Theoretical Approaches to Strongly Correlated Materials

Christopher Lane

Physics of Condensed Matter and Complex Systems, Theoretical Division
Los Alamos National Laboratory
Los Alamos, NM

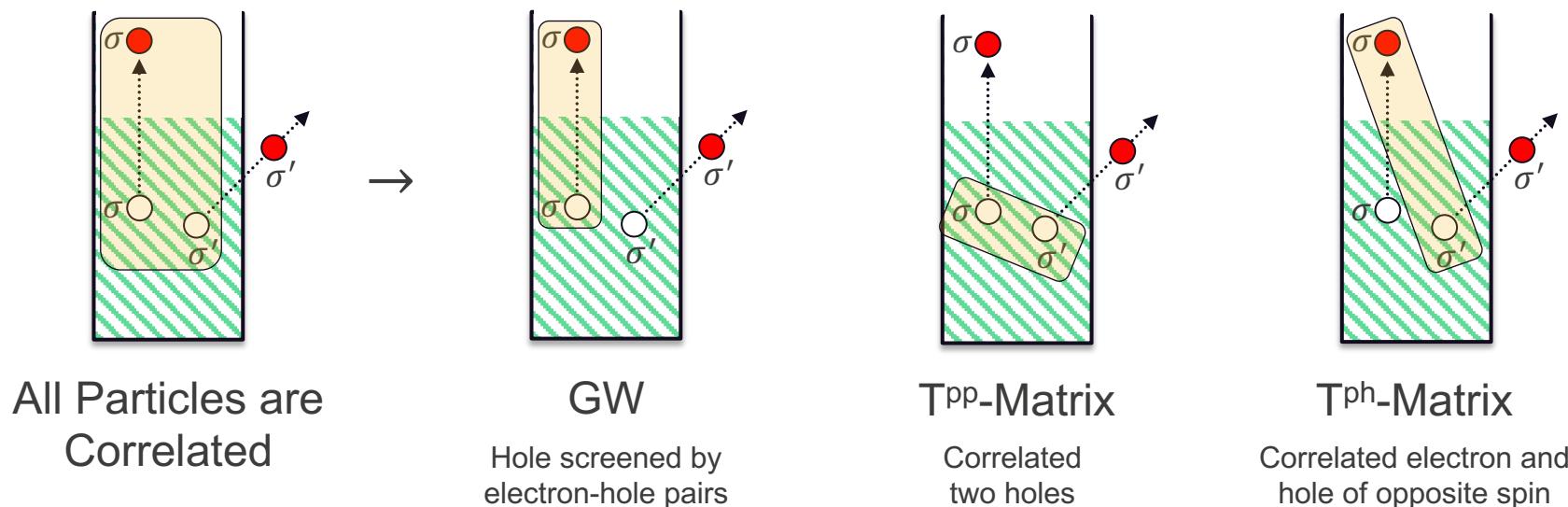# Do we need to go beyond the GW approximation?

Many approximations are based on a picture where a quasi-particle is dressed by pairs of particles. This splits the many-body problem into one effective particle and a correlated two-body part.

$$\Delta E_s = \underbrace{E_N - E_{N-1,t}}_{\text{quasi-particle excitation}} + \underbrace{E_{N-1,t} - E_{N-1,s}}_{\text{quasi-particle excitation}}$$

All Particles are Correlated

GW
Hole screened by electron-hole pairs

T^{pp}-Matrix
Correlated two holes

T^{ph}-Matrix
Correlated electron and hole of opposite spin

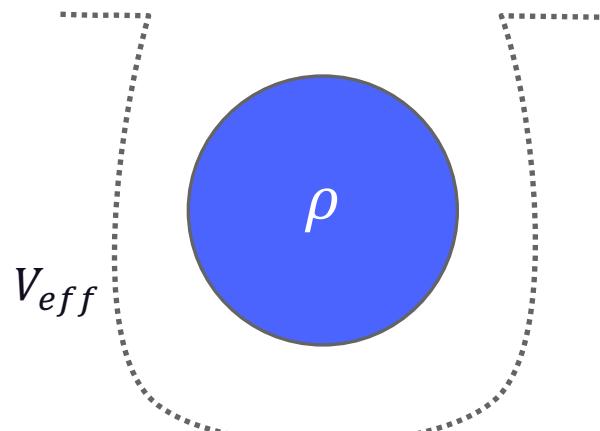**Are there other approaches to address this problem?**

Theoretical Approaches to Interacting Many-Electron Systems

Many-body Hamiltonian

$$\widehat{H} = \sum_{\alpha\beta} \int d^3r \; \hat{\psi}_\alpha^\dagger(r) \left(\frac{-\hbar^2 \nabla^2}{2m} + v_{ext}^{\alpha\beta}(r) \right) \hat{\psi}_\beta(r) + \frac{1}{2} \sum_{\alpha\beta} \iint d^3r \, d^3r' \; \hat{\psi}_\alpha^\dagger(r) \hat{\psi}_\beta^\dagger(r') v(r,r') \hat{\psi}_\beta(r') \hat{\psi}_\alpha(r)$$
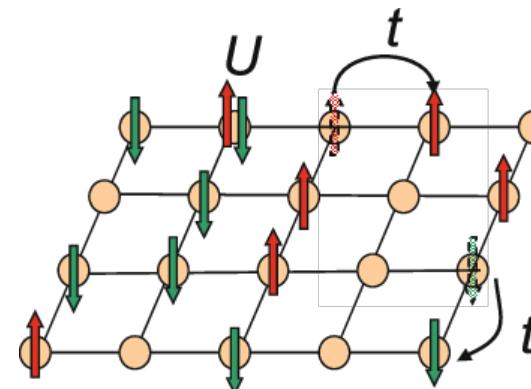
$\alpha\beta \in$ spin

Electronic Kinetic Energy

Interactions

Reduced quantity based approaches

Key Quantities: Simpler physical quantitiy, e.g., $\rho(r), \gamma(r,r'), G(r,r'), \cdots$

