Computational challenges in condensed matter theory

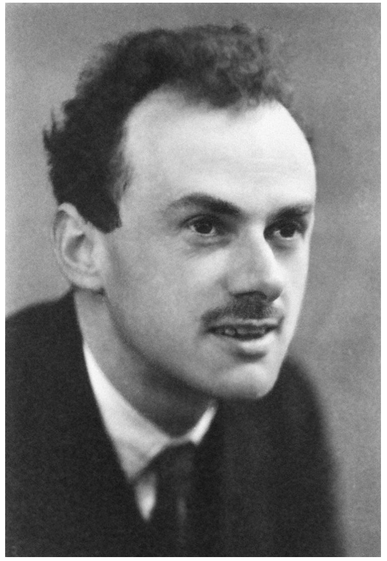
From strongly correlated electrons to quantum information methods

Giacomo Mazza

Congresso Dipartimento 2026

Dipartimento di Fisica “E. Fermi”
Università di Pisa

The Quantum Many-Body Problem



Quantum Mechanics of Many-Electron Systems.

By P. A. M. Dirac, St. John's College, Cambridge.

(Communicated by R. H. Fowler, F.R.S.—Received March 12, 1929.)

The underlying physical laws [...] are completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

The quantum many-body problem is exponentially challenging

Need to find clever approximation schemes

Computational power helps, but not game changer

Example: The N-electrons atom

- N-electrons wavefunction $\Psi(\vec{r}_1, \ldots, \vec{r}_N) = \sum_{\{n_\alpha\}} C_{\{n_\alpha\}} \phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$

  single electron orbitals (e.g. hydrogen) $\varphi_{\alpha_i}(\vec{r})$

  orbital occupations $\{n_\alpha\} = [n_{\alpha_1}, \ldots, n_{\alpha_L}, \times \ldots] \quad n_{\alpha_i} = 0, 1$

  Hilbert space truncation

  $\phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$ Slater determinant for a given set of orbital occupations

$$\sum_{i=1}^{L} n_{\alpha_i} = N$$

Example: The N-electrons atom

- N-electrons wavefunction $\Psi(\vec{r}_1, \ldots, \vec{r}_N) = \sum_{\{n_\alpha\}} C_{\{n_\alpha\}} \phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$

single electron orbitals (e.g. hydrogen) $\varphi_{\alpha_i}(\vec{r})$

orbital occupations $\{n_\alpha\} = [n_{\alpha_1}, \ldots, n_{\alpha_L}, \times \ldots] \quad n_{\alpha_i} = 0, 1$

Hilbert space truncation

2^L coefficients

$L \geq N$

$$\sum_{i=1}^{L} n_{\alpha_i} = N$$

$\phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$ Slater determinant for a given set of orbital occupations

Example: The N-electrons atom

- N-electrons wavefunction $\Psi(\vec{r}_1, \ldots, \vec{r}_N) = \sum_{\{n_\alpha\}} C_{\{n_\alpha\}} \phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$

  single electron orbitals (e.g. hydrogen) $\varphi_{\alpha_i}(\vec{r})$

  orbital occupations $\{n_\alpha\} = [n_{\alpha_1}, \ldots, n_{\alpha_L}, \times .]$ $n_{\alpha_i} = 0, 1$

  Hilbert space truncation

  2^L coefficients

  $L \geq N$

  $\sum_{i=1}^{L} n_{\alpha_i} = N$

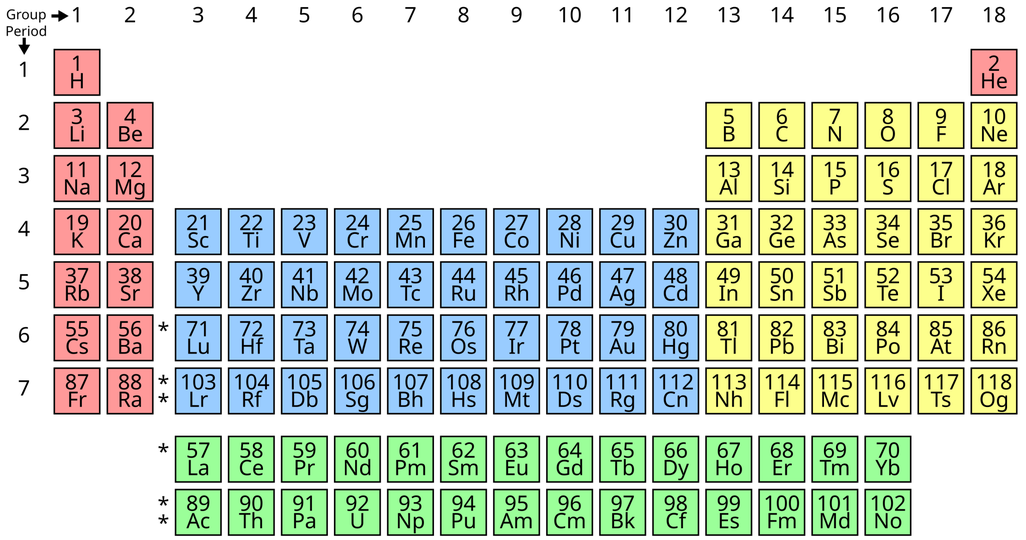
  $\phi_{\{n_\alpha\}}(\vec{r}_1, \ldots, \vec{r}_N)$ Slater determinant for a given set of orbital occupations

- Self-consistent methods (eg. Hartree-Fock)

  non-interacting electrons in an effective potential
  self-consistently determined by the other N-1 electrons

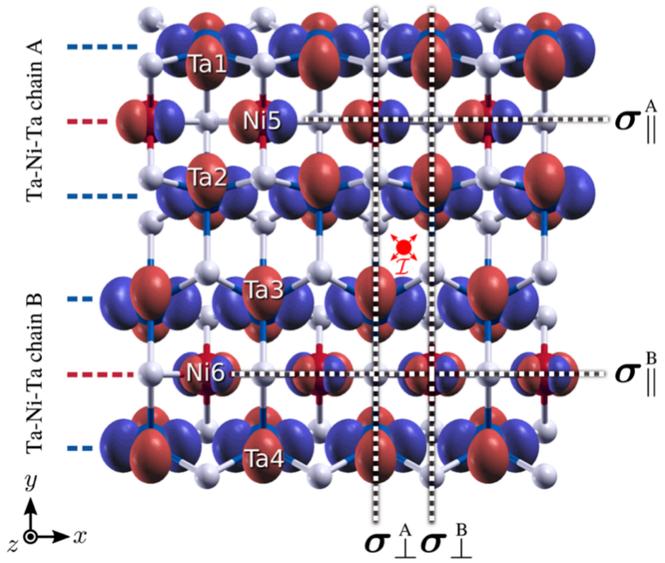
  ↓

  periodic table build up



From single atoms to complex materials

Ab-initio



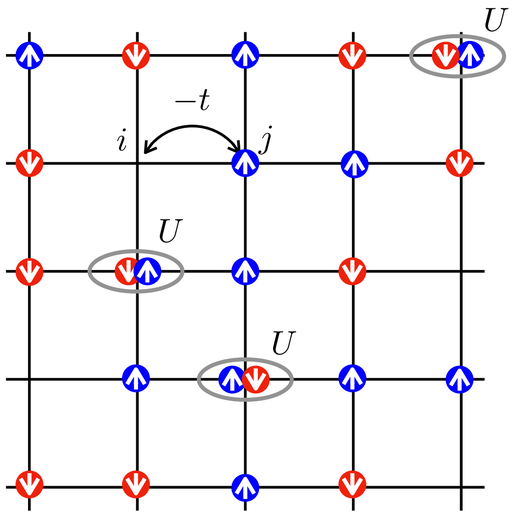
Density Functional Theories
molecular dynamics
Quantum chemistry

