Dynamical mean-field theory

Marcus Kollar

Theoretical Physics III, University of Augsburg, Germany

Autumn School: *Hands-On DMFT*

DFG-Forschergruppe 1346

Forschungszentrum Jülich

August 4 - 7, 2011

Outline

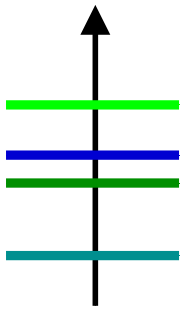
I. Introduction
   - Green functions
   - Useful concepts

II. Fermions in infinite dimensions
   - Free fermions
   - Many-body theory

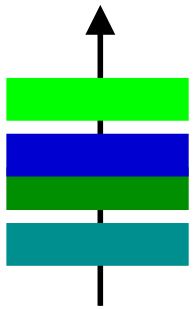
III. Dynamical mean-field theory
   - Mapping onto impurity models
   - A solvable example
   - Impurity solvers

Electrons in solids

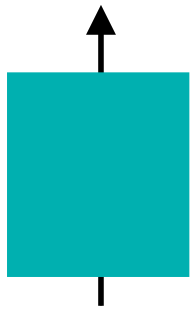
condensed matter: electrons in a ionic potential



individual atoms
$\phi_\alpha(\boldsymbol{r})$
s, p, d, f, ...



condensed matter
Bloch: $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$
Wannier: $\phi_n(\boldsymbol{r}-\boldsymbol{R})$



unbound electrons
Jellium, $\frac{1}{\sqrt{V}}e^{i\boldsymbol{k}\boldsymbol{r}}$

Coulomb interaction: $V_{\text{ee}}(\boldsymbol{r}-\boldsymbol{r}') \propto \dfrac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}$

$\Rightarrow$ important for strongly localized 3d, 4d, 4f, ... electrons

Hubbard model: e.g. 1 band, only $U = V_{iiii}$

$$H_{\text{Hubbard}} = \sum_{ij\sigma} t_{ij}\, c^+_{i\sigma} c_{j\sigma} \;+\; U \sum_i n_{i\uparrow} n_{i\downarrow}$$

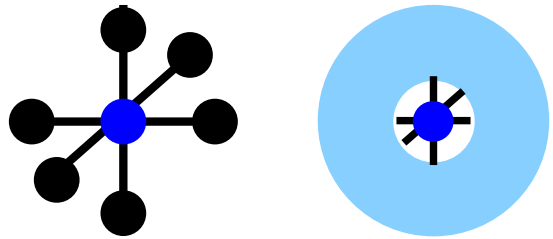
→ lectures

Dynamical mean-field theory

limit of large coordination number z or large dimension d:

- scaling: $t = t^\star \,/\, \sqrt{z}$ with $z \propto d \to \infty$
- Green function: $G_{ij}(\omega) \propto d^{-||\boldsymbol{R}_i - \boldsymbol{R}_j||/2}$
- self energy: $\Sigma_{ij}(\omega) = \delta_{ij}\, \Sigma(\omega)$ $\Rightarrow$ local!

mapping onto single-site problem:



- self-energy $\Sigma_{ii}[G_{ii}]$
  $\Rightarrow$ same as for dynamical single-site problem
- e.g. Anderson impurity model $\Rightarrow$ numerical methods

$\Rightarrow$ Dynamical mean-field theory

Metzner & Vollhardt '89; Müller-Hartmann '89; Georges & Kotliar '92; Georges et al. RMP '96, ...

Part I
Introduction

1. Green functions
   - Spectral representations
   - Self-energy
   - Path-integral formulation

2. Useful concepts
   - Quasiparticles
   - Hubbard bands
   - Mott-Hubbard transition

1. Green functions

e.g., Negele & Orland

imaginary-time-ordered fermionic Green function $G_{\alpha\beta}(\tau)$:

$$G_{\alpha\beta}(\tau) = -\langle T_\tau c_\alpha(\tau) c_\beta^+(0)\rangle = -\begin{cases} \langle c_\alpha(\tau) c_\beta^+(0)\rangle & \tau > 0 \\ -\langle c_\beta^+(0) c_\alpha(\tau)\rangle & \tau \le 0 \end{cases}$$
$$= -G_{\alpha\beta}(\tau+\beta) \quad \text{for } -\beta < \tau < 0$$

with Heisenberg operators $A(\tau) = e^{H\tau} A e^{-H\tau}$

Matsubara Green function:

$$G_{\alpha\beta}(\tau) = T \sum_{n=-\infty}^{+\infty} G_{\alpha\beta}(i\omega_n)\, e^{-i\omega_n\tau}$$

$$G_{\alpha\beta}(i\omega_n) = \int_0^\beta d\tau\, G_{\alpha\beta}(\tau)\, e^{i\omega_n\tau}$$

with fermionic Matsubara frequencies $i\omega_n = 2\pi T(n + \frac{1}{2})$

Spectral representations

spectral function:

$$G_{\alpha\beta}(i\omega_n) = \int_{-\infty}^{\infty} d\omega \frac{A_{\alpha\beta}(\omega)}{i\omega_n - \omega}$$

$$A_{\alpha\beta}(\omega) = -\frac{1}{\pi}\mathrm{Im}\,\underbrace{G_{\alpha\beta}(\omega + i0)}_{\text{retarded Green function}}$$

$$= \sum_{n,m} \langle n|c_\beta^+|m\rangle\langle m|c_\alpha|n\rangle \frac{e^{-\beta E_m} - e^{-\beta E_n}}{Z} \delta(E_n - E_m - \omega)$$

local Green function:

$$G_{ii\sigma}(i\omega_n) = G_\sigma(i\omega_n) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k}\sigma}(i\omega_n)$$

$$A_{ii\sigma}(\omega) = A_\sigma(\omega) = -\frac{1}{\pi}\mathrm{Im}\,\frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k}\sigma}(\omega + i0)$$

$$= \text{interacting density of states}$$

Free particles

free particles: $H - \mu N = \sum_{\boldsymbol{k}\sigma} (\epsilon_{\boldsymbol{k}} - \mu)\, c^{+}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$

$$\Rightarrow \quad G^{(0)}_{\boldsymbol{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}}}$$

local Green function:

$$G_\sigma(i\omega_n) = \frac{1}{L}\sum_{\boldsymbol{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}}} = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{i\omega_n + \mu - \epsilon}$$

$$A_\sigma(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} \delta(\omega + \mu - \epsilon_{\boldsymbol{k}}) = \rho(\omega + \mu)$$

with free density of states (which characterizes $\epsilon_{\boldsymbol{k}}$)

$$\rho(\omega) = \sum_{\boldsymbol{k}} \delta(\omega - \epsilon_{\boldsymbol{k}})$$