V_{eff}

ρ

Many-body Hamiltonian Community

Key: Replace Hamiltonian with a simplified model Hamiltonian, hoping this leads to qualitative understanding

U t t

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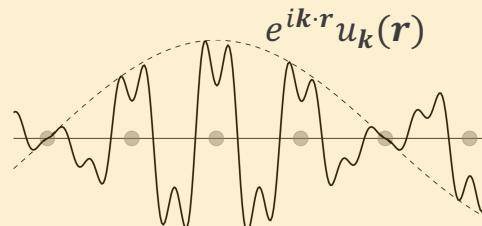
Reduction of the Interacting Many-Electron Hamiltonian

Many-body Hamiltonian

$$\widehat{H} = \sum_{\alpha\beta} \int d^3r \; \hat{\psi}_\alpha^\dagger(r) \left(\frac{-\hbar^2 \nabla^2}{2m} + v_{ext}^{\alpha\beta}(r) \right) \hat{\psi}_\beta(r) + \frac{1}{2} \sum_{\alpha\beta} \iint d^3r \; d^3r' \; \hat{\psi}_\alpha^\dagger(r) \hat{\psi}_\beta^\dagger(r') v(r,r') \hat{\psi}_\beta(r') \hat{\psi}_\alpha(r)$$

$\alpha\beta \in$ spin

Electronic Kinetic Energy

Interactions

The field operators can be expressed in an arbitrary complete representation.

Bloch Representation

$$\hat{\psi}_\alpha(\boldsymbol{r}) = \sum_{n,\boldsymbol{k}} \hat{c}_{nk\alpha} \phi_{nk\alpha}(\boldsymbol{r})$$

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} u_{\boldsymbol{k}}(\boldsymbol{r})$$

Tight-Binding Representation

$$\hat{\psi}_\alpha(\boldsymbol{r}) = \sum_{n,I} \hat{c}_{nI\alpha} \phi_{nI\alpha}(\boldsymbol{r} - \boldsymbol{R}_I)$$

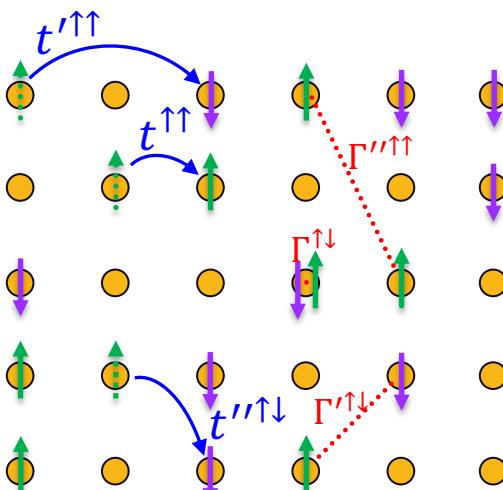$$\phi_{n0\alpha}(r - R_0)$$

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Reduction of the Interacting Many-Electron Hamiltonian

$$\hat{H} = -\sum_{\alpha\beta ijRR'} t_{ij}^{\alpha\beta}(R,R')\hat{c}_{i\alpha}^{\dagger}(R)\hat{c}_{j\beta}(R') + \frac{1}{2}\sum_{\alpha\beta ijmn} \hat{c}_{i\alpha}^{\dagger}(R)\hat{c}_{j\beta}^{\dagger}(R')\Gamma_{\alpha\beta}^{ijmn}(R''',R'';R,R')\hat{c}_{m\beta}(R'')\hat{c}_{n\alpha}(R''')$$

where

$$t_{ij}^{\alpha\beta}(R,R') = \int d^3r\, \phi_{i\alpha}^*(r-R_i)\left(\frac{\hbar^2\nabla^2}{2m}+v_{ext}^{\alpha\beta}(r)\right)\phi_{j\beta}(r-R_j)$$

$$\Gamma_{\alpha\beta}^{ijmn}(R''',R'';R,R') = \iint d^3r\, d^3r'\, \phi_{i\alpha}^*(r-R_i)\phi_{j\beta}^*(r-R_j)v(r,r')\phi_{m\beta}(r-R_m)\phi_{n\alpha}(r-R_n)$$
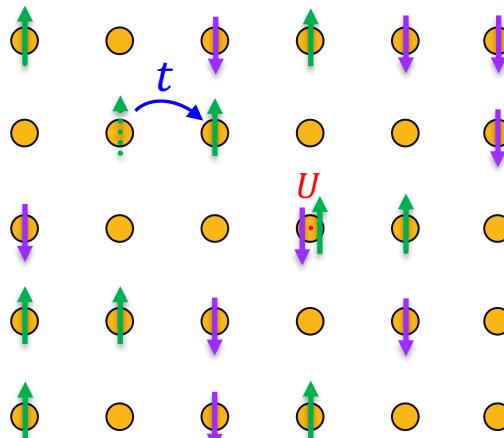
Effective Model Hamiltonians

For problems of strong correlation in narrow band systems,
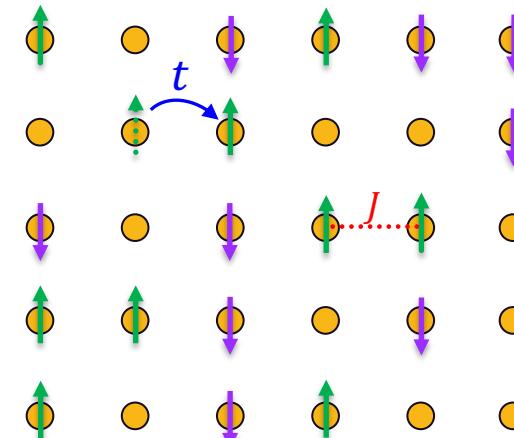it is convenient to use the tight-binding representation

Hubbard Model

$$\hat{H} = -\sum_{\alpha ij} t_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