Quantum Many-body problems in Condensed Matter

Not only electrons!
phonons, light/e.m. environments

Minimal models

$$H = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

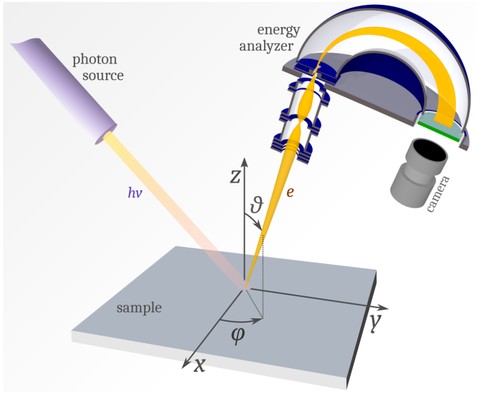


DMFT,
QMC,
DMRG, Neural Networks,
Exact Diag,
…

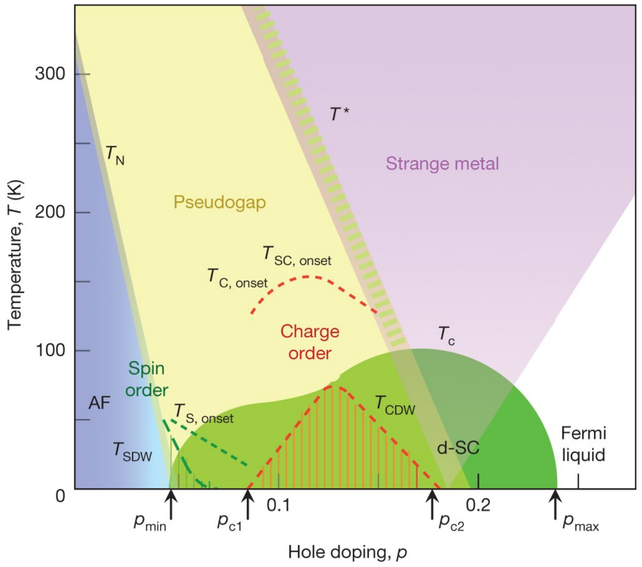
Solving Quantum Many-Body Problems

Determine the full spectrum, and carry out some calculations with that!

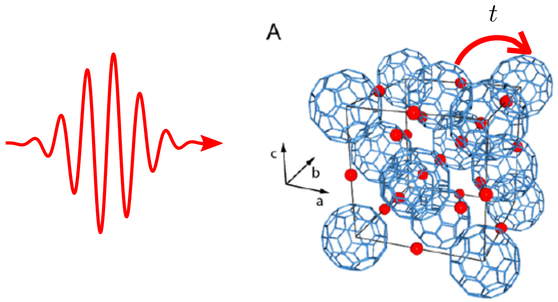
- Experimentally measurable spectral function (e.g. optics, photoemission spectroscopy…)



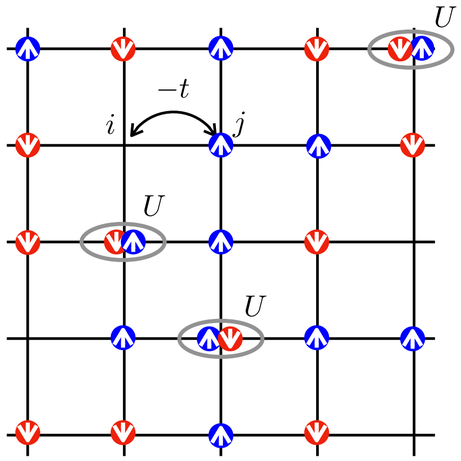
- Spontaneous symmetry breaking/Ordering temperatures



- Non-equilibrium dynamics



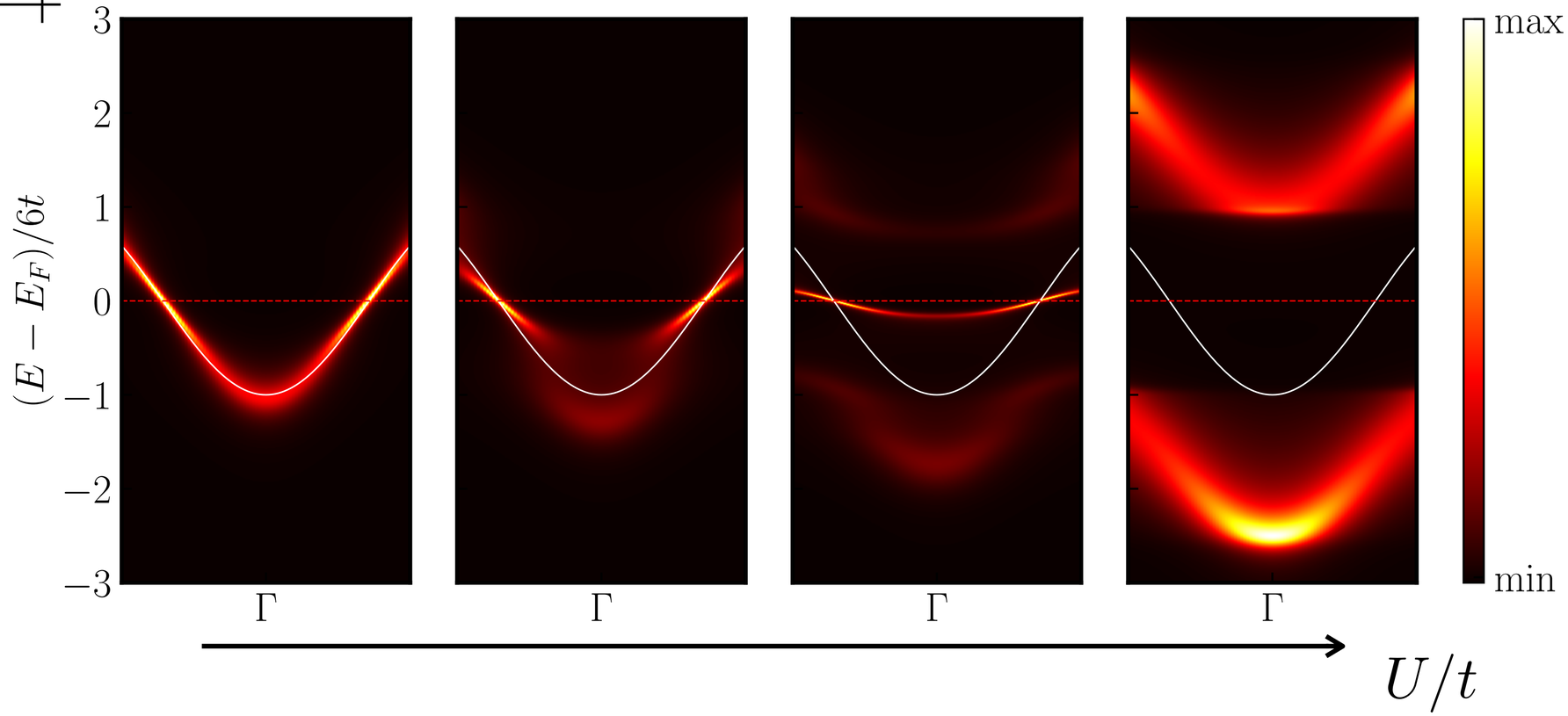
Example: The Mott Transition in the Hubbard model



