Lecture 4:
Generalizations of Dynamical-Mean Field Theory and Improved Solvers

André-Marie Tremblay

Collège de France, 30 mars 2015
17h00 à 18h30
• Quantum cluster methods
  – Cluster Perturbation Theory
  – Self-energy functional
    • Variational cluster approximation
    • Cellular (cluster) Dynamical Mean-Field Theory
  – Dynamical Cluster Approximation

• Remark on other materials
  – Organics
  – Heavy fermions
• Extensions: dual fermions
• Impurity solvers
  – Exact diagonalization
  – Quantum Monte Carlo
    • 3 improvements
• Maximum entropy analytic continuation
• Formal considerations with self-energy functional
Some references

- Reviews
  - Maier, Jarrell et al., RMP. (2005)
  - Kotliar et al. RMP (2006)
  - A.-M.S. Tremblay, B. Kyung and D. Sénéchal
    Low Temperature Physics 32, 424 (2006)
    (arXiv:cond-mat/0511334)
Partitioning the infinite system
Perturbation theory in hopping (Hubbard I)

\[ t_{\mu\nu}^{mn} = t_{\mu\nu}^{(c)} \delta_{mn} + V_{\mu\nu}^{mn} \]

\[ \left[ \hat{G}^{-1}(\tilde{k}, z) \right]_{\mu\nu} = \left[ \hat{G}^{(c)-1}(z) - \hat{V}(\tilde{k}) \right]_{\mu\nu} \]

\[ \hat{G}^{(c)-1}(z) = z + \mu - \hat{t}^{(c)} - \hat{\Sigma}^{(c)} \]

\[ \hat{G}^{(0)-1}(\tilde{k}, z) = z + \mu - \hat{t}^{(c)} - \hat{V}(\tilde{k}) \]

\[ \hat{G}^{-1}(\tilde{k}, z) = \hat{G}^{(0)-1}(\tilde{k}, z) - \hat{\Sigma}^{(c)}(z) \]

Exact \( t = 0 \) and \( U = 0 \)

Periodization

\[ \mathbf{k} = \tilde{\mathbf{k}} + \mathbf{K} \]

Four values of \( \mathbf{K} \)

\( \tilde{\mathbf{k}} \) Runs over \( \frac{1}{4} \) of the Brillouin zone

All the information is in

\[ G(\tilde{\mathbf{k}} + \mathbf{K}, \tilde{\mathbf{k}} + \mathbf{K}'; i\omega_n) \]

\[
\begin{align*}
    n &= T \sum_n \sum_{\tilde{k}, \mathbf{K}} G(\tilde{\mathbf{k}} + \mathbf{K}, \tilde{\mathbf{k}} + \mathbf{K}; i\omega_n) \\
    \text{Periodization:} \\
    G(\tilde{\mathbf{k}} + \mathbf{K}, \tilde{\mathbf{k}} + \mathbf{K}'; i\omega_n) &\rightarrow G(\tilde{\mathbf{k}} + \mathbf{K}, \tilde{\mathbf{k}} + \mathbf{K}; i\omega_n) \equiv G(\mathbf{k}; i\omega_n)
\end{align*}
\]
FIG. 3: Intensity plot of the spectral function at the Fermi level, in the first quadrant of the Brillouin zone, for $U = 8t$ on a $L = 8$ cluster. Left: Hole-doped system ($n = 0.93$). Right: Electron-doped systems ($n = 1.10$). A Lorentzian broadening of $0.2t$ is used. Wave-particle
Cluster Perturbation Theory

Benchmarks
1d Hubbard

$U = 2$ vs Bethe ansatz

Sénéchal et al. PRL 84, 522 (2000)
Sénéchal et al. PRB 66, 075129 (2002)
Self-energy functional
DMFT as a stationary point
Three different types of approximations

I. Approximate the Euler equations
II. Approximate the functional (finite set of diagrams or other method, analogy to DFT)
III. Take and the exact functional but for a limited set of possible functions ($G, \Sigma \ldots$)
SFT : Self-energy Functional Theory