T-J Model

$$\hat{H} = -\sum_{\alpha ij} t_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\alpha} + J \sum_{\langle ij \rangle} \hat{S}_i \cdot \hat{S}_j$$

Lage-U limit

Consider a partially field
single band or "orbital"

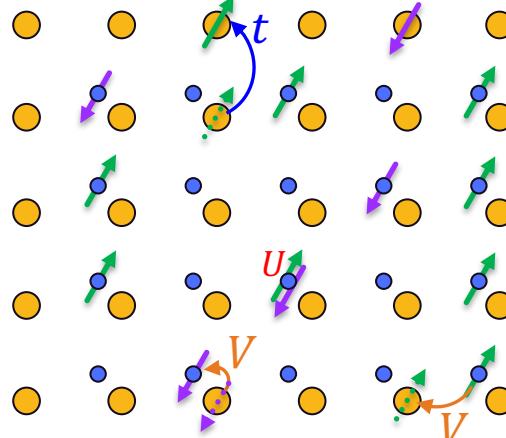$$J = \frac{4t^2}{U}$$

For hopping restricted
to nearest-neighbors

Effective Model Hamiltonians

For problems of strong correlation in narrow band systems,
it is convenient to use the tight-binding representation
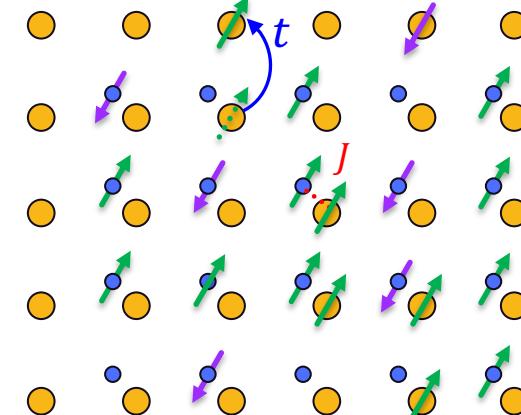
Periodic Anderson Lattice Model

$$\widehat{H} = \sum_{\alpha ij} t_{ij}\hat{c}_{i\alpha}^{\dagger}\hat{c}_{j\alpha} + V_{ij}\hat{c}_{i\alpha}^{\dagger}\hat{f}_{j\alpha} + V_{ji}^{*}\hat{f}_{j\alpha}^{\dagger}\hat{c}_{i\alpha}$$

$$+ \sum_{\alpha i} \varepsilon_f \hat{f}_{i\alpha}^{\dagger}\hat{f}_{i\alpha} + U \sum_{i} \hat{n}_{i\uparrow}^{f}\hat{n}_{i\downarrow}^{f}$$

Kondo Lattice Model

$$\widehat{H} = \sum_{\alpha ij} t_{ij}\hat{c}_{i\alpha}^{\dagger}\hat{c}_{j\alpha} + J_K \sum_{i} S_i \cdot \hat{s}_i$$
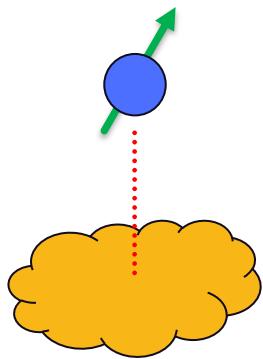

Lage-U limit

Consider a system with
localized f-orbitals hybridized
with dispersive conduction
band electrons

Impurity models are
correlated systems!

For $T \ll T_K$ system displays asymptotic
freedom similar to QCD

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Numerical Methods to Solve Effective Models

- Exact diagonalization method
  - Exact
  - *Limited to finite sizes*
- Quantum Monte Carlo method
  - Non-perturbative and thermodynamic limit
  - *Negative sign problem for fermions*
- Density matrix renormalization group (DMRG) theory
  - Capturing both quantum temporal and spatial fluctuations
  - *Limited to one dimensional (1D) or quasi-1D systems*
- Hartree-Fock mean-field (HMF)
  - Computationally efficient for ordered phases
  - *Neglecting temporal and spatial fluctuations*
- Dynamical mean-field theory (DMFT)
  - Capturing quantum temporal fluctuations
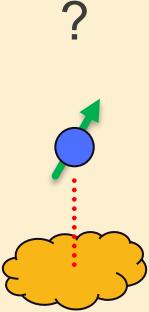 - *Neglecting spatial quantum fluctuations*

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DMFT: An atom in a
self-consistent bath.

Mean-Field Theories

Theory	Kohn–Sham DFT	Weiss MFT	Hubbard Static Alloy Approximation	DMFT
Local observable	Density $n(\boldsymbol{r})$ at point $\boldsymbol{r}$	Magnetization $\boldsymbol{m}_i$ at site i	Disorder averaged $G_{ii}(\omega)$ at site i	?
Auxiliary system	Independent particles	Embedded spin	Embedded sites independent particles	
Effective field	Kohn–Sham local potential $v_{KS}(r)$	Weiss local field $\boldsymbol{h}_i^{eff}$	effective medium $G_0(\omega)$	
Exact formulation	Universal $E_{xc}[n]$ $$v_{xc}(r) = \frac{\delta E_{xc}}{\delta n(r)}$$	Exact $\Omega[\{\boldsymbol{m}\}]$ $$\boldsymbol{h}^{eff} = \frac{\delta \Omega}{\delta \boldsymbol{m}}$$	None	
Canonical local approximation	LDA $E_{xc}[n] = \int n(\boldsymbol{r})\varepsilon_{xc}^{hom}(n(\boldsymbol{r}))$ $$v_{xc}(r) = \frac{\delta E_{xc}}{\delta n(r)}$$	Weiss MFA $$\boldsymbol{h}^{eff} = zJ\langle\boldsymbol{m}\rangle$$	CPA $$G_{00}(\omega) = \mathfrak{G}(\omega)$$	