Self-energy

self-energy $\Sigma_{\boldsymbol{k}}(i\omega_n)$:

$$G_{\boldsymbol{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_{\boldsymbol{k}\sigma}(i\omega_n)}$$

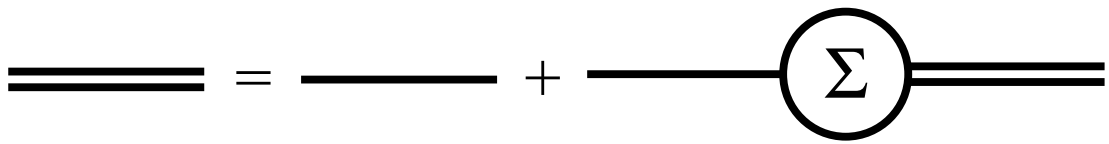
$$G_{\boldsymbol{k}\sigma}(i\omega_n)^{-1} = G^{(0)}_{\boldsymbol{k}\sigma}(i\omega_n)^{-1} - \Sigma_{\boldsymbol{k}\sigma}(i\omega_n) \qquad \text{Dyson equation}$$

matrix notation: $G_{ij\sigma}(i\omega_n) = (\boldsymbol{G})_{ij,\sigma,n}$

$$\boldsymbol{G}^{-1} = \boldsymbol{G}^{(0)\,-1} - \boldsymbol{\Sigma}$$

or $$\boldsymbol{G} = \boldsymbol{G}^{(0)} + \boldsymbol{G}^{(0)}\boldsymbol{\Sigma}\boldsymbol{G}$$

diagrammatic notation:



Path-integral formulation

partition function for fermionic Hamiltonian $H(\{c_\alpha^+\},\{c_\alpha\})$:

$$Z = \mathrm{Tr} e^{-\beta(H-\mu N)} = \int_{\phi_\alpha(\beta)=-\phi_\alpha(0)} \mathcal{D}(\phi_\alpha^*(\tau),\phi_\alpha(\tau)) \quad \exp(\mathcal{A})$$

$$= \text{functional integral over Grassmann variables } \phi_\alpha(\tau)$$

action:

$$\mathcal{A} = -\int_0^\beta d\tau \left[\sum_\alpha \phi_\alpha^* \left(\partial_\tau - \mu\right) \phi_\alpha + H(\{\phi_\alpha^*\},\{\phi_\alpha\}) \right]$$

e.g., Negele & Orland

imaginary-time-ordered fermionic Green function:

$$G_{\alpha\beta}(\tau) = \frac{1}{Z} \int_{\text{APBC}} \mathcal{D}(\phi^*\phi) \quad \phi_\alpha(\tau)\phi_\beta^*(0) \quad \exp(\mathcal{A})$$

Part I
Introduction

1. Green functions
   - Spectral representations
   - Self-energy
   - Path-integral formulation

2. Useful concepts
   - Quasiparticles
   - Hubbard bands
   - Mott-Hubbard transition

2. Useful concepts. Quasiparticles

spectral function: describes single-particle excitations

$$A_{\boldsymbol{k}}(\omega) = \frac{1}{\pi} \frac{\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega)}{[\omega - \epsilon_{\boldsymbol{k}} + \mu - \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega)]^2 + [\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega)]^2}$$

real part vanishes if

$$\omega = \epsilon_{\boldsymbol{k}} - \mu + \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega) \quad \Rightarrow \quad \text{solutions} \;\; \omega = E_{\boldsymbol{k}}$$

2. Useful concepts. Quasiparticles

spectral function: describes single-particle excitations

$$A_{\boldsymbol{k}}(\omega) = \frac{1}{\pi} \frac{\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega)}{[\omega - \epsilon_{\boldsymbol{k}} + \mu - \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega)]^2 + [\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega)]^2}$$

real part vanishes if

$$\omega = \epsilon_{\boldsymbol{k}} - \mu + \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega) \quad \Rightarrow \quad \text{solutions} \quad \omega = E_{\boldsymbol{k}}$$

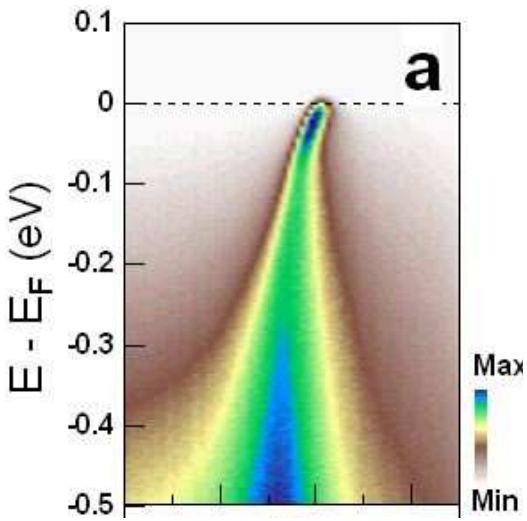
for $\omega \approx E_{\boldsymbol{k}}$:

$$G_{\boldsymbol{k}}(\omega) \approx \frac{Z_{\boldsymbol{k}}(E_{\boldsymbol{k}})}{\omega - E_{\boldsymbol{k}} + i\tau_{\boldsymbol{k}}(E_{\boldsymbol{k}})^{-1}}$$

$$Z_{\boldsymbol{k}}(\omega) = 1/[1 - \frac{\partial}{\partial\omega}\mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega)]$$

$$\tau_{\boldsymbol{k}}(\omega) = 1/[-Z_{\boldsymbol{k}}\mathrm{Im}\Sigma(\omega)]$$

LSCO Zhou et al. (2006)