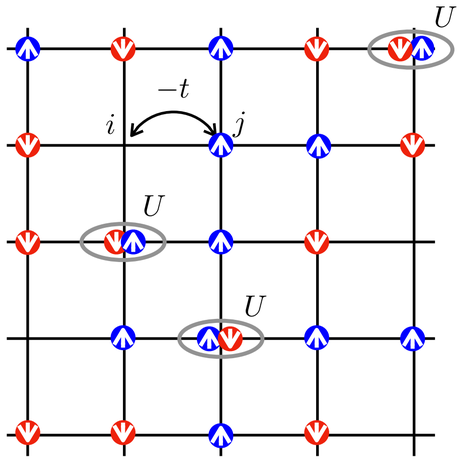
$$H = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$\langle n \rangle = 1$ average of one electron per lattice site

$A(\mathbf{k}, \omega)$



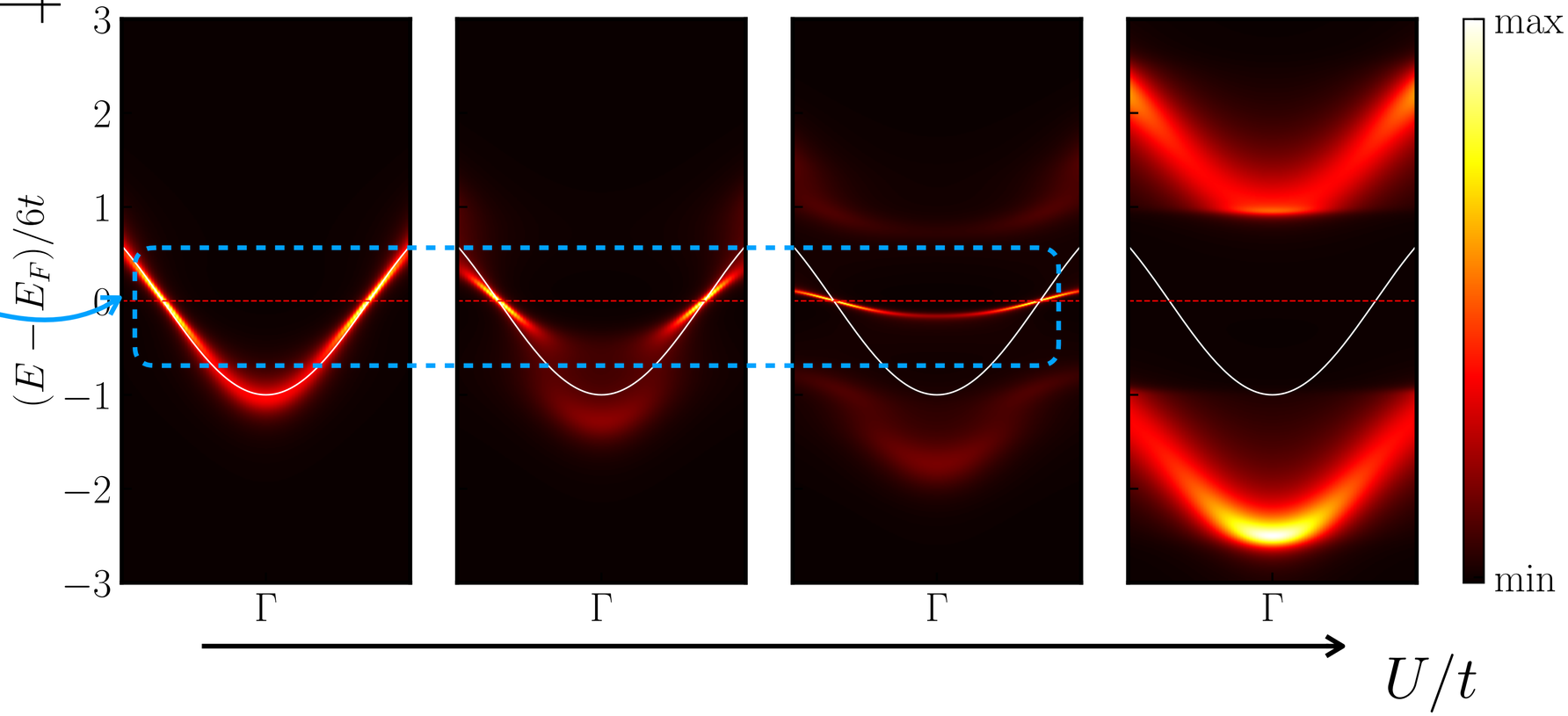
Example: The Mott Transition in the Hubbard model



$$H = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

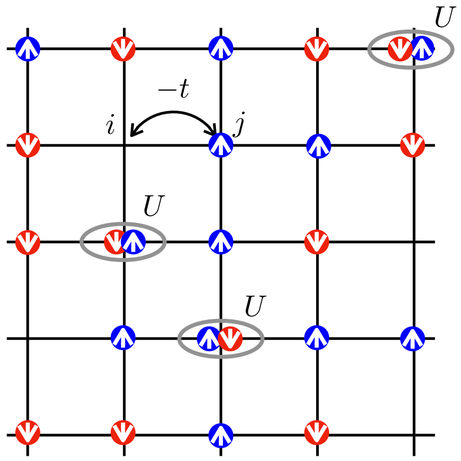
$\langle n \rangle = 1$ average of one electron per lattice site