Hubbard Model

$$H = -\sum_{\alpha i j} t_{ij} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$
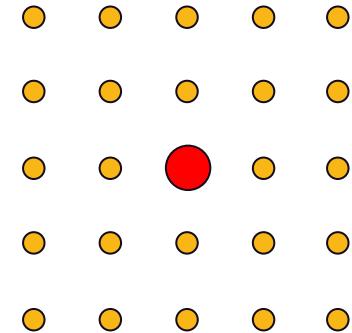
Cavity Method: we focus on one site $i = 0$ and separate the Hamiltonian into three parts

$$H = H_0 + H_h + H^b$$

$$H_0 = -\sum_{\alpha} (\varepsilon_0 - \mu) \hat{c}_{0\alpha}^\dagger \hat{c}_{0\alpha} + U \hat{n}_{0\uparrow} \hat{n}_{0\downarrow}$$

$$H^b = \sum_{i \neq 0, \alpha} (\varepsilon_i - \mu) \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} + \sum_{i \neq 0, j \neq 0, \alpha} t_{ij} \hat{c}_{i\alpha}^\dagger \hat{c}_{j\alpha} + U \sum_{i \neq 0} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$H_h = \sum_{i \neq 0, \alpha} t_{i0} \hat{c}_{i\alpha}^\dagger \hat{c}_{0\alpha} + t_{0i} \hat{c}_{0\alpha}^\dagger \hat{c}_{i\alpha}$$

DMFT Mapping

The three parts of the Hamiltonian correspond to the action $\mathbb{S}_0$ of site 0, the action $\mathbb{S}_h$ for the interaction between site 0 and the lattice, and the action $\mathbb{S}^b$ of the lattice without site 0.

Action:

$$\mathbb{S} = \mathbb{S}_0 + \mathbb{S}^b + \mathbb{S}_h \qquad Z = \int \mathcal{D}\bar{c}_{0\alpha}\mathcal{D}c_{0\alpha}(\tau)e^{-\mathbb{S}_0} \int \prod_{i\neq 0} \mathcal{D}\bar{c}_{0\alpha}\mathcal{D}c_{0\alpha}(\tau)e^{-\mathbb{S}^b}e^{-\int_0^\beta \mathbb{S}_h(\tau)}$$

$$\mathbb{S}_0 = \int_0^\beta d\tau \left[\sum_\alpha \bar{c}_{0\alpha}\left(\frac{\partial}{\partial\tau} - \mu\right)c_{0\alpha} + \frac{U}{2}\sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \bar{c}_{0\alpha}(\tau)c_{0\alpha}(\tau)\bar{c}_{0\alpha'}(\tau)c_{0\alpha'}(\tau) \right]$$

$$\mathbb{S}_h = -\int_0^\beta d\tau \left[\sum_{i\alpha} t_{i0}\bar{c}_{i\alpha}(\tau)c_{0\alpha}(\tau) + t_{0i}\bar{c}_{0\alpha}(\tau)c_{i\alpha}(\tau) \right]$$

$$\mathbb{S}^b = \int_0^\beta d\tau \left[\sum_{i\neq 0,\alpha} \bar{c}_{i\alpha}\left(\frac{\partial}{\partial\tau} - \mu\right)c_{i\alpha} - \sum_{i\neq 0,j\neq 0,\alpha} t_{ij}\bar{c}_{i\alpha}(\tau)c_{j\alpha}(\tau) + \frac{U}{2}\sum_{\substack{i\neq 0,\alpha\alpha' \\ \alpha\neq\alpha'}} \bar{c}_{i\alpha}(\tau)c_{i\alpha}(\tau)\bar{c}_{i\alpha'}(\tau)c_{i\alpha'}(\tau) \right]$$

The aim is now to integrate out all lattice degrees of freedom except those of site 0 in order to find the effective dynamics at site 0. In that process, the action $\mathbb{S}_0$ remains unchanged, the terms of $\mathbb{S}_h$ are expanded in terms of the hopping t which becomes small with increasing dimension and averaged with respect to the action $\mathbb{S}^b$.

Partition Function:

$$Z = \int \mathcal{D}\bar{c}_{0\alpha}\mathcal{D}c_{0\alpha}e^{-\mathbb{S}_0} \int \prod_{i \neq 0} \mathcal{D}\bar{c}_{0\alpha}\mathcal{D}c_{0\alpha}e^{-\mathbb{S}^b}e^{-\int_0^\beta d\tau \mathbb{S}_h(\tau)}$$

$$e^{-\int_0^\beta \mathbb{S}_h(\tau)} = 1 - \int_0^\beta d\tau \mathbb{S}_h(\tau) + \frac{1}{2!}\int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \mathbb{S}_h(\tau_1)\,\mathbb{S}_h(\tau_2) - \cdots$$

In general an operator average with respect to an action S can be expressed as:

$$\langle \mathcal{A} \rangle_S = \frac{\int \prod_i \mathcal{D}\bar{c}_{i\alpha}\mathcal{D}c_{i\alpha}e^{-S}\mathcal{A}[\bar{c}_{i\alpha}, c_{i\alpha}]}{\int \prod_i \mathcal{D}\bar{c}_{i\alpha}\mathcal{D}c_{i\alpha}e^{-S}} = Z_S^{-1}\int \prod_i \mathcal{D}\bar{c}_{i\alpha}\mathcal{D}c_{i\alpha}e^{-S}\mathcal{A}[\bar{c}_{i\alpha}, c_{i\alpha}]$$