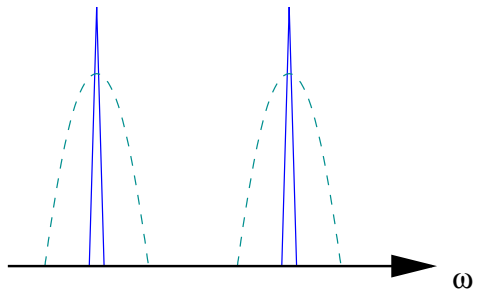
Fermi liquid: coherent quasiparticles for sufficiently small ω

Hubbard bands, Mott transition

atomic limit: $H^{\text{at}} = \sum_i [U\, n_{i\uparrow} n_{i\downarrow} - \mu(n_{i\uparrow} + n_{i\downarrow})]$

$$\Rightarrow \qquad G_\sigma^{\text{at}}(i\omega_n) = \frac{n_{-\sigma}}{i\omega_n + \mu - U} + \frac{1 - n_{-\sigma}}{i\omega_n + \mu}$$

spectral function:



- peaks broaden for $t_{ij} \neq 0 \;\Rightarrow$ Hubbard bands — Hubbard '63
- Hubbard bands merge for large enough $|t_{ij}|$
- quasiparticle bands develops gaps for large enough U

$\Rightarrow$ (non-magnetic) Mott-Hubbard transition at $U = U_c$ and $n = 1$

Mott '46

Part II
Fermions in infinite dimensions

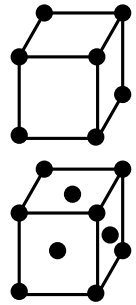
1. Free fermions
   - Scaling of hopping amplitudes
   - Density of states

2. Many-body theory
   - Diagrammatic expansions
   - Power-counting in $1/d$
   - Simplifications in $d = \infty$

1. Free fermions

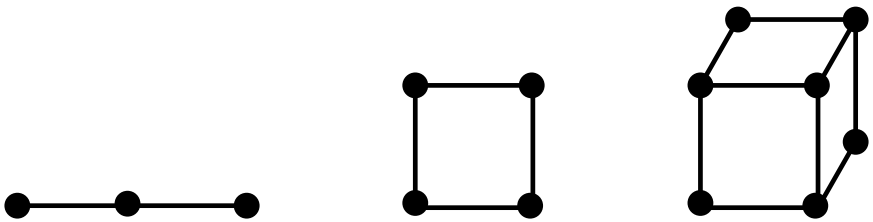
crystal lattices in $d = 3$:

- simple cubic lattice ($Z = 8$)
- face-centered cubic lattice ($Z = 12$)
- ...



$\Rightarrow$ generalized lattices for any (large) dimension d?

easy for hypercubic lattice:



in d dimensions:

$$\begin{aligned} \boldsymbol{e}_1 &= (1, 0, 0, \ldots \quad) \\ \boldsymbol{e}_2 &= (0, 1, 0, \ldots \quad) \\ \ldots &= \ldots \\ \boldsymbol{e}_d &= (0, 0, 0, \ldots, 1) \end{aligned}$$

Next-neighbor hopping

kinetic energy: $H_{\text{kin}} = \sum_{ij\sigma} t_{ij}\, c^+_{i\sigma} c_{j\sigma} = \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}}\, c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}$

NN hopping: $t_{ij} = t(\boldsymbol{R}_i - \boldsymbol{R}_j) = \begin{cases} -t & \text{if } \boldsymbol{R}_i - \boldsymbol{R}_j = \pm \boldsymbol{e}_n \\ 0 & \text{else} \end{cases}$

dispersion: $\epsilon_{\boldsymbol{k}} = -2t \sum_{i=1}^{d} \cos k_i$

nontrivial limit $d \to \infty$?

density of states:

$$\rho(\epsilon) = \frac{1}{L} \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}}) \qquad \overset{L \to \infty}{=} \qquad \int \frac{d^d k}{(2\pi)^d} \delta(\epsilon - \epsilon_{\boldsymbol{k}})$$

Scaling of hopping amplitudes

elegant answer:

Metzner & Vollhardt '89

- random variables $X_i = \sqrt{2}\cos k_i$ (mean=0, variance=1)
- $X_d := \frac{1}{\sqrt{d}} \sum_{i=1}^{d} \cos k_i$

central limit theorem:

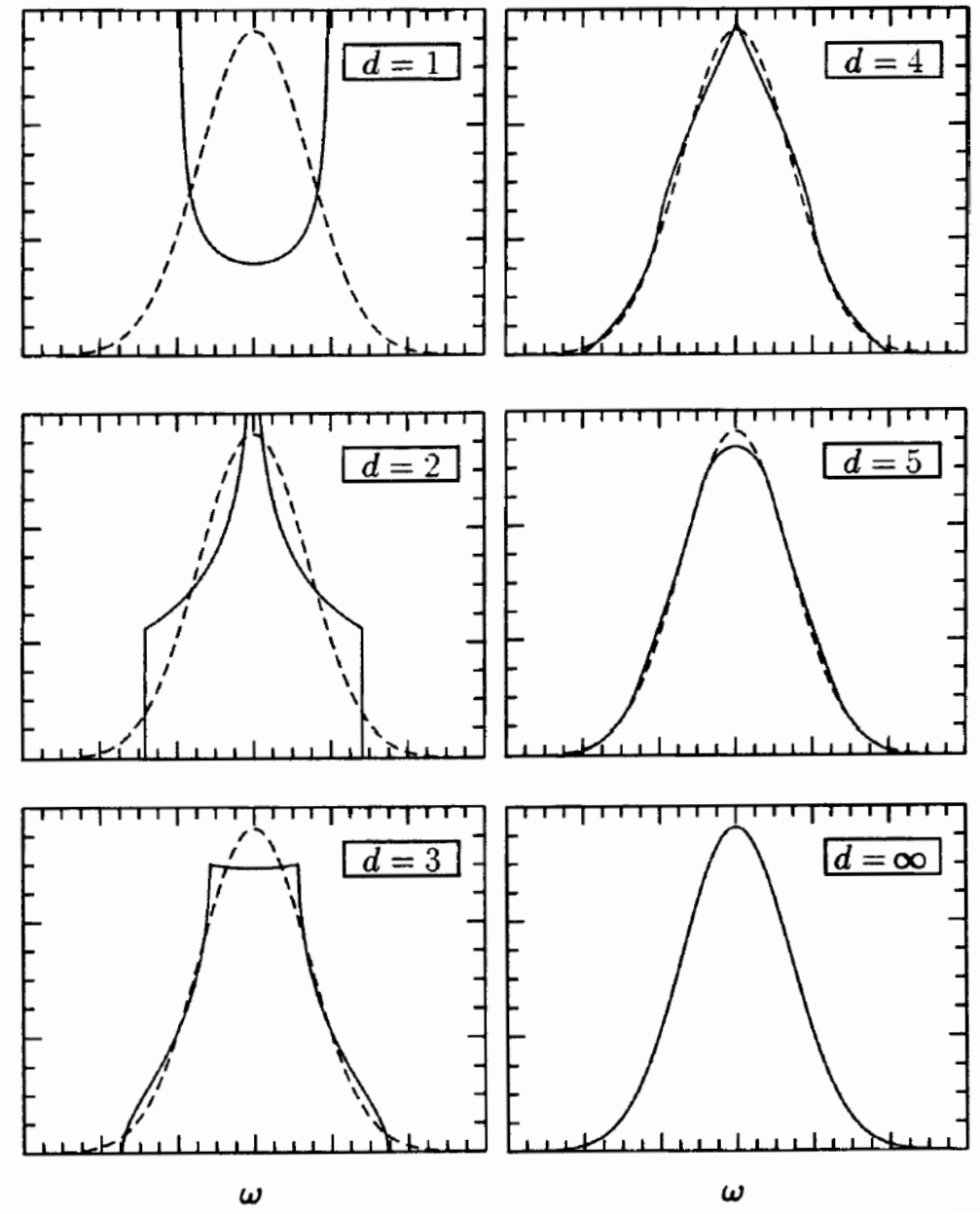
for $d \to \infty$: $X_d \xrightarrow{\text{in law}}$ Gaussian r.v. (mean=0, variance=1)