$A(\mathbf{k}, \omega)$



"heavier" quasiparticles

Example: The Mott Transition in the Hubbard model

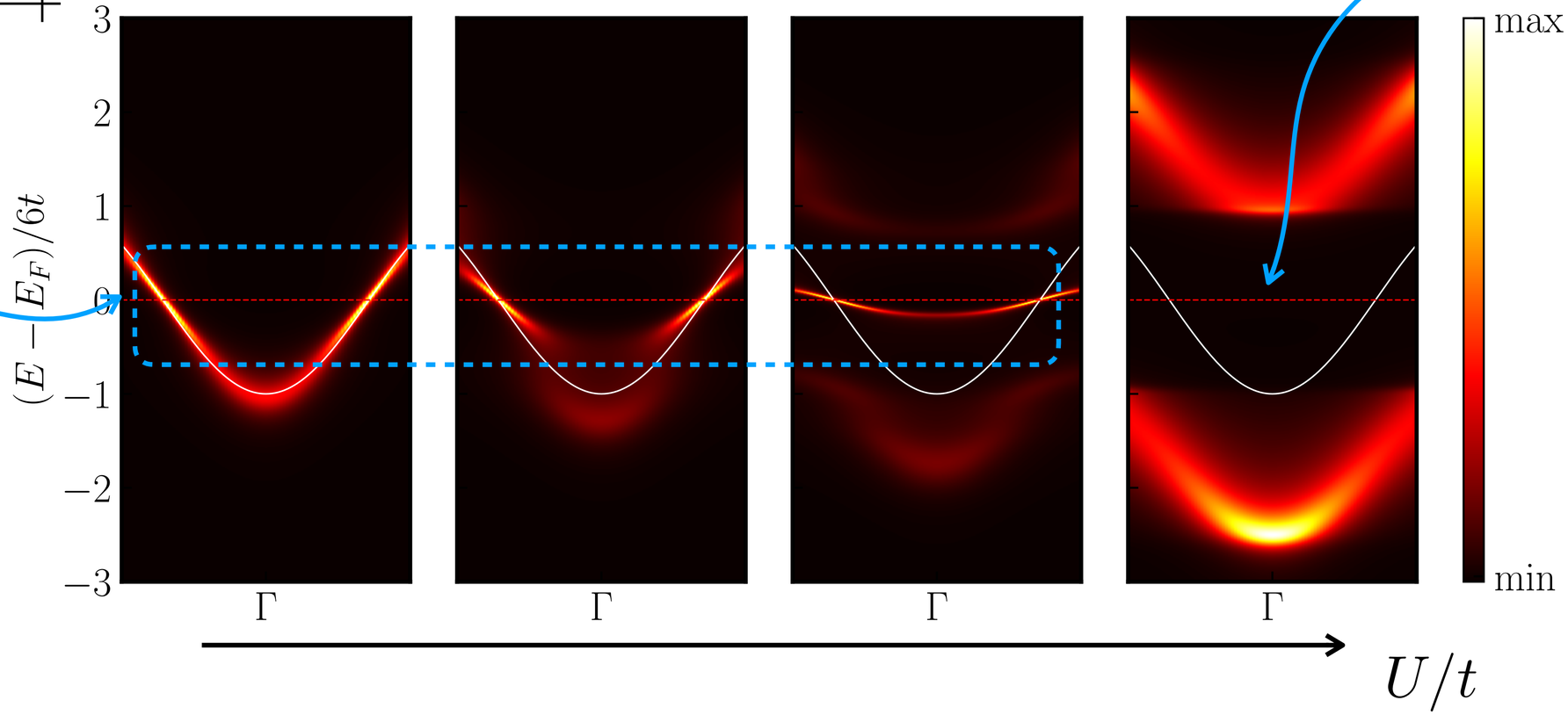


$$H = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$\langle n \rangle = 1$ average of one electron per lattice site

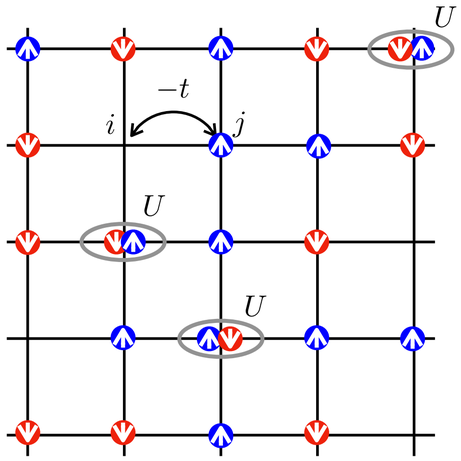
No quasiparticles
“Mott Insulator”

