$, $\rho^2 \leq \rho$, *equilibrium* $[\rho, \hat{H}] = 0$

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The *one-body time-ordered Green's function* $\tilde{G}$ of a quantum system $\mathcal{H}, \hat{H}$ in a state Γ is the *matrix-valued* function with

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- *Experimentally* "measurable" : ARPES (see Lucia's talk)

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Green's functions without interaction

Non-interacting Green's function

The *non-interacting Green's function* G^0 is the Green's function of $(\mathcal{H}, \hat{H}^0, \Gamma)$.

Non-interacting Green's functions are Green's functions

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In the time domain, equivalent to $\boxed{(i\partial_t - h)\, \tilde{G}^0 = \delta.}$

DMFT ustensil : the self-energy Σ.

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- Etymology : (1) $\iff$ $G(z) = (z - \underbrace{(h + \Sigma(z))}_{\text{effective } h'})^{-1}$
- $-\Sigma$ is a Herglotz function.
- If $\dim(\mathcal{H})$ is finite (see M.Lindsey's thesis),$\exists a_k \in \mathcal{S}(\mathbb{C})^+, \epsilon_k \in \mathbb{R}$ s.t. $\forall z \in \mathbb{C}+$,

$$\Sigma(z) = \Sigma_{HF} + \sum_k^{?} \frac{1}{z - \epsilon_k} a_k \tag{2}$$

DMFT ustensil : the hybridization function Δ.

DMFT is formulated with Green's functions *blocks* : for an Anderson impurity model we have

$$G^0_{\text{imp}} = (z-h)^{-1}_{\text{imp}} = \left(z - h_{\mathrm{imp}} - \sum_{k=1}^{Bathsize} \frac{1}{z-\epsilon_k} V_k V_k^\dagger \right)^{-1} \quad (3)$$

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The *hybridization function* Δ associated to an Anderson impurity model is the *matrix-valued* map defined for all $z \in \mathbb{C}+$ by

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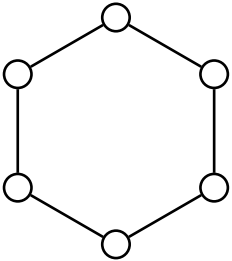
Δ *fully characterizes* the bath and its coupling to the impurity

DMFT recipe: from one Hubbard to several small Anderson



$$G = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \end{bmatrix}$$

DMFT recipe : find the Greens function G of a Hubbard model $(\mathcal{F}_H, \hat{H}_H)$ in a state Γ.

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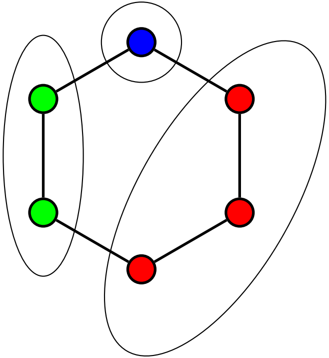

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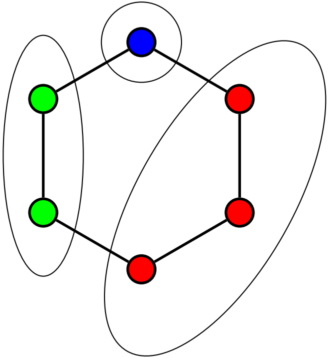
Step 1 : *partition* the vertices $\Lambda = \sqcup_{i=1}^{N} \Lambda_i$ of the original Hubbard graph $\mathcal{G} = (\Lambda, E)$ and focus on the blocks $(G_i)_{i=1,N}$.



$$G = \begin{bmatrix} G_1 & & & & & \\ & * & * & * & & \\ & * & G_2 & * & & \\ & * & * & * & & \\ & & & & G_3 & * \\ & & & & * & * \end{bmatrix}$$

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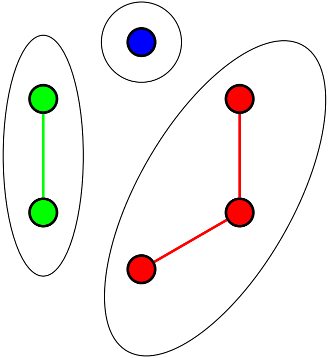

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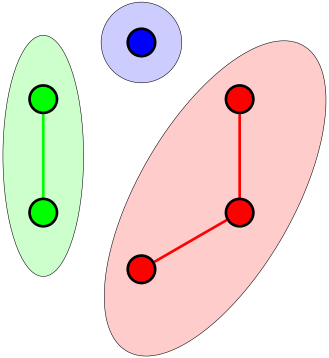
G of $\hat{H}_H$ with $\mathcal{G}_i \neq G_i$ of $\hat{H}_H$ with $\mathcal{G}$! *Even if not interacting* !