DMFT Mapping

The second functional integral over $\mathbb{S}^b$ is used to average the terms of the $\mathbb{S}_h$ expansion

$$Z = \int \mathcal{D}\bar{c}_{0\alpha} \mathcal{D}c_{0\alpha} e^{-\mathbb{S}_0} Z_{\mathbb{S}^b} \left\{ 1 - \int_0^\beta d\tau \langle \mathbb{S}_h(\tau) \rangle_{\mathbb{S}^b} + \frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \langle \mathbb{S}_h(\tau_1) \mathbb{S}_h(\tau_2) \rangle_{\mathbb{S}^b} - \cdots \right\}$$

$$\langle \mathbb{S}_h(\tau) \rangle_{\mathbb{S}^b} = \sum_{i\alpha} t_{0i} \langle \bar{c}_{i\alpha}(\tau) \rangle_{\mathbb{S}^b} c_{0\alpha}(\tau) + t_{i0} \bar{c}_{0\alpha}(\tau) \langle c_{i\alpha}(\tau) \rangle_{\mathbb{S}^b} = 0 \qquad \text{Average only acts on all sites except 0}$$

$$\langle \mathbb{S}_h(\tau) \mathbb{S}_h(\tau) \rangle_{\mathbb{S}^b} = 2 \sum_{i\alpha} t_{0i} t_{j0} \bar{c}_{0\alpha}(\tau_1) \langle \mathcal{T}_\tau c_{i\alpha}(\tau_1) \bar{c}_{j\alpha}(\tau_2) \rangle_{\mathbb{S}^b} c_{0\alpha}(\tau_2)$$

$$= -2 \sum_{i\alpha} t_{0i} t_{j0} \bar{c}_{0\alpha}(\tau_1) G_{ij\alpha}^b(\tau_1 - \tau_2) c_{0\alpha}(\tau_2) \qquad \text{Assume a paramagnetic state } \delta_{\alpha\alpha'}$$

$$Z = \int \mathcal{D}\bar{c}_{0\alpha} \mathcal{D}c_{0\alpha} e^{-\mathbb{S}_0} Z_{\mathbb{S}^b} \left\{ 1 - \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{ij\alpha} t_{0i} t_{j0} \bar{c}_{0\alpha}(\tau_1) G_{ij\alpha}^b(\tau_1 - \tau_2) c_{0\alpha}(\tau_2) + \cdots \right\}$$

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We write the bracket $\{\cdots\}$ as an exponential function in order to identify an effective action $\mathbb{S}_{eff}$

$$Z = \int \mathcal{D}\bar{c}_{0\alpha}\mathcal{D}c_{0\alpha}e^{-\mathbb{S}_{eff}}$$

$$\mathbb{S}_{eff} = \int_0^\beta d\tau \left[\sum_\alpha \bar{c}_{0\alpha}\left(\frac{\partial}{\partial\tau} - \varepsilon_0 - \mu\right)c_{0\alpha} + \frac{U}{2}\sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \bar{c}_{0\alpha}(\tau)c_{0\alpha}(\tau)\bar{c}_{0\alpha'}(\tau)c_{0\alpha'}(\tau) \right]$$

$$+ \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \sum_{ij\alpha} t_{0i}t_{j0}\bar{c}_{0\alpha}(\tau_1)G^b_{ij\alpha}(\tau_1 - \tau_2)c_{0\alpha}(\tau_2)$$

$$= -\sum_\alpha \int_0^\beta\int_0^\beta d\tau_1 d\tau_2 \bar{c}_{0\alpha}(\tau_1)\mathfrak{G}_\alpha^{-1}(\tau_1 - \tau_2)c_{0\alpha}(\tau_2) + \int_0^\beta d\tau \frac{U}{2}\sum_{\substack{\alpha\alpha' \\ \alpha\neq\alpha'}} \bar{c}_{0\alpha}(\tau)c_{0\alpha}(\tau)\bar{c}_{0\alpha'}(\tau)c_{0\alpha'}(\tau)$$

Where we define the Weiss field:

$$\mathfrak{G}_\alpha^{-1}(\tau_1 - \tau_2) = -\left(\frac{\partial}{\partial\tau} - \varepsilon_0 - \mu\right)\delta_{\tau_1,\tau_2} - \sum_{i\neq 0, j\neq 0} t_{0i}G^b_{ij\alpha}(\tau_1 - \tau_2)t_{j0}$$

DMFT Mapping

Fourier transform the Weiss field:

$$\mathfrak{G}_\alpha^{-1}(i\omega_n) = i\omega_n - \varepsilon_0 + \mu - \sum_{i\neq 0, j\neq 0} t_{0i} G_{ij\alpha}^b(i\omega_n) t_{j0} \qquad i\omega_n = (2n+1)\pi T$$

Identity relation between the cavity Green's function and Green's function on the lattice:

$$G_{ij\alpha}^b(i\omega_n) = G_{ij\alpha}(i\omega_n) - G_{i0\alpha}(i\omega_n) G_{00\alpha}^{-1}(i\omega_n) G_{0j\alpha}(i\omega_n)$$

$$G_{ij\alpha}(i\omega_n) = \frac{1}{N_L} \sum_k G_\alpha(k, i\omega_n) e^{ik\cdot R_{ij}} \qquad G_\alpha^{-1}(k, i\omega_n) = i\omega_n - \varepsilon_0 + \mu - t_k - \Sigma_\alpha(k, i\omega_n)$$

