

A Multiorbital Quantum Impurity Solver for General Interactions and Hybridizations

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Outline

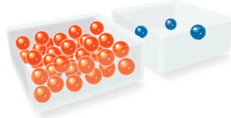
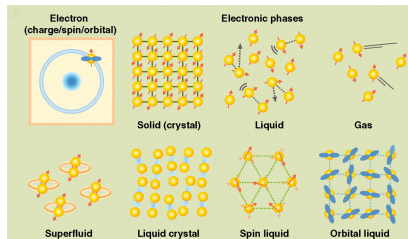
- 1 Strongly Correlated Materials
- 2 Quantum Impurity Models
- 3 Inchworm Monte Carlo
- 4 The Multiorbital Sign Problem

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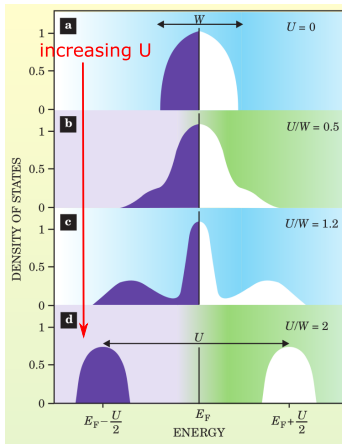
Strongly correlated materials

- Goal: simulate materials with various electronic phases.¹



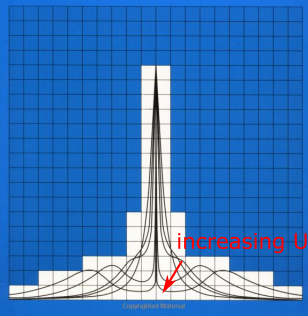
¹H. Takagi and H. Y. Hwang, Science 327, 1601 (2010).

Mott metal–insulator transition



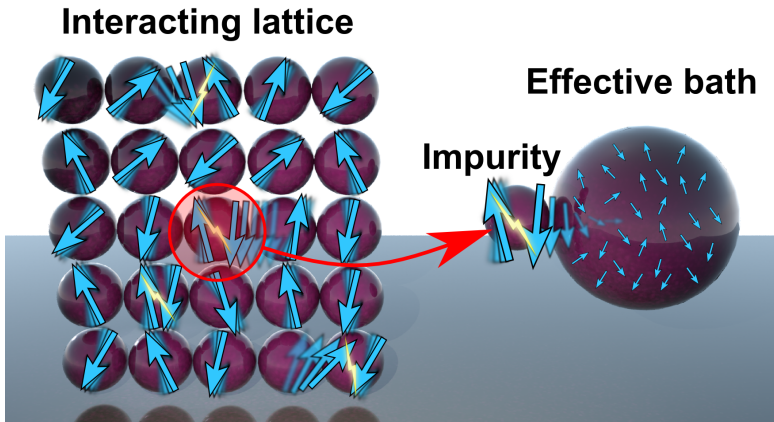
The Kondo Problem to Heavy Fermions

A.C. HEWSON

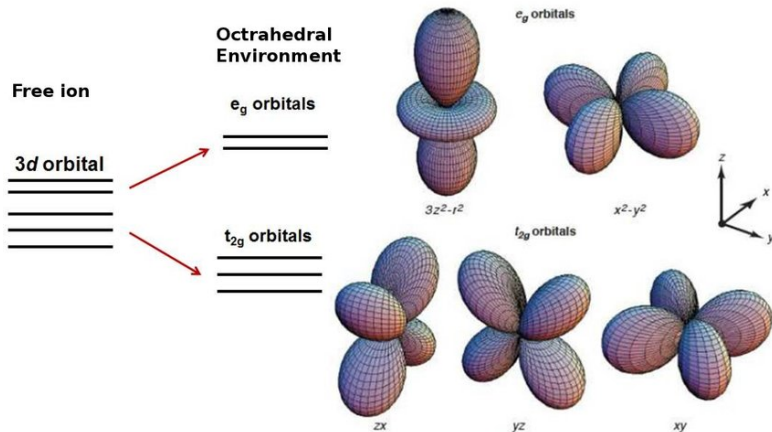


Dynamical Mean Field Theory (DMFT)