With $F[\Sigma]$  Legendre transform of Luttinger-Ward funct.

$$\Omega_t[\Sigma] = F[\Sigma] + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1})$$

is stationary with respect to $\Sigma$ and equal to grand potential there.

$$\Omega_t[\Sigma] = \Omega_{t'}[\Sigma] - \text{Tr} \ln(-(G_0'^{-1} - \Sigma)^{-1}) + \text{Tr} \ln(-(G_0^{-1} - \Sigma)^{-1})$$

Vary with respect to parameters of the cluster (including Weiss fields)

Variation of the self-energy, through parameters in $H_0(t')$

Variational Cluster Approximation
(Variational Cluster Perturbation Theory)

M. Potthoff, M. Aichhorn, and C. Dahnken

C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff
Adding and subtracting Weiss fields

No mean-field factorization of interaction

\[ H_0^{(\text{intra})}(\mathbf{R}) \rightarrow H_0^{(\text{intra})}(\mathbf{R}) + \Delta(\mathbf{R}), \]
\[ H_0^{(\text{inter})}(\mathbf{R}, \mathbf{R}') \rightarrow H_0^{(\text{inter})}(\mathbf{R}, \mathbf{R}') - \delta_{\mathbf{R}, \mathbf{R}'} \Delta(\mathbf{R}) \]

\[ \Delta(\mathbf{R}) = \sum_{a,b} \Delta_{a,b} c_{R_a}^\dagger c_{R_b} \]

e.g. antiferromagnétisme alternating field proportional to \( h \)

In the presence of interactions result depends on \( h \): optimize

\[ \Omega_t(t') = \Omega' - \int_{c} \frac{d\omega}{2\pi} \sum_{K} \ln \det[1 + (G_0^{-1} - G_0'^{-1})G'] \]
$Q = \frac{\text{# of sites in cluster}}{\text{# of sites/unit cell in infinite cluster}}$
Ground state energy, $n = 1$, 2-d Hubbard

C. Dahnken, M. Aichhorn, W. Hanke, E. Arrigoni, and M. Potthoff
Cellular Dynamical Mean-Field Theory
CDMFT

Gabriel Kotliar, Sergej Y. Savrasov, Gunnar Pálsson, and Giulio Biroli
Methods of derivation for DMFT

- Cavity method
- Local nature of perturbation theory in infinite dimensions
- Expansion around the atomic limit
- Effective medium theory
- Local approximation for Luttinger Ward
- Potthoff self-energy functional

Mott transition and Dynamical Mean-Field Theory. The beginnings in $d = \infty$

- Compute scattering rate (self-energy) of impurity problem.
- Use that self-energy ($\omega$ dependent) for lattice.
- Project lattice on single-site and adjust bath so that single-site DOS obtained both ways be equal.

W. Metzner and D. Vollhardt, PRL (1989)
A. Georges and G. Kotliar, PRB (1992)
M. Jarrell PRB (1992)

DMFT, $(d = 3)$
2d Hubbard: Quantum cluster method

Hettler ...Jarrell...Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar et al. RMP (2006)
AMST et al. LTP (2006)
Hybridization function

$$G_{\text{full}}^{-1}(\omega) = \frac{1}{\omega - T}$$

$$T = \begin{pmatrix} -t & \theta \\ \theta^\dagger & -\varepsilon \end{pmatrix}$$

$$G^{-1} = \omega - t - \theta \frac{1}{\omega - \varepsilon} \theta^\dagger$$
Self-consistency

\[ \mathcal{G}_\sigma^{\text{imp}}(i\omega_n)^{-1} = \mathcal{G}_\sigma^{0-\text{imp}}(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n) \]

Impurity \( \mathcal{G}^0 \) depends on hybridization function

\[ N_c \int \frac{d^d \vec{k}}{(2\pi)^d} \frac{1}{\mathcal{G}_k^{0-\text{imp}}(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n)} = \mathcal{G}_\sigma^{\text{imp}}(i\omega_n) \]