$A(\mathbf{k}, \omega)$



“heavier”
quasiparticles

Example: The Mott Transition in the Hubbard model

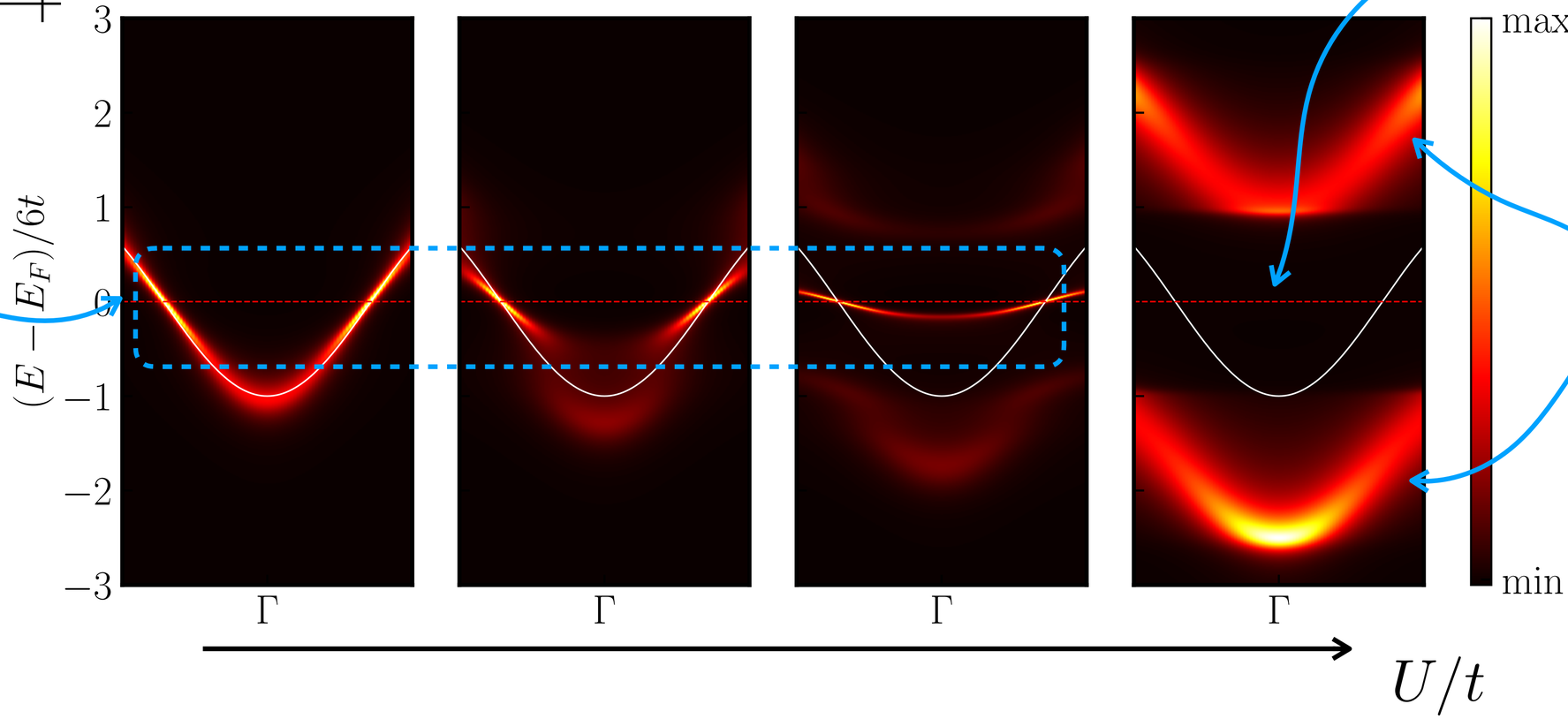


$$H = -t \sum_{\langle ij \rangle} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$\langle n \rangle = 1$ average of one electron per lattice site

No quasiparticles
“Mott Insulator”

$A(\mathbf{k}, \omega)$



~ eV
“high-energy”
incoherent
excitations

“heavier”
quasiparticles

Dynamical Mean Field Theory for Strongly Correlated Electrons

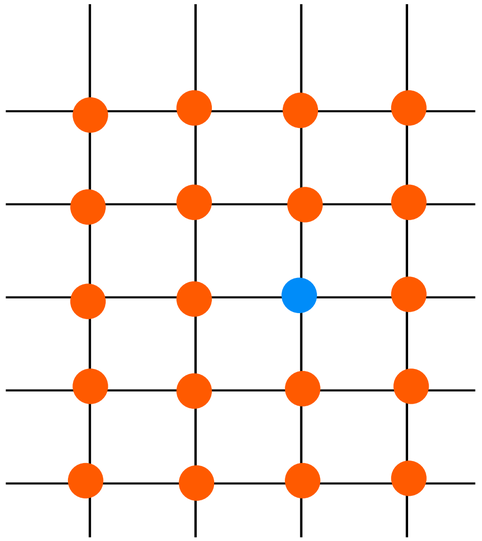
mean-field theory for a dynamical object

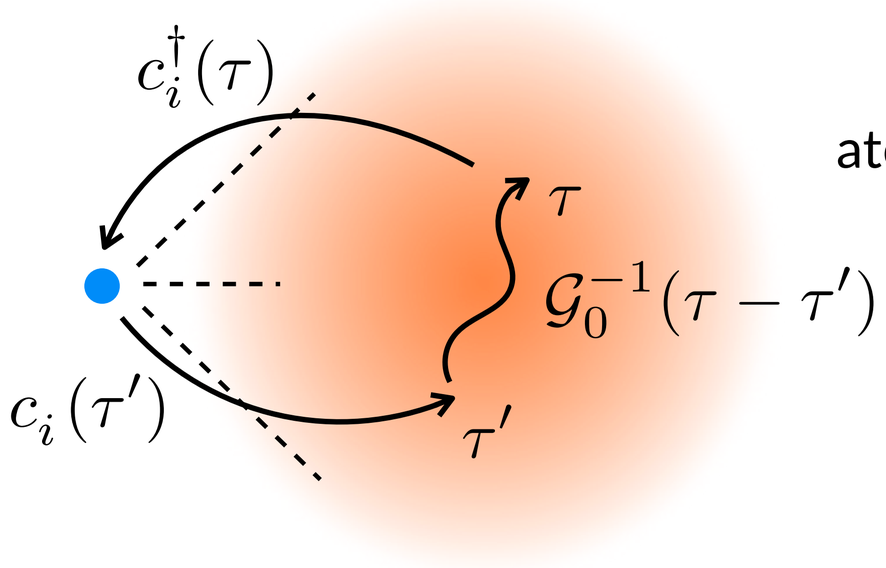
single-particle Green's function

$$G_i(\tau) = -\left\langle T_\tau c_i(\tau) c_i^\dagger(\tau') \right\rangle$$

$$H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

lattice model





atom in a bath

effective action $$\mathcal{S}_i = \int_0^\beta d\tau d\tau' c_{i\sigma}^\dagger(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{i\sigma}(\tau') + U \int_0^\beta d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)$$

A. Georges, G. Kotliar, W. Krauth, M. Rozenberg Review Modern Physics 1996

Dynamical Mean Field Theory for Strongly Correlated Electrons

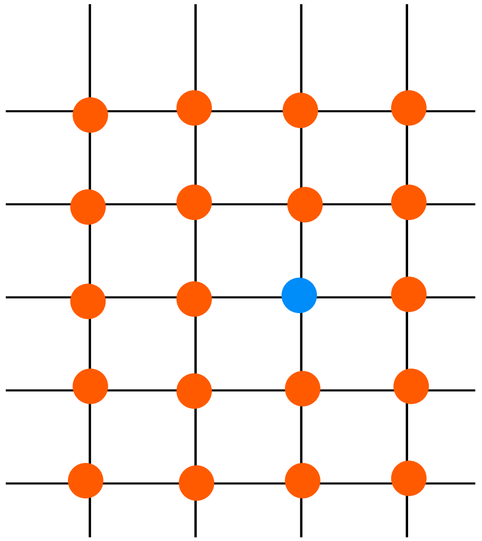
mean-field theory for a dynamical object

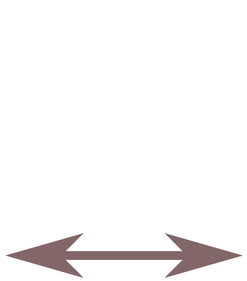
single-particle Green's function

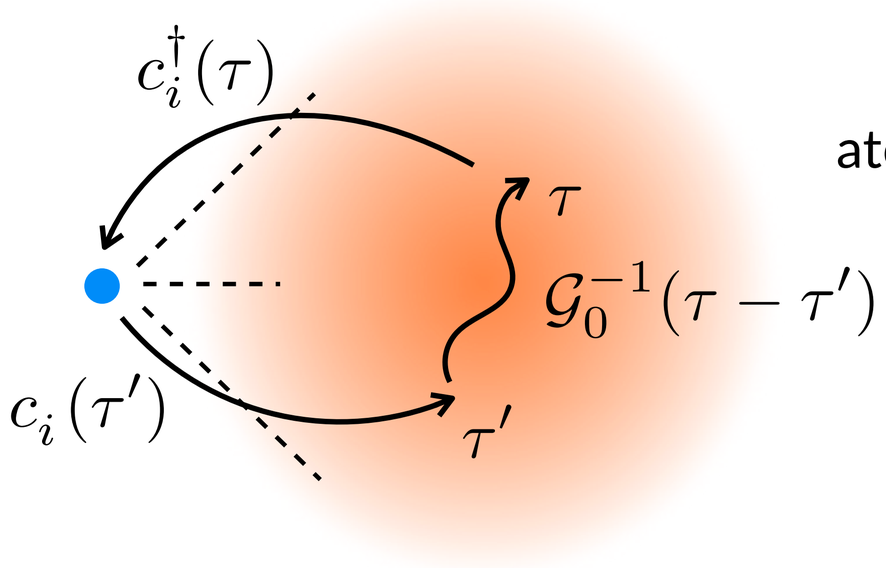
$$G_i(\tau) = -\left\langle T_\tau c_i(\tau) c_i^\dagger(\tau') \right\rangle$$