- 1992—Georges, Kotliar:



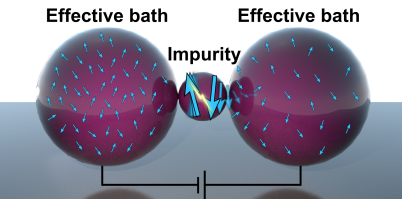
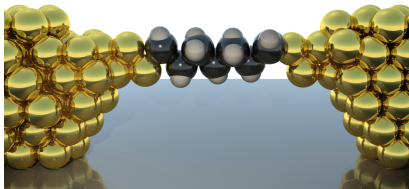
Multiple local orbitals



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Transport in junctions

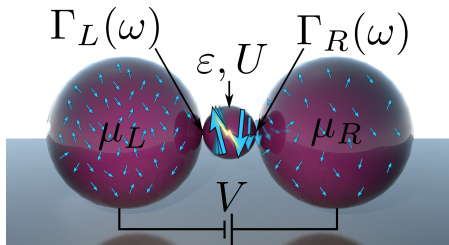


$$\hat{H} = \hat{H}_{\text{dot}} + \hat{H}_{\text{leads}} + \hat{H}_{\text{hyb}}$$

We would like to understand:

Electronic populations and transport; the effects of many-body correlation; magnetic and optical properties; elastic properties and heat transport; ...

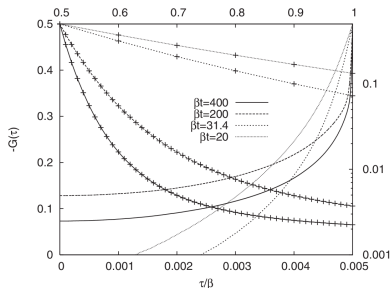
An example: the Anderson impurity model



$$\begin{aligned}
 H &= \hat{H}_{\text{dot}} + \hat{H}_{\text{leads}} + \hat{H}_{\text{hyb}} \\
 &= \sum_{\sigma} \epsilon_{\sigma} d_{\sigma}^{\dagger} d_{\sigma} + U d_{\uparrow}^{\dagger} d_{\uparrow} d_{\downarrow}^{\dagger} d_{\downarrow} + \sum_{\sigma k} \sum_{\ell \in \{L, R\}} \epsilon_{\sigma \ell k} a_{\sigma \ell k}^{\dagger} a_{\sigma \ell k} \\
 &\quad + \sum_{\sigma k} \sum_{\ell \in \{L, R\}} t_{\sigma \ell k} a_{\sigma \ell k}^{\dagger} d_{\sigma} + t_{\sigma \ell k}^{*} d_{\sigma}^{\dagger} a_{\sigma \ell k}.
 \end{aligned}$$

Monte Carlo methods: sampling contributions

- Continuous time (hybridization) solvers;² usually formulated in imaginary time (expand $e^{-\beta H}$). This:
 - Limits us to equilibrium.
 - Requires uncontrolled analytical continuation for dynamics.
- Despite this, QMC has dominated DMFT for decades.



²Werner et. al., Phys. Rev. Lett. 97, 076405 (2006)

Monte Carlo methods: nonequilibrium

- Continuous time solvers can also be formulated in real time (expand $e^{\pm iHt}$).^{3, 4, 5}

Nonequilibrium / exact dynamics require real time QMC

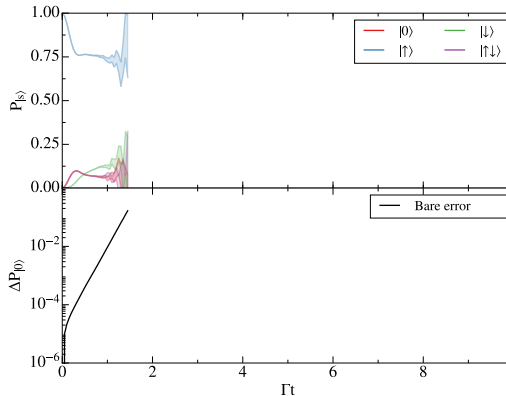
This results in dynamical sign problems.