DMFT recipe: from one Hubbard to several small Anderson



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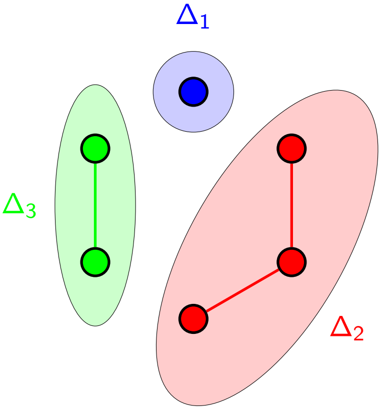

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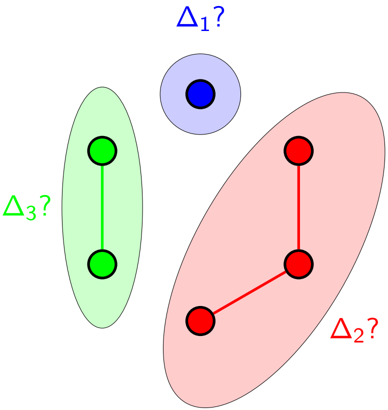

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Step 3 : define $G_{\mathrm{imp},i}$ of an Anderson impurity model with an *electronic bath* for each impurity $(\Delta_i)_{i=1,N}$. *Which one ?*

Self-consistent equation on (Δ_i)

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$$\boxed{\Sigma_{\mathrm{DMFT}} = \bigoplus_{i=1}^{N} \Sigma_{\mathrm{imp},i}} \tag{5}$$

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The impurity solver : $\Delta_i \longrightarrow \Sigma_{\mathrm{imp},i}$

Impurity solver : $\Delta_i \to \Sigma_i$ for each impurity.

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For each impurity, $\Sigma_i = \mathrm{IPT}(\Delta_i)$

DMFT equations (1)

We are looking for Δ_i such that for all $z \in \mathbb{C}+$,

$$G_{\mathrm{imp},i}(z) = G_{DMFT,i}(z) \tag{6}$$

(7)

(8)

(9)

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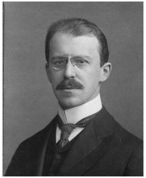
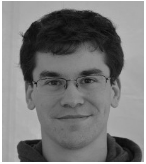


Schur-Levitt complement !



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$$z - h_i - \Sigma_i(z) - \Delta_i(z) = z - h_i - \Sigma_i(z) - h_{i,\bar{i}} \left(z - h_{\bar{i}} - \bigoplus_{j\neq i, j=1}^{N} \Sigma_j(z)\right)^{-1} h^{\dagger}_{i,\bar{i}} \tag{9}$$

DMFT equations (2)

DMFT equations : for all $i = 1, N$

$$\boxed{\Delta_i = h_{i,\bar{i}} \left(\cdot - h_{\bar{i}} - \bigoplus_{j \neq i, j=1}^{N} \Sigma_j \right)^{-1} h_{i,\bar{i}}^{\dagger}}, \quad (\Sigma_i)_{i=1,N} \mapsto \Delta_i \quad \text{(Self-consistent, global)}$$

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Mathematical question : $\mathfrak{D}, \mathfrak{S}$ s. t. well posed and existing solution ?