Modify the bath (hybridization) for the impurity until this equality is satisfied
Self-consistency condition

- Obtain Green’s function for the « impurity » (cluster) in a bath
- Extract $\Sigma$
- Substitute $\Sigma$ in lattice Green’s function
- Project lattice Green’s function on impurity (cluster).
- If the two Green’s functions are not equal, modify the bath until they are.
• Long range order:
  – Allow symmetry breaking in the bath (mean-field)
• Included:
  – Short-range dynamical and spatial correlations
• Missing:
  – Long wavelength p-h and p-p fluctuations
CDMFT

Benchmarks
Systematic study on cluster-size dependence in the cellular dynamical mean-field theory

Shiro Sakai, Giorgio Sangiovanni, Marcello Civelli, Yukitoshi Motome, Karsten Held, and Masatoshi Imada

Size dependence near FS

$T = 0.06t, U=8t, t'=-0.2,$
$1\%, 3\%, 5\%$ doping


Main conclusions:
- 4 site close to 16 site
- (0,0) and ($\pi/2$, $\pi/2$) converge faster
Their preferred periodization

$M$ is irreducible with respect to all intersite terms in $H$

$$M_{\mu,\nu} = \left( \frac{1}{i\omega_n - \mu - \Sigma} \right)_{\mu,\nu}$$

$$M(k) = \sum_{\mu,\nu} e^{i(\tilde{k} + K) \cdot (R_{\mu} - R_{\nu})} M_{\mu,\nu}$$

$$G^{-1}(k) = M^{-1}(k) - t(k)$$

Periodizing the self-energy is bad! (Sénéchal)
Dynamical Cluster Approximation
DCA

M. H. Hettler, A. N. Tahvildar-Zadeh, M. Jarrell, T. Pruschke, and H. R. Krishnamurthy
**2d Hubbard: Quantum cluster method**

Hettler ...Jarrell...Krishnamurty PRB 58 (1998)
Kotliar et al. PRL 87 (2001)

**REVIEWS**
Maier, Jarrell et al., RMP. (2005)
Kotliar et al. RMP (2006)
AMST et al. LTP (2006)
Cannot be derived from self-energy functional
Based on mapping on a translationally invariant cluster

\[ t_{\mu,\nu}^{m,n} = \sum_{\tilde{k},K} e^{i(\tilde{k} + K) \cdot (r_{m,n} + R_{\mu,\nu})} t(\tilde{k} + K) \]

\[ t_{\mu,\nu}(\tilde{k}) = \sum_{K} e^{iK \cdot R_{\mu,\nu}} t(\tilde{k} + K) ; \quad K \cdot r_{m,n} = 0 \text{ (Modulo } 2\pi) \]

\[ t^{m,n}(K) = \sum_{\tilde{k}} e^{i\tilde{k} \cdot (r_{m,n} + R_{\mu,\nu})} t(\tilde{k} + K) \]

\[ t^{DCA}(K) = \sum_{\tilde{k}} e^{i\tilde{k} \cdot R_{\mu,\nu}} t(\tilde{k} + K) \]
DCA self-consistency

Matrix vs scalar
For large systems, fewer terms in DC self-consistency
Dynamical Cluster Approximation
DCA

Benchmarks
Taking advantage of liberty in choice of patch

E. Gull, M. Ferrero, O. Parcollet, A. Georges, and A. J. Millis

\[ T = 0.05t, \ U=7t, \ t'=-0.15, \]

Many dopings

**FIG. 1**: Qualitative sketch of doping regimes for parameters considered in this paper.
Thinking locally: reflections on Dynamical Mean-Field Theory from a high-temperature/high energy perspective.