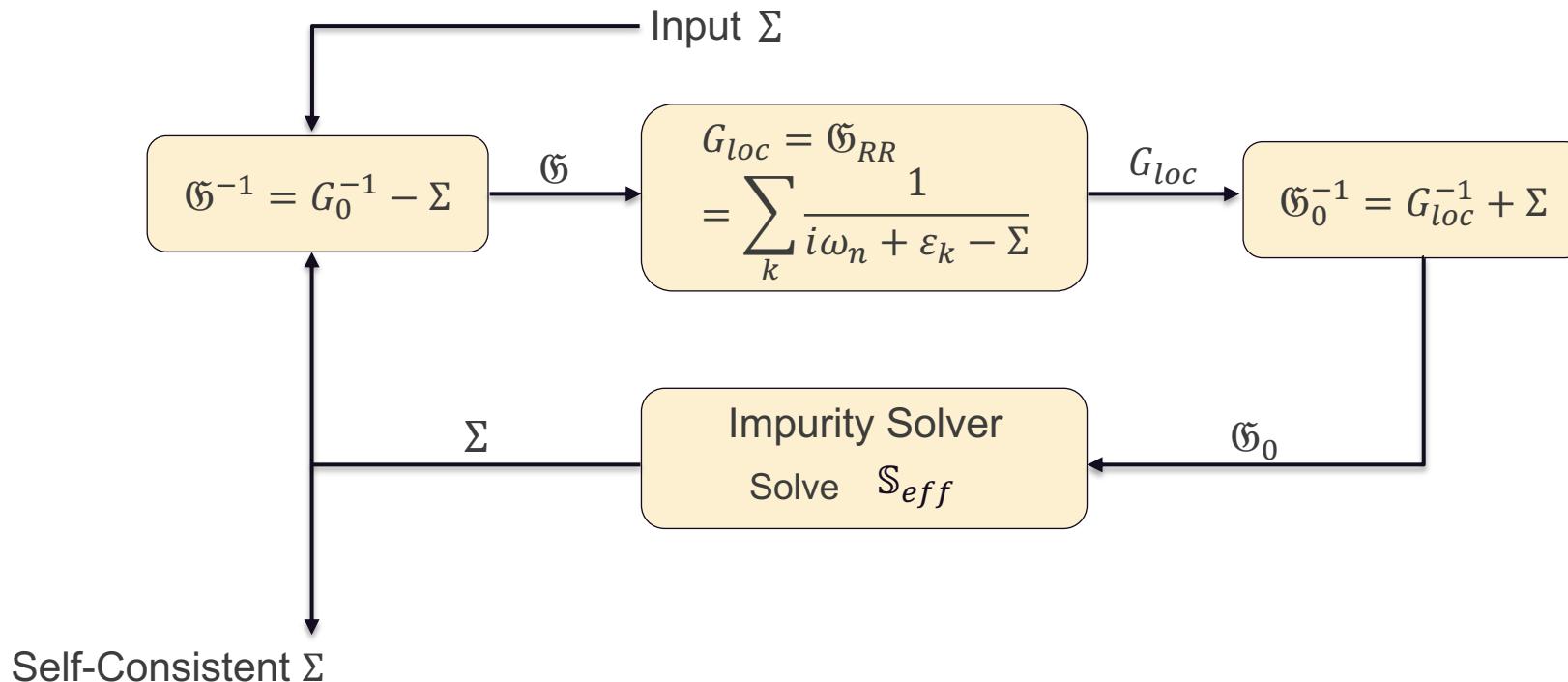In DMFT, we neglect the spatial quantum fluctuation:

$$\Sigma_\alpha(k, i\omega_n) \approx \Sigma_\alpha(i\omega_n)$$

Weiss field satisfies the local Dyson equation:

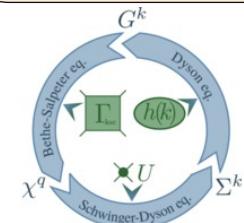$$\mathfrak{G}_\alpha^{-1}(i\omega_n) = G_{00\alpha}^{-1}(i\omega_n) + \Sigma_\alpha(i\omega_n)$$

DMFT Self-Consistency Procedure

Dynamical Mean Field Theory

Input Σ

$$\mathfrak{G}^{-1} = G_0^{-1} - \Sigma$$

$\mathfrak{G}$

$$G_{loc} = \mathfrak{G}_{RR}$$
$$= \sum_k \frac{1}{i\omega_n + \varepsilon_k - \Sigma}$$

G_{loc}

$$\mathfrak{G}_0^{-1} = G_{loc}^{-1} + \Sigma$$

Σ

Impurity Solver

Solve $\mathbb{S}_{eff}$

$\mathfrak{G}_0$

Self-Consistent Σ

Mean-Field Theories

Theory	Kohn–Sham DFT	Weiss MFT	Hubbard Static Alloy Approximation	DMFT
Local observable	Density $n(\boldsymbol{r})$ at point $\boldsymbol{r}$	Magnetization $\boldsymbol{m}_i$ at site i	Disorder averaged $G_{ii}(\omega)$ at site i	Green's function $G_{ii}(\omega)$ at site i
Auxiliary system	Independent particles	Embedded spin	Embedded sites independent particles	Embedded site interacting particles
Effective field	Kohn–Sham local potential $v_{KS}(r)$	Weiss local field $\boldsymbol{h}_i^{eff}$	effective medium $G_0(\omega)$	effective medium $\mathfrak{G}(\omega)$
Exact formulation	Universal $E_{xc}[n]$ $$v_{xc}(r) = \frac{\delta E_{xc}}{\delta n(r)}$$	Exact $\Omega[\{\boldsymbol{m}\}]$ $$\boldsymbol{h}^{eff} = \frac{\delta \Omega}{\delta \boldsymbol{m}}$$	None	Exact $\Phi_{\text{local}}[G_{00}]$ $$\Sigma(\omega) = \frac{\delta \Phi_{\text{local}}}{\delta G_{00}}$$
Canonical local approximation	LDA $E_{xc}[n] = \int n(\boldsymbol{r})\varepsilon_{xc}^{hom}(n(\boldsymbol{r}))$ $$v_{xc}(r) = \frac{\delta E_{xc}}{\delta n(r)}$$	Weiss MFA $$\boldsymbol{h}^{eff} = zJ\langle\boldsymbol{m}\rangle$$	CPA $$G_{00}(\omega) = \mathfrak{G}(\omega)$$	Single-site DMFA

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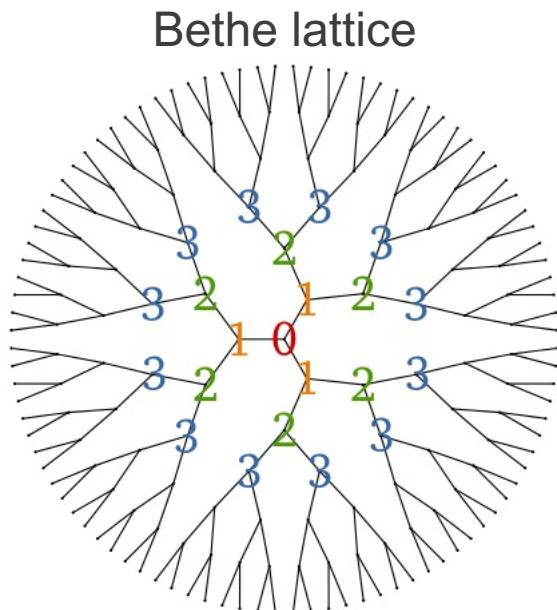
Numerical Approaches for Impurity Solver