density of states: distribution function of $\sqrt{2d}\,t\,X_d$

$$\rho(\epsilon) = \frac{1}{2\pi|t_*|}\, e^{-\frac{\epsilon^2}{2t_*^2}} \qquad \text{for} \qquad t = \frac{t_*}{\sqrt{2d}}$$

Density of states

$\rho(\omega)$



Vollhardt '93

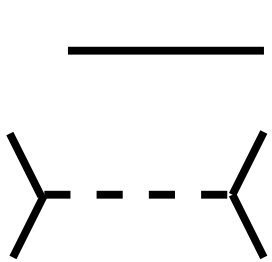
Part II
Fermions in infinite dimensions

1. Free fermions
   - Scaling of hopping amplitudes
   - Density of states
   - Generalized lattices

2. Many-body theory
   - Diagrammatic expansions
   - Power-counting in $1/d$
   - Simplifications in $d = \infty$

2. Many-body theory

Feynman diagrams for Green functions:

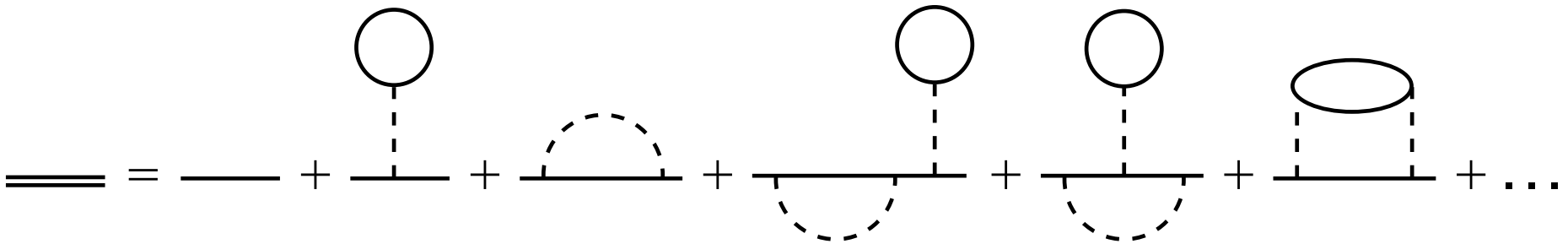


= non-interacting Green function line $\boldsymbol{G}^{(0)}$

= interaction vertex

= full (interacting) Green function line $\boldsymbol{G}$

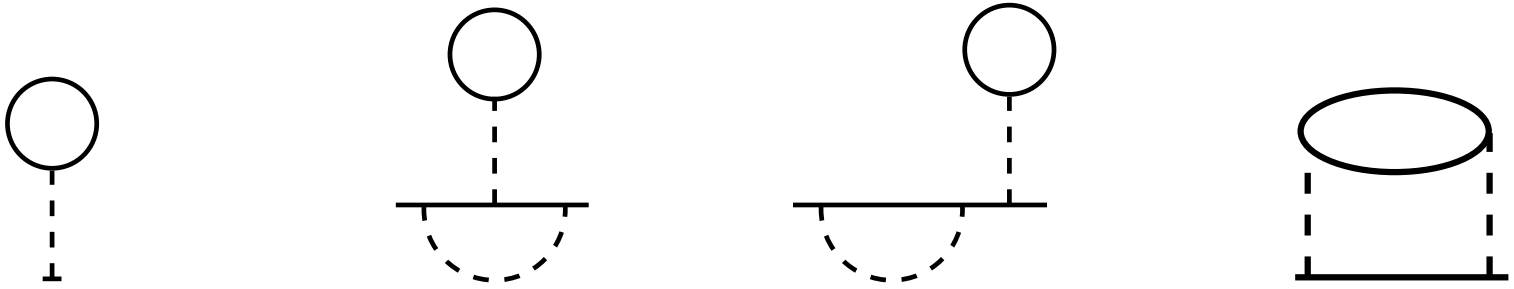
perturbation expansion:



Self-energy

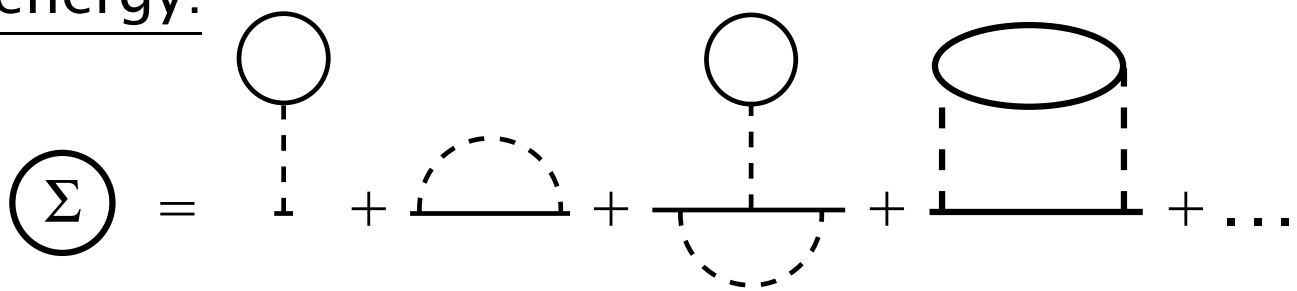
proper self-energy diagrams:

- external vertex amputated
- cannot be cut in two pieces



proper proper not proper proper

self-energy:

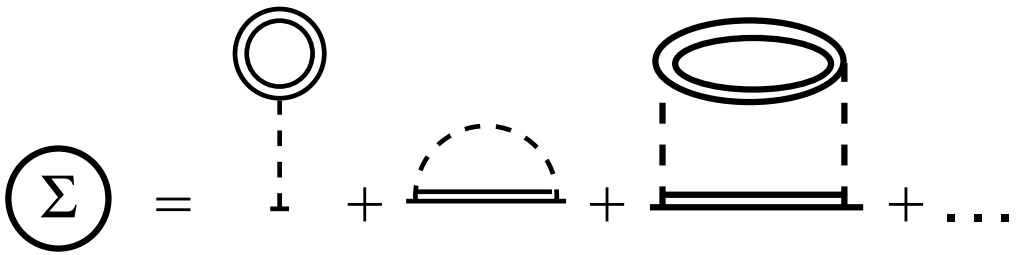


Skeleton expansion

so far: $\boldsymbol{\Sigma}[\boldsymbol{G}^{(0)}]$

now: omit self-energy insertions,  etc.

$\Rightarrow$ skeleton expansion $\boldsymbol{\Sigma}[\boldsymbol{G}]$



- avoid double counting
- should be equivalent when summing all diagrams
- not equivalent when summing some diagrams

Power counting in 1/d

d dependence of $G_{ij\sigma}(\omega)$ for $d \to \infty$?

hopping amplitudes:

$$t_{ij} = t_{ij}^* \; d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||}$$

kinetic energy:

$$E_{\text{kin},\sigma} = \sum_{ij} t_{ij} \langle c_{i\sigma}^+ c_{j\sigma} \rangle = \underbrace{\sum_{ij} t_{ij}}_{O(d^{||\boldsymbol{R}_i - \boldsymbol{R}_j||})} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \; G_{ij\sigma}(\omega) \; e^{i\omega 0^+} = O(d^0)$$

Green function:

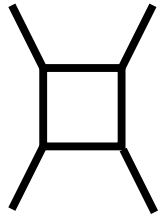
$$G_{ij\sigma}(\omega) = O(d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||}), \qquad G_{ii\sigma}(\omega) = O(d^0)$$

$\Rightarrow$ simplifications for Feynman diagrams!

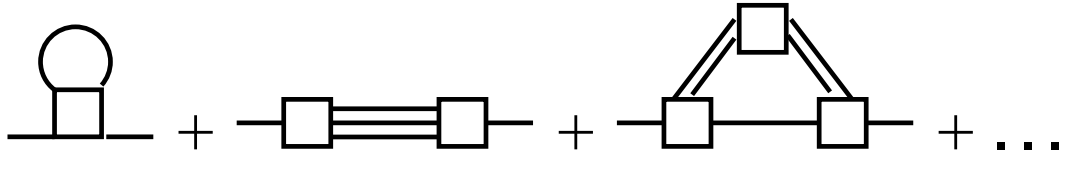
Diagrammatic simplifications

Hugenholtz diagrams: (Hubbard model: no exchange diagrams)

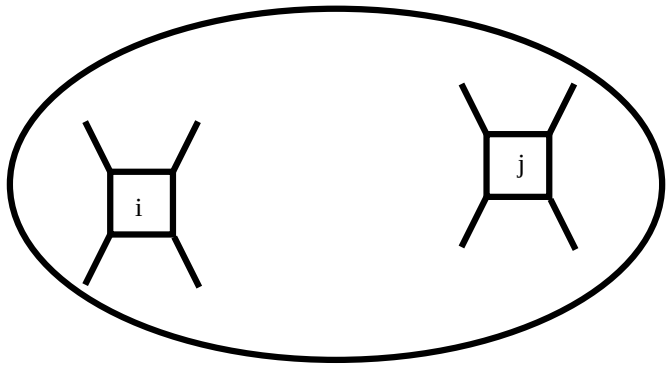
i,σ - - - $i,-\sigma$ $= U n_{i\uparrow} n_{i\downarrow} =$



skeleton expansion:

$\Sigma =$  $+ \ldots$ (1)

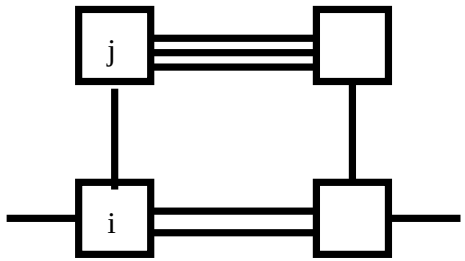
consider fixed i: compare $j \neq i$ with $j = i$



Collapse of position space diagrams

skeleton expansion: ≥ 3 independent paths from i to j

- Green function lines: $O(d^{-\frac{3}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||})$
- summation over j: $O(d^{||\boldsymbol{R}_i - \boldsymbol{R}_j||})$



$\Rightarrow$ skeleton diagram is $O(d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||})$

in $d = \infty$:

all vertices in $\boldsymbol{\Sigma}[\boldsymbol{G}]$ have the same site label!

self-energy is local!

$$\Sigma_{ij\sigma}(\omega) = \delta_{ij}\,\Sigma_{ii\sigma}(\omega) = \delta_{ij}\,\Sigma_{\sigma}(\omega)$$

$$\Sigma_{\boldsymbol{k}\sigma}(\omega) = \Sigma_{\sigma}(\omega) \qquad \text{independent of } \boldsymbol{k}!$$