Antoine Georges$^{1,2,*}$

$^1$ Collège de France, 11 place Marcelin Berthelot, 75005 Paris
$^2$ Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France
DMFT vs High temperature series: 3-d Hubbard

Double occupancy, square lattice various methods

\[ U = 4t \]

A. Reymbaut et al. unpublished
Crossovers square lattice: DCA, CDMFT, DMFT

A. Reymbaut et al. unpublished

- Non particle-hole symmetric system:
  \[ n = 1 + T \left[ N(\mu_+) e^{\beta(\mu_+ - \mu_-)} - N(\mu_-) e^{-\beta(\mu_+ - \mu_-)} \right] \]

- Particle-hole symmetric system:
  \[ n = 1 + 2T N\left(\frac{E_g}{2}\right) e^{-\beta \frac{E_g}{2}} \sinh \left( \beta \left[ \mu - \frac{U}{2} \right] \right) \]
CDMFT vs DCA, 1-d Hubbard model

Kyung, Kotliar, AMST, PRB 73, 205106 (2006)

\( U = 4t, \ T = 1/5, \ n = 1 \) (strong correlations)

Filled symbols from DCA. Pseudogap at \( L = 8 \) only

S. Moukouri, C. Huscroft, and M. Jarrell, in
CDMFT vs DCA, 2-d Hubbard model

Pseudogap from long-wavelengths takes large system sizes to converge

\[ N = L \times L \]

\[ L = 2, 3, 4, 6 \]

Kyung, Kotliar, AMST, PRB 73, 205106 (2006)

\[ U = 4.4t, T = 1/4, n = 1 \] (weak correlations)

Filled symbols from DCA. Pseudogap at \( L = 8 \) only

Jarrell et al. PRB 64, 195130 (2001)
Comparisons DCA-CDMFT with a large $N$ model

Local quantities (double occupancy etc…) converge exponentially fast with CDMFT (Take center of cluster)
Otherwise $1/L$

DCA faster for long wavelength quantities

Other materials
Generic case highly frustrated case

(a)

Mott Insulator

Strongly correlated state

\( U/W \)

Mott transition

\( U/W \) = 1.07 at 0.5 GPa

\( U/W \) = 0.88 at 0.15 GPa

\( \kappa(ET)_2Cu_x(CN)_y \)

\( \kappa(ET)_4Hg_{2.89}Br_8 \)

Fermi liquid

Band filling

Half filled

10% doped

20% doped

\( T \)

\( n \)

\( t/U \)
Heavy fermions

3D metals tuned by pressure, field or concentration

$\text{CeRhIn}_5$

Magnetic superconductivity

Quantum criticality

Knebel et al. (2009)

Mathur et al., Nature 1998
Heavy fermions

\[ H = \sum_{k,\sigma} \epsilon_{k\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k,\sigma} \epsilon^f_{k,\sigma} f_{k,\sigma}^\dagger f_{k,\sigma} + \sum_{k,\sigma} V_k (f_{k,\sigma}^\dagger c_{k,\sigma} + h.c.) + \sum_i U (n_i^\dagger - \frac{1}{2})(n_i - \frac{1}{2}) \]

\[ V_k = V + 2V'[\cos(k_x) + \cos(k_y)] \]

Phase diagram

\( U = 4 \)

AFM: antiferro-magnetism
SC: superconducting

\( V'/V = 2 \): more frustrated case
\( V'/V = 5 \): less frustrated case

Challenges
Challenges

• Weak to intermediate coupling (TPSC)
  – Generalize to broken symmetry states
  – Multiband states
  – Use in realistic calculations

• Strong coupling
  – Include long-wavelength fluctuations (vertex)
  – Feedback observable on double occupancy
Bio break
Dual fermions
Some references