³Mühlbacher, L. & Rabani, 2008, E. Phys. Rev. Lett. 100, 176403.

⁴Werner, P., Oka, T., Millis, A.J., 2009. Phys. Rev. B 79, 035320.

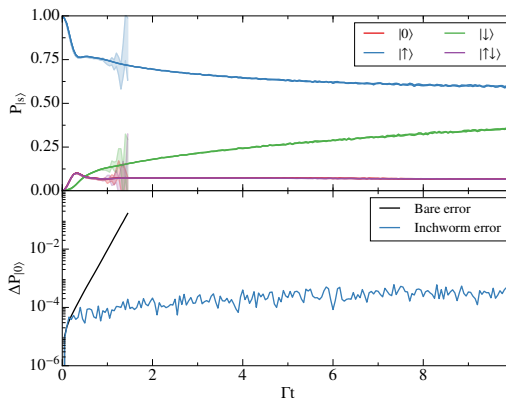
⁵Schiró, M., Fabrizio, M., 2009. Phys. Rev. B 79, 153302.

What a dynamical sign problem looks like



G. Cohen, E. Gull, D. R. Reichman, A. J. Millis, PRL 115, 266802 (2015)

Getting around the dynamical sign problem

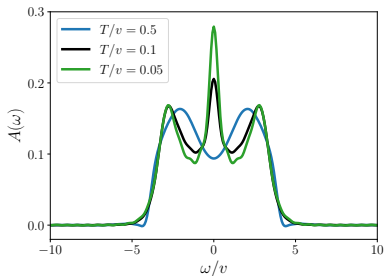
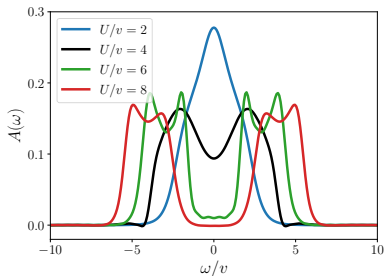


$$U = 8\Gamma, \beta_K \Gamma \simeq 50.$$

G. Cohen, E. Gull, D. R. Reichman, A. J. Millis, PRL 115, 266802 (2015)

Dynamical mean field theory: single orbital in real time

First polynomial scaling calculation!



Q. Dong, I. Krivenko, J. Kleinhenz, A. E. Antipov, G. Cohen and E. Gull, PRB 96, 155126 (2017)

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Hybridization expansion

Partitioning the Hamiltonian

- We separate the Hamiltonian into:
 - V : the hybridization between the dot and the fermionic leads.
 - H_0 : everything else.
- To evaluate an auxiliary propagator $G(t) \equiv \langle e^{iHt} \rangle$, we expand it in a Dyson series:

$$G(t) = \text{Tr} \left\{ \rho_0 T \left(U^\dagger(t) e^{-iH_0 t} \right) \right\},$$

$$U(t) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar} \right)^n \int_0^t ds_1 \int_0^{s_1} ds_2 \dots \int_0^{s_{n-1}} ds_n$$

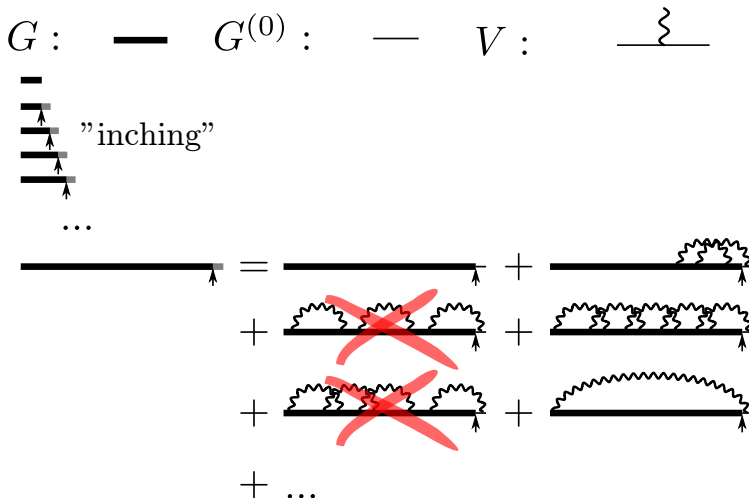
$$\times V_I(s_1) V_I(s_2) \dots V_I(s_n).$$