Consequences of local self-energy

simple $\boldsymbol{k}$ dependence:

$$G_{\boldsymbol{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(i\omega_n)}$$

local Green function:

$$G_\sigma(i\omega_n) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(i\omega_n)} \quad \text{Dyson equation}$$

$$= \int_{-\infty}^{\infty} d\epsilon \, \frac{\rho(\epsilon)}{i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon} \quad \text{Hilbert transform}$$

(later: “self-consistency equation”)

Part III
Dynamical mean-field theory

1. Mapping onto impurity models
2. A solvable example
3. Impurity solvers

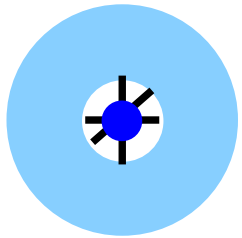
1. Mapping onto impurity models

Effective single-site action: $\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2$

Kotliar & Georges '92, Jarrell '92

$$\mathcal{A}_1 = \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^*(\tau)\, \mathcal{G}_\sigma^{-1}(\tau,\tau')\, c_\sigma(\tau')$$

$$= \sum_{n,\sigma} c_\sigma^*(i\omega_n)\, \mathcal{G}_\sigma(i\omega_n)^{-1}\, c_\sigma(i\omega_n)$$



$$\mathcal{A}_2 = -U \int_0^\beta d\tau\; c_\uparrow^*(\tau) c_\uparrow(\tau) c_\downarrow^*(\tau) c_\downarrow(\tau)$$ local Hubbard interaction

Weiss field $\boldsymbol{\mathcal{G}}$: $(\boldsymbol{\mathcal{G}}^{-1})_{\tau,\tau'} = \mathcal{G}_\sigma^{-1}(\tau,\tau')$

Green function: $G_\sigma(i\omega_n) = \langle c_\sigma(i\omega_n) c_\sigma^*(i\omega_n) \rangle_{\mathcal{A}[\boldsymbol{\mathcal{G}}]}$

Dynamical mean-field theory

- in general $\mathcal{A}_1$ is not due to a single-site Hamiltonian
  - $\mathcal{G}$ is a dynamical mean field
  - only single-site Hamiltonian H^{at} for $\mathcal{G}^{-1} = -\partial_\tau + \mu$

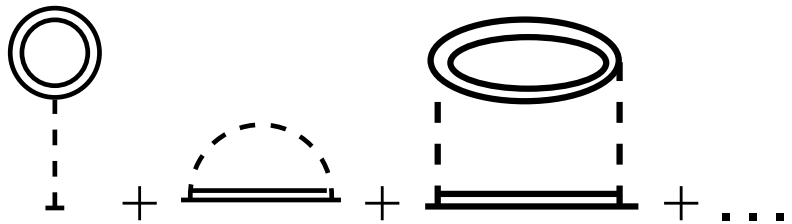
- define impurity self-energy $\tilde{\boldsymbol{\Sigma}}$ via

$$\boldsymbol{G} = \left[\mathcal{G}^{-1} - \tilde{\boldsymbol{\Sigma}}\right]^{-1}$$

impurity Dyson equation

- skeleton expansion:

$$\tilde{\boldsymbol{\Sigma}}[\boldsymbol{G}] =$$



$+ \ldots$

one site only!

$$= \boldsymbol{\Sigma}[\boldsymbol{G}]$$

same as for Hubbard model in $d = \infty$!

Dynamical mean-field equations

lattice Dyson equation:

$$G_\sigma(i\omega_n) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(i\omega_n)}$$

$$= \int_{-\infty}^{\infty} d\epsilon \, \frac{\rho(\epsilon)}{i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon} \qquad \text{self-consistency} \qquad (1)$$

together with

$$G_\sigma(i\omega_n) = \left[\mathcal{G}_\sigma(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n) \right]^{-1} \qquad (2)$$

$$G_\sigma(i\omega_n) = \langle c_\sigma(i\omega_n) c_\sigma^*(i\omega_n) \rangle_{\mathcal{A}[\mathcal{G}]} \qquad \text{(solve numerically)} \qquad (3)$$

$\Rightarrow$ three equations for unknowns G, $\mathcal{G}$, Σ

Some simple limits

non-interacting case, $U = 0$: $\quad \Sigma_\sigma(i\omega_n) = 0$

$$(1) \Rightarrow \qquad G_\sigma(i\omega_n) = G^{(0)}_\sigma(i\omega_n) = \frac{1}{L}\sum_{\boldsymbol{k}} G^{(0)}_{\boldsymbol{k}}(i\omega_n)$$

$$(2) \Rightarrow \qquad \mathcal{G}_\sigma(i\omega_n) = G_\sigma(i\omega_n) \qquad \Rightarrow \quad (3) \quad \checkmark$$

atomic limit, $t_{ij} = 0$, $\epsilon_{\boldsymbol{k}} = 0$: $\quad \rho(\epsilon) = \delta(\epsilon)$

$$(1) \Rightarrow \qquad G_\sigma(i\omega_n) = \frac{1}{i\omega_n + \mu - \Sigma_\sigma(i\omega_n)}$$

$$(2) \Rightarrow \qquad \mathcal{G}_\sigma(i\omega_n)^{-1} = i\omega_n + \mu$$

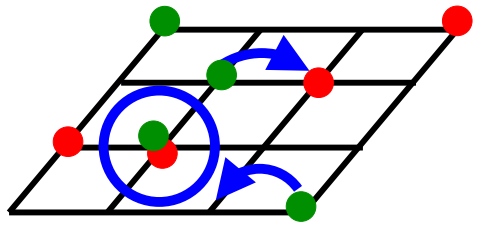
$$\Rightarrow \qquad \mathcal{G}^{-1}_\sigma(\tau) = -\partial_\tau + \mu \qquad \Rightarrow \quad (3) \quad \checkmark$$

2. A solvable example

Falicov-Kimball model: hopping only for d spin species

$$H = \sum_{ij} t_{ij}\, d_i^+ d_j + E_f \sum_i f_i^+ f_i + U \sum_i d_i^+ d_i\, f_i^+ f_i$$

- d electrons hop on background of f electrons
- f configuration optimizes the free energy