Fermionic HS transformation

S. Pairault, D. Senechal, A.-M.S. Tremblay
   PRL 80, 5389 (1998); EPJ (2000)

Dual fermions in quantum clusters

A.N. Rubtsov, M. I. Katsnelson, A. I. Lichtenstein, and A. Georges
   PRB 79, 045133 2009
A fermionic Hubbard-Stratonovich transformation for strong coupling

\[ h_i(c_{i\sigma}^\dagger, c_i) = U c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger c_i c_i^\uparrow \]

\[ \mathcal{H}^1 = \sum_\sigma \sum_{ij} V_{ij} c_{i\sigma}^\dagger c_{j\sigma} \]

\[ Z = \int [d\gamma^* d\gamma] \exp - \int_0^\beta d\tau \left\{ \sum_{i\sigma} \gamma_{i\sigma}^*(\tau) \left( \frac{\partial}{\partial \tau} - \mu \right) \gamma_{i\sigma}(\tau) \right. \]

\[ + \sum_i h_i(\gamma_{i\sigma}^*(\tau), \gamma_{i\sigma}(\tau)) + \sum_{ij\sigma} V_{ij} \gamma_{i\sigma}^*(\tau) \gamma_{j\sigma}(\tau) \left\} \right. \cdot (5) \]

\[ \int_0^\beta d\tau \sum_{ij\sigma} V_{ij} \gamma_{i\sigma}^*(\tau) \gamma_{j\sigma}(\tau) = \sum_{ab} V_{ab} \gamma_a^* \gamma_b = \langle \gamma | V | \gamma \rangle \]

\[ \int [d\psi^* d\psi] e^{\langle \psi | V^{-1} | \psi \rangle + \langle \gamma | \psi \rangle + \langle \gamma | \psi \rangle} = \text{det}(V^{-1}) e^{-\langle \gamma | V | \gamma \rangle} \]

\[ Z = Z_0 \int [d\psi^* d\psi] e^{\langle \psi | V^{-1} | \psi \rangle + \left\langle e^{\langle \psi | \gamma \rangle + \langle \gamma | \psi \rangle} \right\rangle_0} \]
Exact diagonalization impurity solver
Parametrization of bath

S. Kancharla

B. Kyung

David Sénéchal
Effect of finite bath

• Minimize a distance function to find bath parameters at iteration $i+1$:
  – Weight (cutoff) needed
  – Effective temperature

\[
d = \sum_{\mu, \nu} \sum_n W(i\omega_n) \left| \Delta_{\mu,\nu}^{(i+1)}(i\omega_n) - \Delta_{\mu,\nu}^{(i)}(i\omega_n) \right|^2
\]
Implementation issues (not trivial!)

• Exact diagonalization code issues
  – Need Lanczos or band Lanczos or Arnoldi
  – Integrations are difficult (do them in imaginary plane in the case of frequency)
  – Value of Lorentzian broadening for dynamics

• General bath difficult to converge
  – Start from known easy solutions and do small change on Hamiltonian parameters
Some references

M. Caffarel and W. Krauth, PRL, 72, 1545 (1994).
A. Liebsch and N.-H. Tong, PRB, 80, 165126 (2009).
D. Sénéchal, “An introduction to quantum cluster methods,”
Lecture notes from the CIFAR - PITP
International Summer School on Numerical Methods
for Correlated Systems in Condensed Matter, Sherbrooke, Canada,
Benchmarks

ED solver

Red, $U/t = 4$, $N_c = 2$, $N_b = 8$
Solid line: Bethe ansatz

Capone, Civelli, et al.
PRB 69, 195105 2004.

QMC solver

Kyung, Kotliar, AMST
PRB 73, 205106 (2006)
CT-QMC impurity solver
Monte Carlo method


\[ Z = \int_{C} dx p(x). \]

\[ \langle A \rangle_p = \frac{1}{Z} \int_{C} dx \mathcal{A}(x)p(x). \]

\[ \langle A \rangle_p \approx \langle A \rangle_{MC} = \frac{1}{M} \sum_{i=1}^{M} \mathcal{A}(x_i). \]

\[ \langle A \rangle = \frac{1}{Z} \int_{C} dx \mathcal{A}(x)p(x) = \frac{\int_{C} dx \mathcal{A}(x)[p(x)/\rho(x)]\rho(x)}{\int_{C} dx [p(x)/\rho(x)]\rho(x)} \equiv \frac{\langle A(p/\rho) \rangle_p}{\langle p/\rho \rangle_p}. \]
Monte Carlo: Markov chain