- Exact diagonalization method [PRL 72, 1545 (1994)]

- Quantum Monte Carlo method
  - Hirsch-Fye implementation [PRL 56, 2521 (1986)]
  - Projective QMC [PRB 40, 506 (1989)]
  - Continuous-time QMC [PRB 72, 035122 (2005); PRL 97, 076405 (2006)]

- Numerical renormalization group (NRG) [RMP 47, 773 (1975); PRB 64, 045103 (2001)]

- Density matrix renormalization group (DMRG) [PRB 96, 085118 (2017)]

- Perturbation theory
  - Iterative perturbation theory [PRB 49, 10181 (1994)]
  - Noncrossing approximation [PRB 47, 3553 (1993)]
  - Equation of motion [PRB 71, 085103 (2005)]

DMFT Equations for Bethe Lattice

For standard lattice systems, the evaluation of the local Green's function involving the summation over momentum k or integral over the band density of states

$$G_{loc} = \sum_k \frac{1}{i\omega_n + \varepsilon_k - \Sigma} \quad \longrightarrow \quad G_{loc} = \int d\xi \frac{\rho_0(\xi)}{i\omega_n + \xi - \Sigma}$$

Bethe lattice

$$\rho_0(\xi) = \frac{1}{2\pi t^2} \sqrt{4t^2 - \xi^2} \qquad |\xi| \leq 2t$$

$$G_{loc}(\Lambda) = \frac{1}{2t^2}(\Lambda - s\sqrt{\Lambda^2 - 4t^2}) \qquad \Lambda(i\omega_n) = i\omega_n + \mu - \Sigma(i\omega_n) \quad s = \text{sgn}[Im\Lambda]$$

Solve for Λ: $\quad \Lambda(i\omega_n) = G_{loc}^{-1}(i\omega_n) + t^2 G_{loc}(i\omega_n)$

DMFT system of equations reduce to a single equation:

$$\mathfrak{G}^{-1}(i\omega_n) = i\omega_n + \mu - t^2 G_{loc}(i\omega_n)$$

Three-peak spectral structure

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}G(\boldsymbol{k}, \omega)$$

D=2t

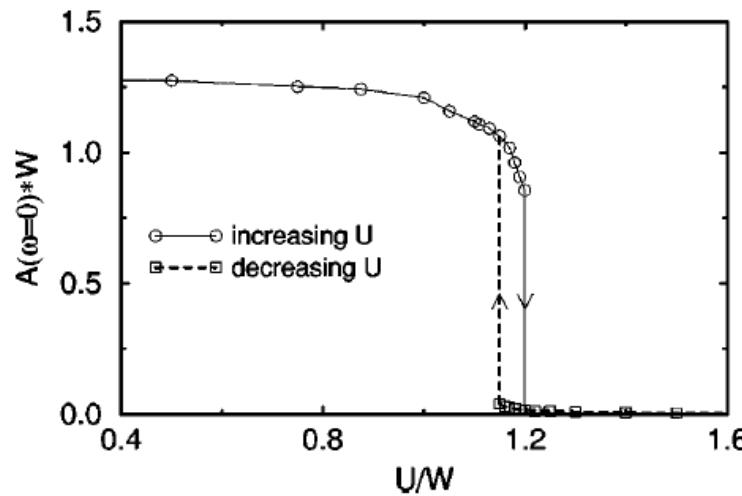# Spectral Function of the Hubbard Model in DMFT

Quasiparticle weight

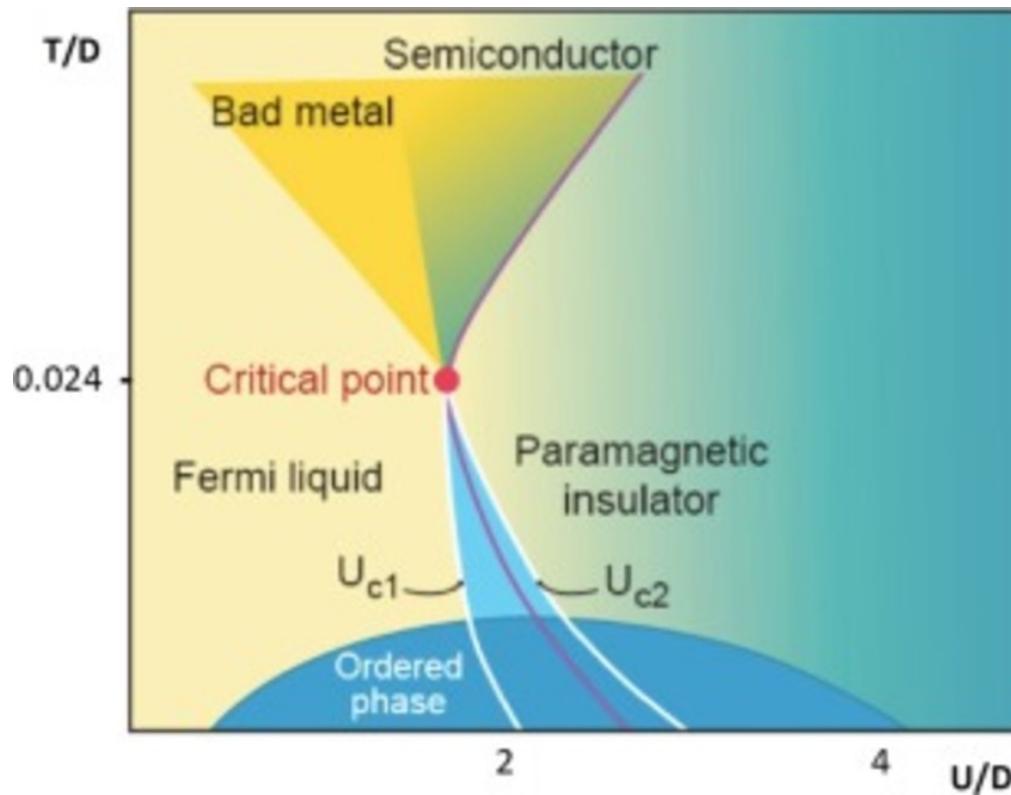$$Z = \frac{1}{1 - \frac{\partial \mathrm{Re}\Sigma(\omega)}{\partial \omega}\big|_{\omega=0}}$$