- half-filling, bipartitie lattice, $d \geq 2$:

  checkerboard phase for $U > 0$ and $T_c > T > 0$ Lieb '86

- DMFT exactly solvable Brandt & Mielsch '89, van Dongen '90, Si et al. '92, Freericks & Zlatic '03

DMFT equations

self-consistency for f electrons: $\mathcal{G}_f^{-1} = -\partial_\tau + \mu$

DMFT action:

$$\mathcal{A} = \int_0^\beta d\tau \int_0^\beta d\tau' d^*(\tau)\, \mathcal{G}_d^{-1}(\tau,\tau')\, d(\tau')$$
$$+ \int_0^\beta d\tau f^*(\tau)(\partial_\tau - \mu + E_f)\, f(\tau) - U \int_0^\beta d\tau\, d^*(\tau) d(\tau) f^*(\tau) f(\tau)$$

integrate out f electrons: (atomic limit!)

$$G_d(i\omega_n) = \langle d(i\omega_n) d^*(i\omega_n) \rangle_{\mathcal{A}}$$
$$= \frac{n_f}{\mathcal{G}_d(i\omega_n)^{-1} - U} + \frac{1 - n_f}{\mathcal{G}_d(i\omega_n)^{-1}}$$

DMFT solution

self-consistency equations:

$$G_d(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\epsilon\ \rho_d(\epsilon)}{i\omega_n + \mu - \Sigma_d(i\omega_n) - \epsilon}$$

$$G_d(i\omega_n)^{-1} = \mathcal{G}_d(i\omega_n)^{-1} - \Sigma_d(i\omega_n)$$

$\Rightarrow$ determines $G_d(i\omega_n)$ for any density of states $\rho_d(\epsilon)$

skeleton functional $\Sigma_d[G_d]$:

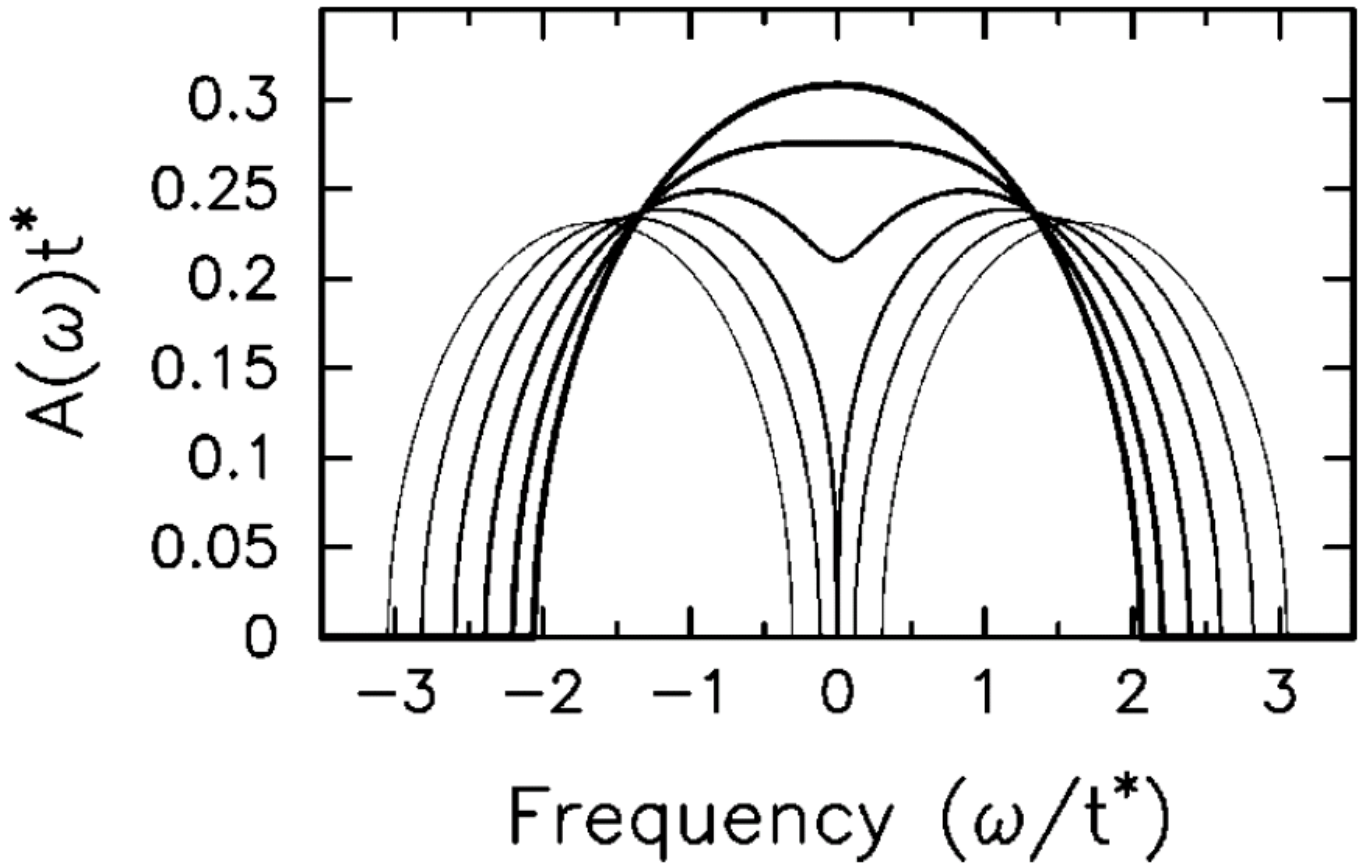
$$\Sigma_d(i\omega_n) = \frac{U}{2} - \frac{1}{2G_d(i\omega_n)} \pm \sqrt{\left(\frac{U}{2} - \frac{1}{2G_d(i\omega_n)}\right)^2 + \frac{Un_f}{G_d(i\omega_n)}}$$

involves all orders in U

Spectral function of itinerant electrons

Bethe lattice, homogeneous phase, $n_d = n_f = \frac{1}{2}$, $U = 0.5,\ 1.0,\ \ldots\ 3.0$

Freericks & Zlatic '03



- Mott metal-insulator transition at $U = 2$
- non-Fermi-liquid
- spectrum T independent in homogeneous phase