$$H = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

lattice model







atom in a bath

effective action $$\mathcal{S}_i = \int_0^\beta d\tau d\tau' c_{i\sigma}^\dagger(\tau) \mathcal{G}_0^{-1}(\tau - \tau') c_{i\sigma}(\tau') + U \int_0^\beta d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)$$

unknown function describing the embedding of the atom in the lattice

A. Georges, G. Kotliar, W. Krauth, M. Rozenberg Review Modern Physics 1996

Static VS Dynamical Mean Field Theory

Static

Local observable

local magnetization

$$m_i = \langle \sigma_i \rangle$$

Static VS Dynamical Mean Field Theory

Static

Local observable

local magnetization

$$m_i = \langle \sigma_i \rangle$$

auxiliary problem

spin in a magnetic field

$$m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$$

Static VS Dynamical Mean Field Theory

Static

Local observable

local magnetization

$$m_i = \langle \sigma_i \rangle$$

auxiliary problem

spin in a magnetic field

$$m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$$

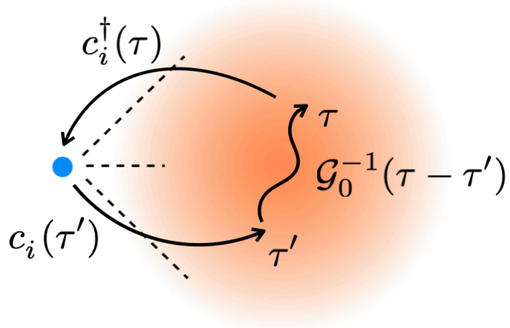
mean-field approx

$z \to \infty$

$$h_i^{\text{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$$

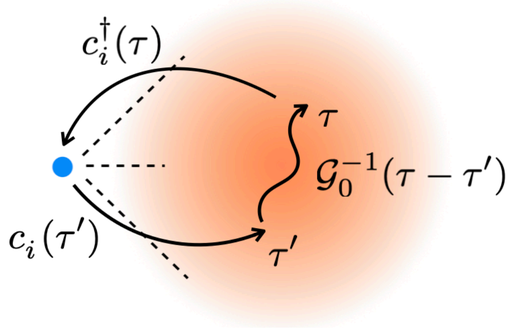
Static VS Dynamical Mean Field Theory

	Static	Dynamical
Local observable	local magnetization $m_i = \langle \sigma_i \rangle$	local Greens function $G_{ii}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(0) \rangle$
auxiliary problem	spin in a magnetic field $m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$	atom in a bath $G^{-1}_{ii}(\tau) = \mathcal{G}_0^{-1}(\tau) - \Sigma_{\text{imp}}[\mathcal{G}_0]$
mean-field approx $z \to \infty$	$h_i^{\text{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$	$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{imp}(\omega)$



Static VS Dynamical Mean Field Theory

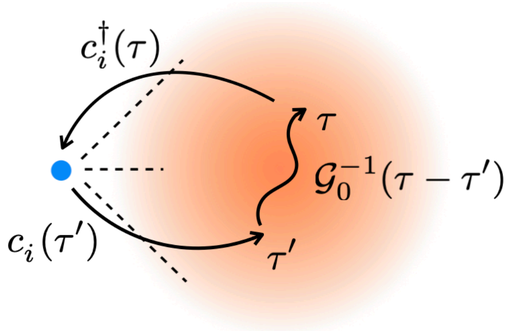
	Static	Dynamical
Local observable	local magnetization $m_i = \langle \sigma_i \rangle$	local Greens function $G_{ii}(\tau) = -\langle T_\tau c_{i\sigma}(\tau) c^\dagger_{i\sigma}(0) \rangle$
auxiliary problem	spin in a magnetic field $m_i = \tanh\left(\beta h_i^{\text{eff}}\right)$	atom in a bath $G^{-1}_{ii}(\tau) = \mathcal{G}_0^{-1}(\tau) - \Sigma_{\text{imp}}[\mathcal{G}_0]$
mean-field approx $z \to \infty$	$h_i^{\text{eff}} = h_i + J \sum_{\langle ij \rangle} m_j$	$\Sigma_{\mathbf{k}}(\omega) = \Sigma_{imp}(\omega)$



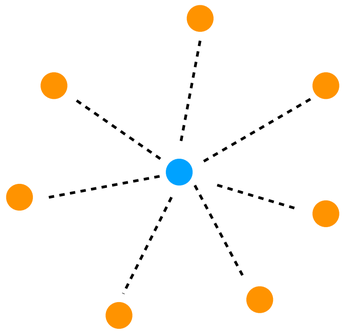
In the Dynamical Mean Field Theory the auxiliary problem is still a quantum many body problem!

Exact diagonalization methods for solving impurity problems

Discretize the “atom-in-a-bath-problem” and solve an interacting Anderson model



discretization



Compute impurity Greens function using Lanczos-based methods

Computer Physics Communications 273 (2022) 108261

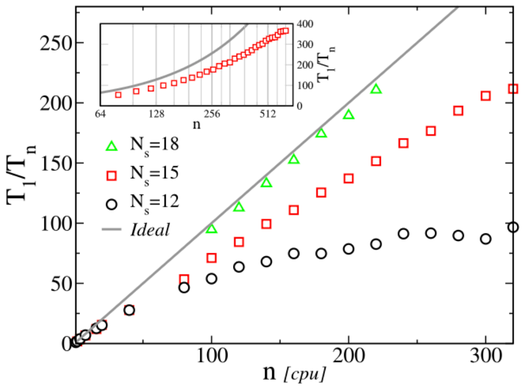
Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

EDIpack: A parallel exact diagonalization package for quantum impurity problems ☆,☆☆

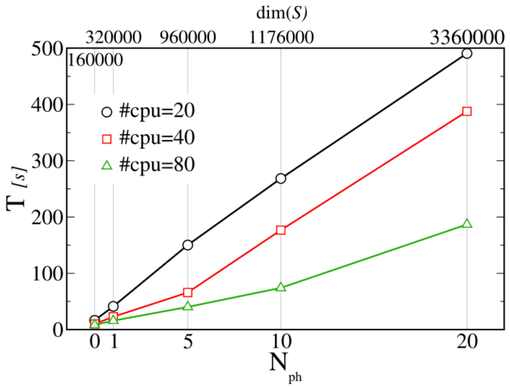
A. Amaricci [a,*], L. Crippa [b,c], A. Scazzola [b], F. Petocchi [d], G. Mazza [e], L. de Medici [f], M. Capone [b]