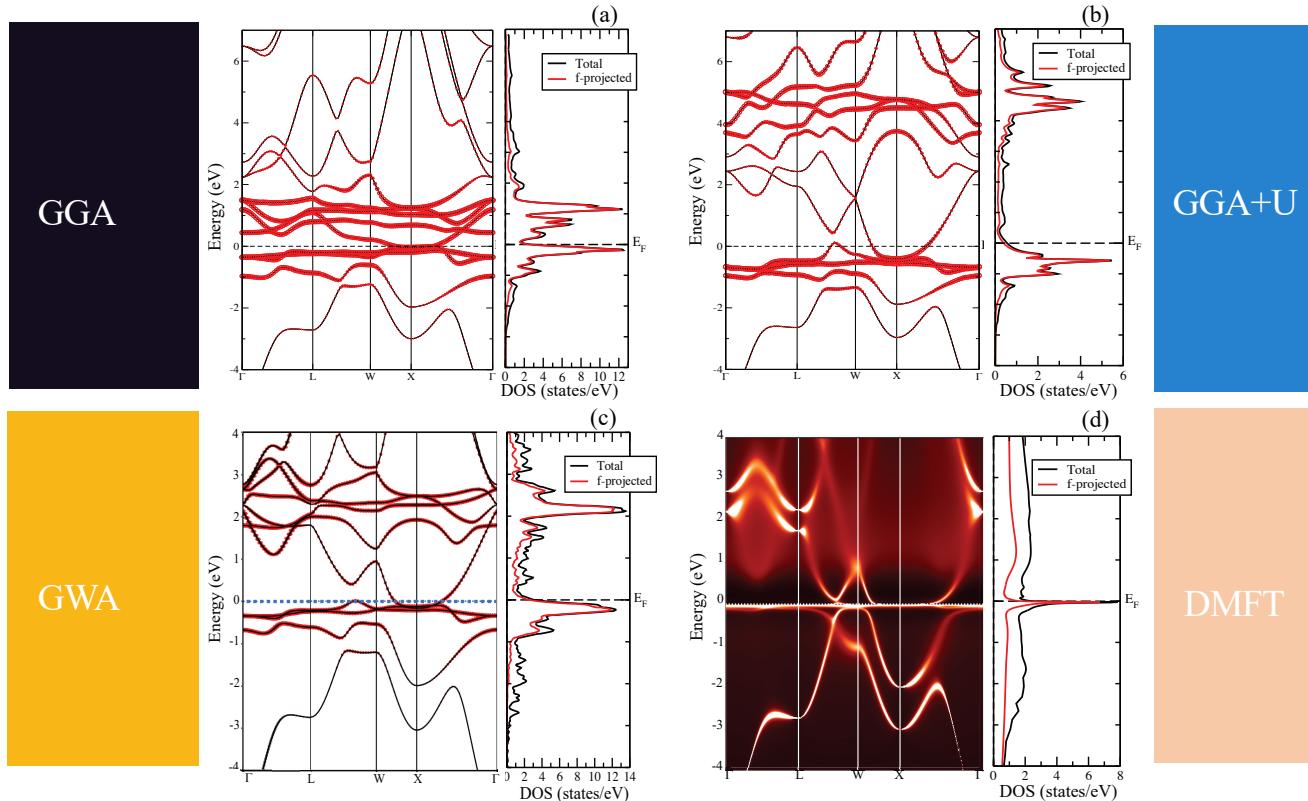Bulla, PRL **83**, 136 (1999)

First-order phase transition

Bulla, PRB **64**, 045103 (2001)

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Kotliar, Science **302**, 67 (2003)
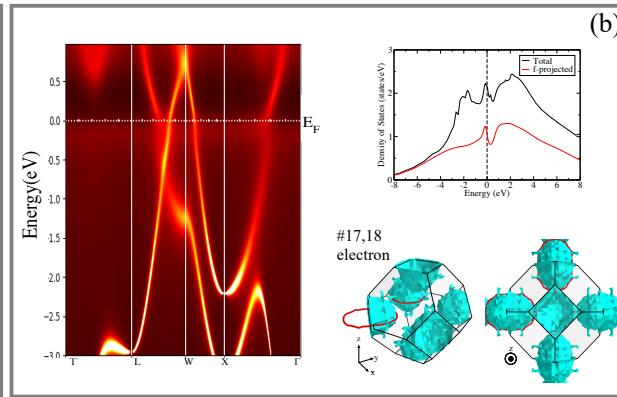
- Consistent band structure from 3 methods with correlation (with no magnetic long-range order)
- Correlation effect narrows the *f*-electron bands

Electronic band structure of δ-Pu at T=0 K

T = 116 K

(a)

T = 1160 K

(b)

Band	T=0 K			T=116 K			T=1160 K		
	f	m^*	V_{FS}	f	m^*	V_{FS}	f	m^*	V_{FS}
15, 16	3.07	1.84	0.95	2.38	1.56	0.57	—	—	—
17, 18	6.18	2.17	0.95	7.02	1.98	1.14	13.80	2.36	3.04