3. Impurity solvers

representation of $\mathcal{G}$ via Anderson impurity model:

$$H = \sum_{\ell\sigma} \epsilon_\ell \, a^+_{\ell\sigma} a_{\ell\sigma} + \sum_{\ell\sigma} V_\ell \, (a^+_{\ell\sigma} c_\sigma + c^+_\sigma a_{\ell\sigma}) + U c^+_\uparrow c_\uparrow \, c^+_\downarrow c_\downarrow$$

integrate out host degrees of freedom $\Rightarrow$ action $\mathcal{A}$ with

$$\begin{aligned} \mathcal{G}^{-1}_\sigma(i\omega_n) &= i\omega_n + \mu - \sum_\ell \frac{V_\ell^2}{i\omega_n - \epsilon_\ell} \\ &= i\omega_n + \mu - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\Delta(\omega)}{i\omega_n - \omega} \end{aligned}$$

$$\Delta(\omega) = \pi \sum_\ell V_\ell^2 \delta(\omega - \epsilon_\ell)$$ hybridization function

3. Impurity solvers

representation of $\mathcal{G}$ via Anderson impurity model:

$$H = \sum_{\ell\sigma} \epsilon_\ell \, a^+_{\ell\sigma} a_{\ell\sigma} + \sum_{\ell\sigma} V_\ell \, (a^+_{\ell\sigma} c_\sigma + c^+_\sigma a_{\ell\sigma}) + U c^+_\uparrow c_\uparrow \, c^+_\downarrow c_\downarrow$$

integrate out host degrees of freedom $\Rightarrow$ action $\mathcal{A}$ with

$$\begin{aligned} \mathcal{G}^{-1}_\sigma(i\omega_n) &= i\omega_n + \mu - \sum_\ell \frac{V_\ell^2}{i\omega_n - \epsilon_\ell} \\ &= i\omega_n + \mu - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\Delta(\omega)}{i\omega_n - \omega} \end{aligned}$$

$$\Delta(\omega) = \pi \sum_\ell V_\ell^2 \delta(\omega - \epsilon_\ell)$$ hybridization function

Numerical methods

Hirsch-Fye QMC

Trotter decomposition of imaginary-time action

Continuous-time QMC

Expansion in hopping or interaction

ED

exact diagonalization for small number of host sites

NRG

logarithmic discretization of host spectrum, sites added successively

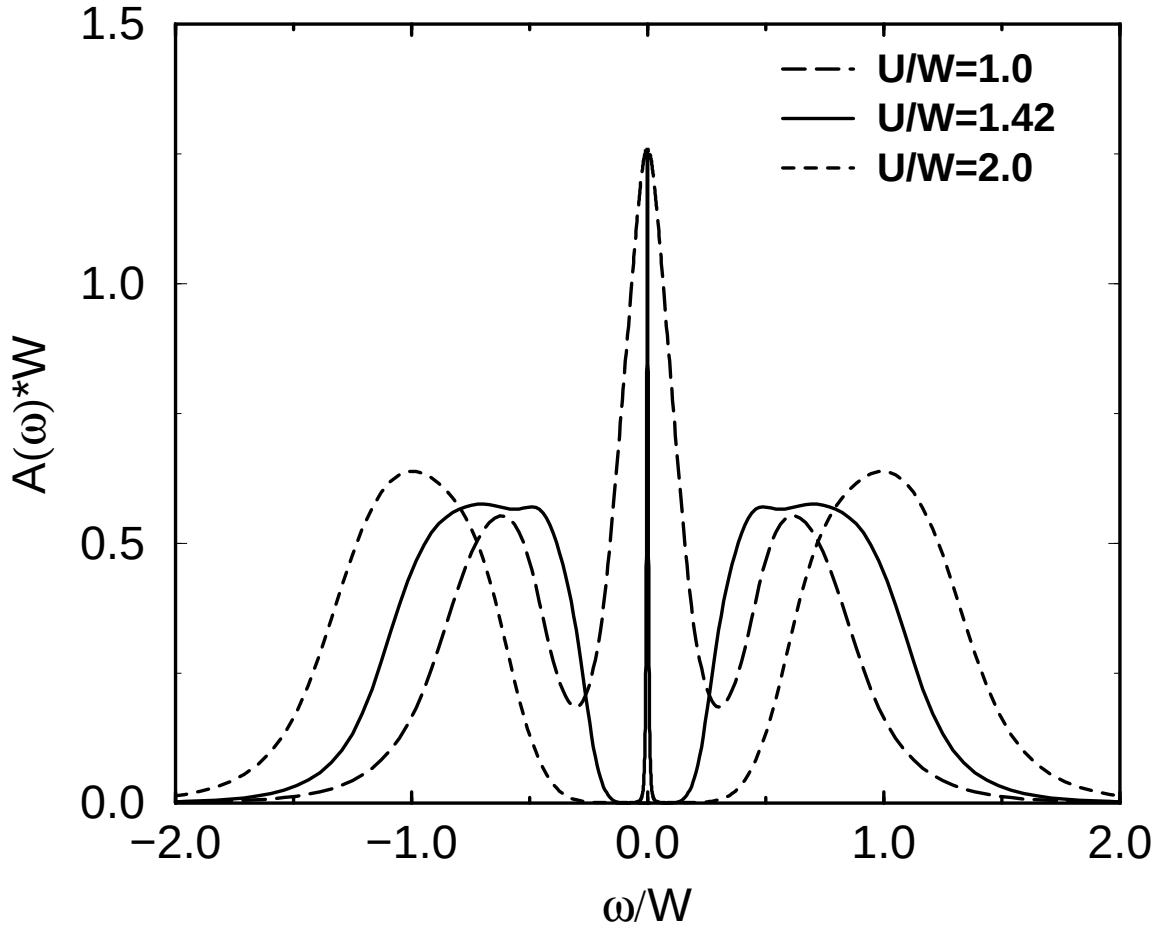
DMRG

blocks with varying number of sites, dynamical quantities available

→ lectures

Metal-insulator transition

Hubbard model, Bethe lattice, homogeneous phase, $n = 1$, DMFT(NRG)



Bulla '99

Summary

DMFT:

- exact for $d \to \infty$
- numerical solution of local dynamical many-body problem
- input: kinetic energy, interactions, band-filling (materials!)

→ lectures

Outlook:

- multiband systems, real materials, LDA+DMFT
- numerical methods
- spatial fluctuations: cluster theories, dual fermions, DΓA, ...

→ lectures