- Ergodicity
- Detailed balance

\[
\frac{W_{xy}}{W_{yx}} = \frac{p(y)}{p(x)}
\]

\[
W_{xy} = W_{xy}^{\text{prop}} W_{xy}^{\text{acc}}
\]

\[
W_{xy}^{\text{acc}} = \min[1, R_{xy}]
\]

\[
R_{xy} = \frac{p(y)W_{yx}^{\text{prop}}}{p(x)W_{xy}^{\text{prop}}}
\]
Reminder on perturbation theory

\[
\exp(-\beta(H_a + H_b)) = \exp(-\beta H_a)U(\beta)
\]

\[
\frac{\partial U(\beta)}{\partial \beta} = -H_b(\beta)U(\beta)
\]

\[
U(\beta) = 1 - \int_0^\beta d\tau H_b(\tau) + \int_0^\beta d\tau \int_0^\tau d\tau' H_b(\tau)H_b(\tau') + \ldots
\]
Partition function as sum over configurations

\[ Z = \text{Tr}[\exp(H_a + H_b)] \]

\[ = \sum_k (-1)^k \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k \text{Tr}[e^{-\beta H_a} H_b(\tau_k) \times H_b(\tau_{k-1}) \cdots H_b(\tau_1)] \]

\[ Z = \sum_{k=0}^{\infty} \sum_{\gamma \in \Gamma_k} \int_0^\beta d\tau_1 \cdots \int_{\tau_{k-1}}^\beta d\tau_k w(k, \gamma, \tau_1, \ldots, \tau_k) \]

\[ x = (k, \gamma, (\tau_1, \ldots, \tau_k)), \quad p(x) = w(k, \gamma, \tau_1, \ldots, \tau_k) d\tau_1 \cdots d\tau_k, \]
Updates

\[
R_{(k, \bar{\tau}), (k+1, \bar{\tau}')} = \frac{p(((k+1, \bar{\tau}'))) W_{(k+1, \bar{\tau}'), (k, \bar{\tau})}^{\text{prop}}}{p((k, \bar{\tau})) W_{(k, \bar{\tau}), (k+1, \bar{\tau}')}^{\text{prop}}}
\]

\[
= \frac{w(k+1) \, d\tau'_1 \cdots d\tau'_{k+1}}{w(k) \, d\tau_1 \cdots d\tau_k} \, \frac{1/(k+1)}{d\tau/\beta}
\]

\[
= \frac{w(k+1)}{w(k)} \frac{\beta}{k+1}.
\]

Solving cluster in a bath problem

- Continuous-time Quantum Monte Carlo calculations to sum all diagrams generated from expansion in powers of hybridization.
  
  
Some Algorithmic details:
3 improvements
Continuous-time QMC : CT-HYB

\[ H_{\text{imp}} = H_{\text{loc}}(d_i^\dagger, d_i) + \sum_{i\mu}(V_{\mu i}a_{\mu}^\dagger d_i + V_{\mu i}^* d_i^\dagger a_{\mu}) \]

\[ + \sum_{\mu} \epsilon_{\mu} a_{\mu}^\dagger a_{\mu}, \]

\[ Z = \text{Tr} T_{\tau} e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))} \]

\[ = \sum_{k \geq 0} \frac{1}{k! 2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau'_1 \cdots d\tau'_k \text{Tr} T_{\tau} e^{-\beta H_0} \]

\[ \times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau'_1) \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau'_k). \]

\[ = \sum_{k \geq 0} \sum_{i_1 \cdots i_k} \sum_{i'_1 \cdots i'_k} \frac{1}{k! 2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau'_1 \cdots d\tau'_k \]

\[ \times \text{Tr} T_{\tau} e^{-\beta H_{\text{loc}}} d_{i_1}(\tau_1) d_{i'_1}^\dagger(\tau'_1) \cdots d_{i_k}(\tau_k) d_{i'_k}^\dagger(\tau'_k) \]

\[ \times Z_{\text{bath}}(\hat{V}_{i_1}(\tau_1) \hat{V}_{i'_1}(\tau'_1) \cdots \hat{V}_{i_k}(\tau_k) \hat{V}_{i'_k}(\tau'_k)), \quad \hat{V}_i = \sum_{\mu} V_{\mu i}^* a_{\mu}. \]