$$G: \text{---} \quad G^{(0)}: \text{---} \quad V: \text{---} \zeta$$

$$\begin{array}{c}
 \text{thick line} = \text{double line} + \text{self-energy} + \text{two self-energies} \\
 + \text{three self-energies} + \dots
 \end{array}$$

$$G : \text{---} \quad G^{(0)} : \text{---} \quad V : \text{---} \zeta$$


The Inchworm algorithm



Explicit notation: two symmetry-protected orbitals

$$\begin{array}{ll}
 G_{00} : \text{===} & G_{00}^{(0)} : \text{====} \\
 G_{11} : \text{==\text{}} & G_{11}^{(0)} : \text{====} \\
 G_{22} : \text{==\text{}} & G_{22}^{(0)} : \text{====} \\
 G_{33} : \text{==} & G_{33}^{(0)} : \text{==}
 \end{array}
 \quad V : \quad
 \begin{array}{cc}
 \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} & \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} & \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} & \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} \\
 \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} & \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array}
 \end{array}$$

$$\begin{array}{c}
 \text{===} = \text{====} + \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} + \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} \\
 + \begin{array}{c} \text{---} \text{ } \text{---} \\ \text{---} \end{array} + \dots
 \end{array}$$

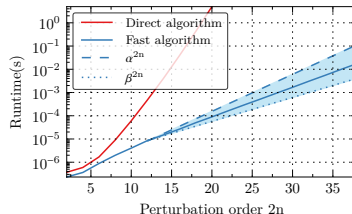
IDET(?)

$$v(V) = \text{diagram 1} + \text{diagram 2} + \text{diagram 3} + \text{diagram 4} + \text{diagram 5} + \text{diagram 6}$$

$$v(S) = \text{diagram 1} + \text{diagram 2}$$

$$\begin{aligned} & \text{diagram 1} = \text{diagram 1.1} - \text{diagram 1.2} - \text{diagram 1.3} \\ & - \text{diagram 1.4} - \text{diagram 1.5} - \text{diagram 1.6} \\ & - \text{diagram 1.7} \\ & + \text{diagram 1.8} + \text{diagram 1.9} + \text{diagram 1.10} \\ & \text{diagram 2} = \text{diagram 2.1} - \text{diagram 2.2} - \text{diagram 2.3} \\ & = 0 \end{aligned}$$

$$\begin{aligned} c(V) &= c_1(V) = \text{diagram 1} \\ c_2(V) &= \text{diagram 2} \\ c_3(V) &= \text{diagram 3} + \text{diagram 4} \\ c(S) &= \text{diagram 5} \end{aligned}$$

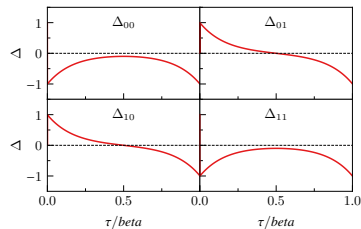
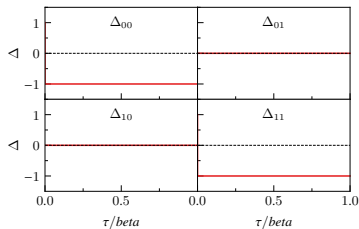
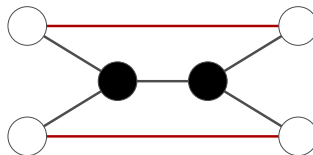
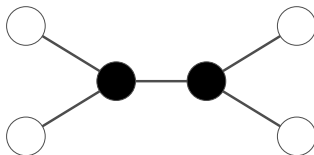