Self-coherent equation well-posedness for finite bath

Finite bath dimension well-posedness (L. Lin, M. Lindsey, R. Schneider, 2019)

Assume $\forall i = 1, n$, $\exists C_i \in \mathcal{S}_{N_i}(\mathbb{C}), L_i \in \mathbb{N}$, $\forall k = 1, L_i, a_k \in \mathcal{S}_{N_i}(\mathbb{C})^+, \epsilon_k \in \mathbb{R}$ s.t. $\forall z \in \mathbb{C}+$,

$$\Sigma_i(z) = C_i + \sum_{k=1}^{L_i} \frac{1}{z - \epsilon_k} a_k \tag{10}$$

Then $\forall i = 1, N$, Δ_i is well-defined and there exists $\tilde{L}_i \in \mathbb{N}$, $\forall k = 1, \tilde{L}_i, \tilde{a}_k \in \mathcal{S}_{N_i}(\mathbb{C})^+, \tilde{\epsilon}_k \in \mathbb{R}$ s.t. $\forall z \in \mathbb{C}+$,

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Issue : $\tilde{L}_i > L_i$, *no finite bath solution with IPT*

Self-coherent equation well-posedness for any bath

Extension : $\Sigma(z) = C + \int_{\mathbb{R}} \frac{1}{z-\epsilon} d\mu(\epsilon)$, μ a $\mathcal{S}(\mathbb{C})^+$-valued measure

Proposition : Self-coherent infinite bath well-posedness

Assume $\forall i = 1, N$, $\exists C_i \in \mathcal{S}_{N_i}(\mathbb{C})^+$ and μ_i a $\mathcal{S}_{N_i}(\mathbb{C})^+$-valued measure (with integrability condition), s.t. $\forall z \in \mathbb{R}$,

$$\Sigma_i(z) = C_i + \int_{\mathbb{R}} \frac{1}{z-\epsilon} d\mu_i(\epsilon) \tag{12}$$

Then $\forall i = 1, N$, Δ_i is well-defined and there exists ν_i a *finite* $\mathcal{S}_{N_i}(\mathbb{C})^+$-valued measure such that

$$\Delta_i(z) = \int_{\mathbb{R}} \frac{1}{z-\epsilon} d\nu_i(\epsilon) \tag{13}$$

The IPT solver

In the litterature : only found with $N = |\Lambda|$ (one site per impurity), with Γ the Gibbs state at β, μ, using *Matsubara*'s Green's functions and frequencies $\omega_n = \frac{\pi(2n+1)}{\beta}$
Given Δ, IPT proceeds in two steps :

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- First compute $\forall n \in \mathbb{N}$,

$$\Sigma_n = \frac{U}{2} + U^2 \int_0^\beta e^{i\omega_n \tau} \left(\frac{1}{\beta} \sum_{n' \in \mathbb{Z}} e^{-i\omega_{n'}\tau} \frac{1}{i\omega_{n'} - h_{\mathrm{imp}} + \mu - \Delta(i\omega_{n'})} \right)^3 d\tau \quad (14)$$

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- "Analytic continue" it : find $\Sigma : \mathbb{C}+ \to \mathbb{C}+$ analytic s.t.

$$\forall n \in \mathbb{N}, \Sigma(i\omega_n) = \Sigma_n \quad (15)$$

IPT well-posedness (1)

Proposition : IPT first-step well-posedness

Given ν a positive measure (w. integrability conditions) s.t. $\forall z \in \mathbb{C}+$,

$$\Delta(z) = \int_{\mathbb{R}} \frac{1}{z-\epsilon} d\nu(\epsilon) \tag{16}$$

Then $\forall n \in \mathbb{N}$, Σ_n is well-defined and $\exists \mu$ a positive and *finite* measure s.t. $\forall n \in \mathbb{N}$,

$$\Sigma_n = \frac{U}{2} + \int_{\mathbb{R}} \frac{1}{i\omega_n - \epsilon} d\mu(\epsilon) \tag{17}$$

IPT well-posedness (2)

Proposition : IPT second-step well-posedness

The analytical continuation problem

$$\text{Find } \Sigma : \mathbb{C}+ \to \mathbb{C}+ \text{ analytic s.t. } \forall n \in \mathbb{N}, \Sigma(i\omega_n) = \Sigma_n \tag{18}$$

admits a unique solution if

- Δ represents a bath of finite dimension
- ν is compactly supported

Solution : ν finite, (probably not compactly supported) ...

Conclusion

Ongoing :

- Necessary conditions on the solution.
- Functional equation on the *density* of ν if $\nu \ll$ Lebesgue.
- Convergence study : *which topology* ?

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(a) S. Perrin-Roussel

(b) É. Cancès

(c) M. Vinteler (M1 student)