SciPost Phys. Codebases 58 (2025)

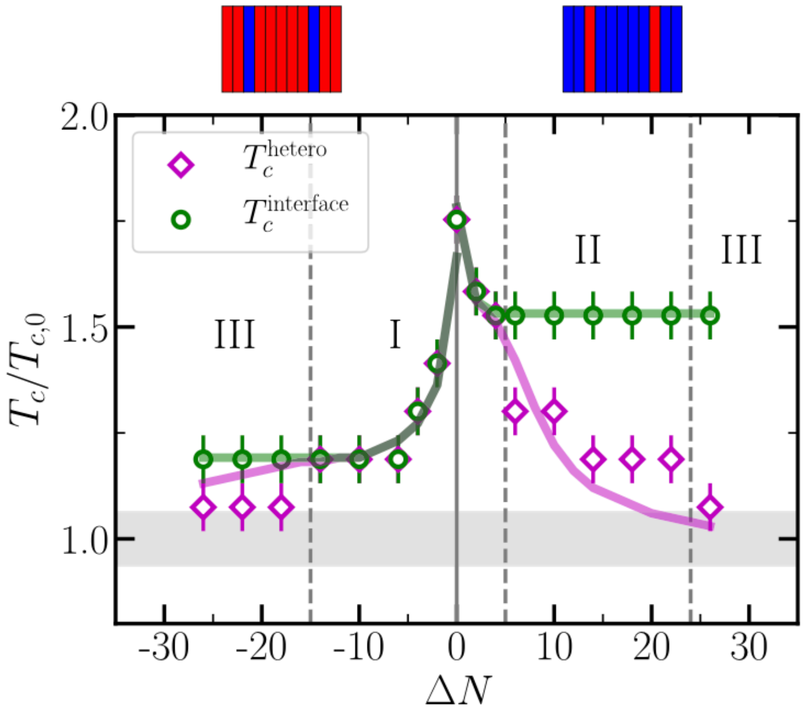
Next-generation EDIpack: A Lanczos-based package for quantum impurity models featuring general broken-symmetry phases, flexible bath topologies and multi-platform interoperability

Lorenzo Crippa[1,2,3], Igor Krivenko[1], Samuele Giuli[4], Gabriele Bellomia[4], Alexander Kowalski[3], Francesco Petocchi[5], Alberto Scazzola[6], Markus Wallerberger[7], Giacomo Mazza[8], Luca de Medici[9], Giorgio Sangiovanni[2,3], Massimo Capone[4,10] and Adriano Amaricci[10]



DMFT-ED - some applications

- Competition between weak and strong coupling superconductivity in layered heterostructures

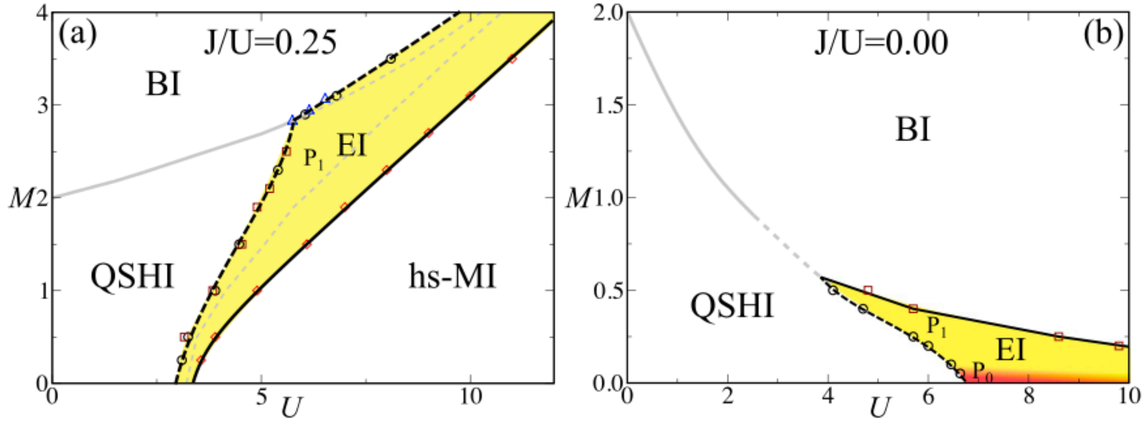


G. Mazza, A. Amaricci, M. Capone PRB (2022)

- Simultaneous breaking of multiple symmetries in Quantum Spin Hall Insulators

Multi-orbital —> Hund's Coupling

- ✗ Tr-symmetry
- ✗ U(1) spin
- ✗ Parity



A. Amaricci, G. Mazza, M. Capone, M. Fabrizio PRB (2023)

Semidefinite Program/bootstrap methods for correlated electrons

F. Vallone, M. Polini, A. Vichi, G. Mazza, and C. Budroni in prep (2026)

Ground state energy as a convex optimization

$$E_{gs} = \min_{\rho} \mathrm{Tr}\left[\rho H\right]$$

such that $\rho \succeq 0$ + linear constraints

$$\mathrm{Tr}\left[\rho\right] = 1$$
$$\mathrm{Tr}\left[\rho \left\{c^{\dagger}_{i\sigma}, c_{j\sigma'}\right\}\right] = \delta_{ij}\delta_{\sigma\sigma'}$$
$$\dots$$

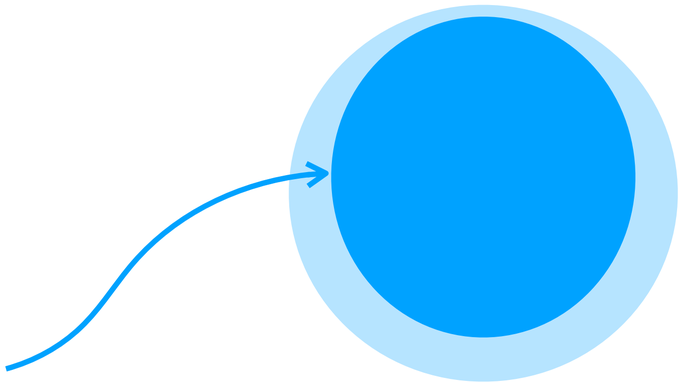
Relaxation of the optimization problem

$$E = \min_{\Gamma} \mathrm{Tr}\left[X_H \Gamma\right]$$

such that $\Gamma \succeq 0$ + linear constraints

Moment matrix $\Gamma = \mathrm{Tr}\left[\rho O_i O_j\right]$

$O_i \in$ set of linear operators acting on the Hilbert space



Original problem: minimization over the set of physical states

Relaxation: Optimization over a larger set

$$E \leq E_{gs}$$

Gao et al PRX 15, 031034 (2025)
Gao, et al PRL 136, 076503 (2026)
Scheer arXiv 2410.00810