A. Boag, E. Gull, and G. Cohen, PRB 98, 115152 (2018)

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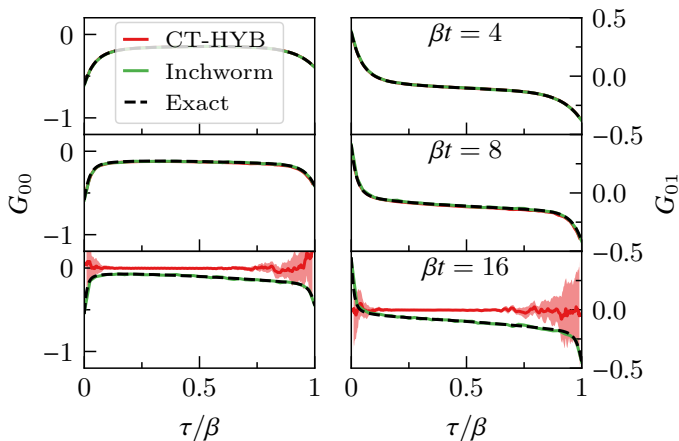
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Spinless Anderson model

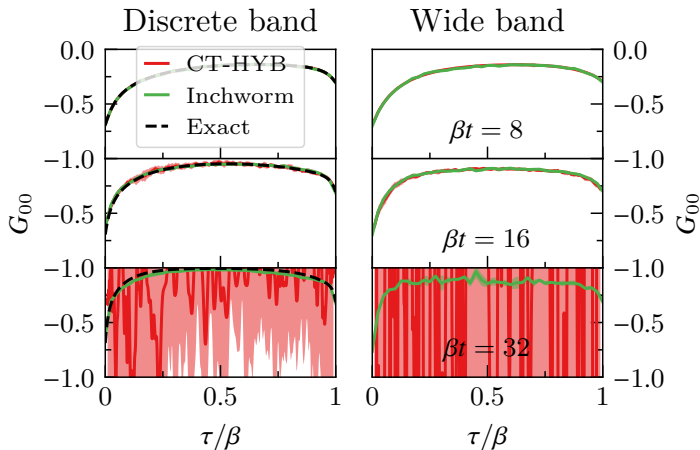


E. Eidelstein, E. Gull, and G. Cohen, arXiv:1907.08570

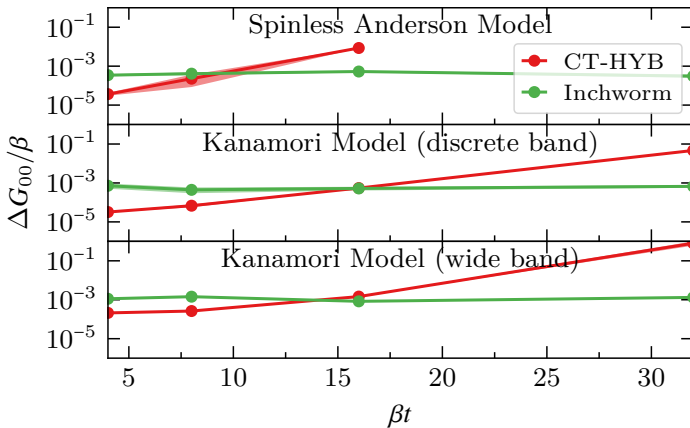
Spinless Anderson model



Two-orbital Kanamori model



Scaling



Summary and future directions

- The old adage that real time QMC suffers from exponential sign problems at long times can be overcome in some cases: **The Inchworm algorithm** eliminates the sign problem quite generally in the Anderson impurity model and spin-boson model, at least where finite-order skeleton expansions are applicable.
- The same idea can be used to eliminate the **multiorbital sign problem**, allowing DMFT to be applied to a much wider class of real materials without additional approximations.