Reducing the sign problem

\[ \cos \theta c'_{A_1\sigma} - \sin \theta c_{A_1\sigma}, \quad \sin \theta c'_{A_1\sigma} + \cos \theta c_{A_1\sigma} \]

\[ C_{2v} \]

\[ 2A_1, B_1, B_2 \]

\[ t'/t = 0.8 \]
Ergodicity of the hybridization expansion with two operator updates and broken symmetry

\[ H_{\text{imp}} = H_{\text{loc}}(d_i^\dagger, d_i) + \sum_{i\mu} (V_{\mu i} a_{\mu}^\dagger d_i + V_{\mu i}^* d_i^\dagger a_{\mu}) + \sum_{\mu} \epsilon_{\mu} a_{\mu}^\dagger a_{\mu}, \]

\[ Z = \text{Tr} \text{Tr}_\tau e^{-\beta H_0} e^{-\int_0^\beta d\tau (H_{\text{hyb}}(\tau) + H_{\text{hyb}}^\dagger(\tau))} = \sum_{k \geq 0} \frac{1}{k!^2} \int_0^\beta d\tau_1 \cdots d\tau_k \int_0^\beta d\tau'_1 \cdots d\tau'_k \text{Tr} \text{Tr}_\tau e^{-\beta H_0} \]

\[ \times H_{\text{hyb}}(\tau_1) H_{\text{hyb}}^\dagger(\tau'_1) \cdots H_{\text{hyb}}(\tau_k) H_{\text{hyb}}^\dagger(\tau'_k). \]

\[ \text{Tr}[d_{\uparrow}(0,\pi) d_{\downarrow}(0,\pi) d_{\downarrow}(\pi,0) d_{\uparrow}(\pi,0)] \]

\[ \times \Delta_{a_{\uparrow}(0,\pi), \downarrow(0,\pi)} \Delta_{a_{\uparrow}(\pi,0), \downarrow(\pi,0)} \]

Lazy Skip-List: 1 Lazy

Fast rejection algorithm: the lazy part

Flip coin

Initial bound

Refined bound: move rejected

MC weights in CT-HYB: some notation

\[ w\{(i_1, \tau_1) \cdots (i_k, \tau_k)\} = \text{Det } \Delta \text{ Tr}_{\text{loc}} \left[ T_\tau e^{-\beta H_{\text{loc}}} \right. \]
\[ \times d_{i_k}^{}(\tau_k) d_{i_k'}^\dagger(\tau'_k) \cdots d_{i_1}^{}(\tau_1) d_{i_1'}^\dagger(\tau'_1) \left. \right] \]

\[ \text{Tr}_{\text{loc}} \ P_{\beta-\tau_k}^{} F_{i_k}^{} P_{\tau_k-\tau_k'}^{} F_{i_k'}^\dagger \cdots F_{i_1}^{} P_{\tau_1-\tau_1'}^{} F_{i_1'}^\dagger P_{\tau_1'}^{} \]
Lazy Skip List : Skip List

Tree structure : E. Gull, ETH thesis
Lazy Skip List : Skip List

Tree structure : E. Gull, ETH thesis
Some more details

Subproducts stored in blue arrows are emptied if tail coincides with red arrow
Lazy Skip-List: Speedup (beat Moore)

LaNiO$_3$

FeTe

(a) LNO

(b) FeTe
continued
Maximum Entropy analytical continuation

Look for cond-mat soon
D. Bergeron, A.-M.S. Tremblay

A new maximum entropy approach and a user friendly software for analytic continuation of numerical data
Mammouth
André-Marie Tremblay

Sponsors:
Merci

Thank you