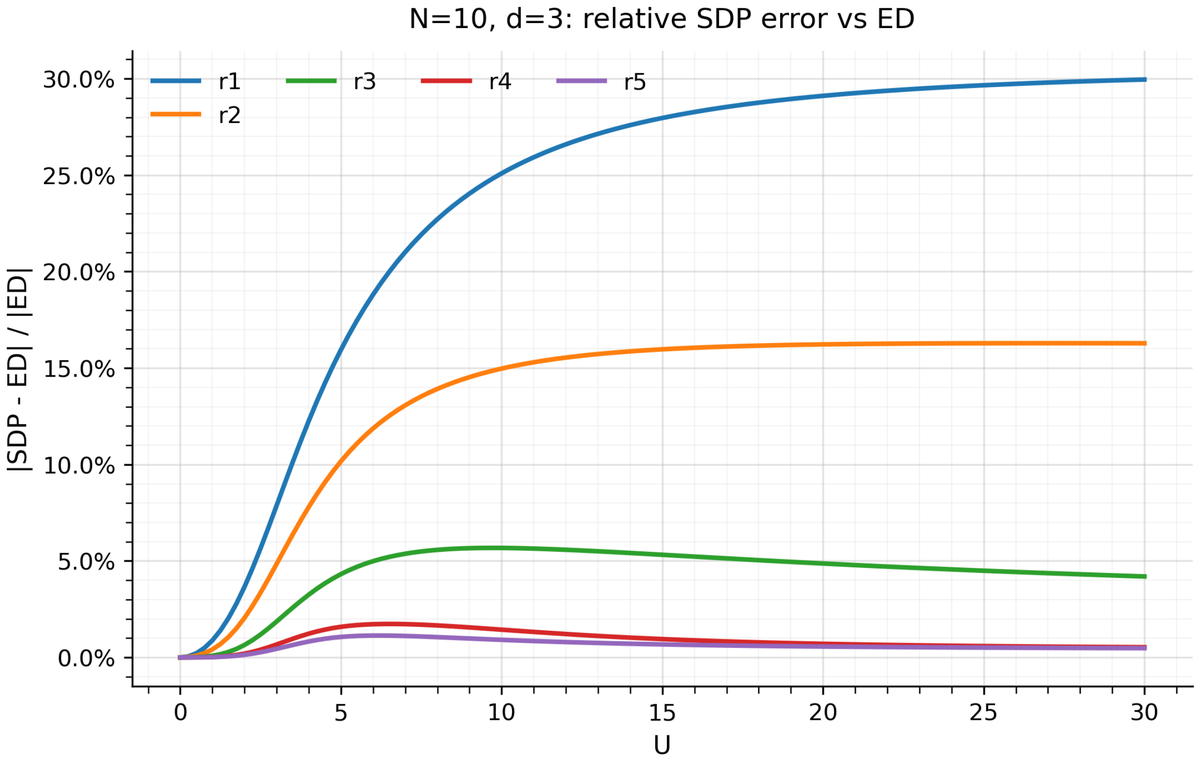
Benchmarking SDP VS Exact Diagonalization for the 1D Hubbard model

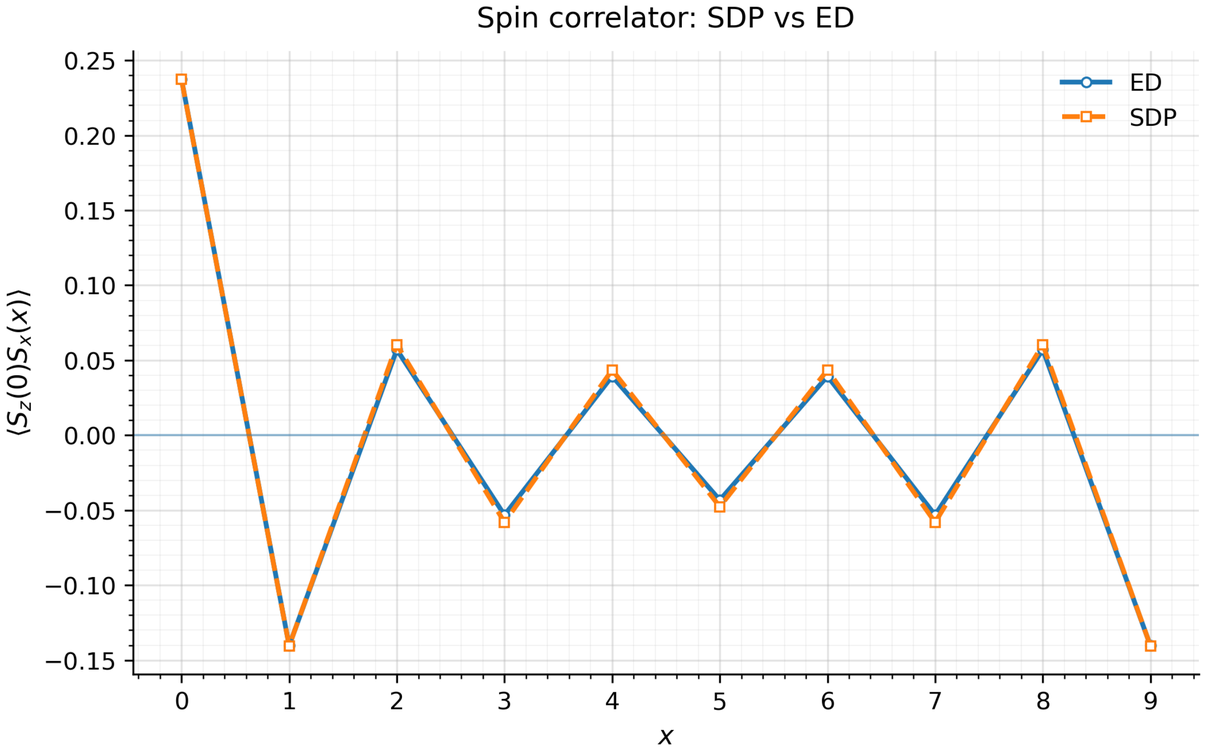
Exploitation of symmetries in the moment matrix

so far up to N = 20 spinfull electrons
(~ state-of-the-art ED)

Physically intuition for truncation of the moment set

moving towards to 2D models





F. Vallone, M. Polini, A. Vichi, G. Mazza, and C. Budroni in prep (2026)

summary

quantum many body problem from a condensed matter point of view

Interplay between approximate schemes and numerically exact methods —> DMFT

interdisciplinary research direction @df.unipi to push SDP/bootstrap methods for strongly correlated electrons

thanks to

Costantino Budroni (unipi)
Marco Polini (unipi)
Fabio Vallone (unipi)
Alessandro Vichi (unipi)
Damiano Marian (unipi)
Giovanni Citeroni (unipi)
Adriano Amaricci (CNR)
Massimo Capone (SISSA)
Michele Fabrizio (SISSA)

Dipartimento di Fisica “E. Fermi”
Università di Pisa