Dynamical mean-field theory

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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
\( \phi_\alpha (\mathbf{r}) \)
s, p, d, f, ...

condensed matter
Bloch: \( \psi_{nk} (\mathbf{r}) \)
Wannier: \( \phi_n (\mathbf{r} - \mathbf{R}) \)

unbound electrons
Jellium, \( \frac{1}{\sqrt{V}} e^{ikr} \)

Coulomb interaction: \( V_{ee}(\mathbf{r} - \mathbf{r}') \propto \frac{1}{|\mathbf{r} - \mathbf{r}'|} \)
\( \Rightarrow \) important for strongly localized 3d, 4d, 4f, ... electrons

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

\[ H_{\text{Hubbard}} = \sum_{ij\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]
Dynamical mean-field theory

limit of large coordination number $Z$ or large dimension $d$:

- scaling: $t = t^* / \sqrt{Z}$ with $Z \propto d \to \infty$
- Green function: $G_{ij}(\omega) \propto d^{-||R_i - R_j||/2}$
- 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
imaginary-time-ordered fermionic Green function $G_{\alpha\beta}(\tau)$:

$$G_{\alpha\beta}(\tau) = -\langle T\tau c_{\alpha}(\tau)c_{\beta}^+(0) \rangle = -\begin{cases} \langle c_{\alpha}(\tau)c_{\beta}^+(0) \rangle & \tau > 0 \\ -\langle c_{\beta}^+(0)c_{\alpha}(\tau) \rangle & \tau \leq 0 \end{cases}$$

$$= -G_{\alpha\beta}(\tau + \beta) \quad \text{for} \quad -\beta < \tau < 0$$

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

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:**

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

\[
A_{\alpha\beta}(\omega) = -\frac{1}{\pi} \text{Im} G_{\alpha\beta}(\omega + i0)
\]

**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:**

\[
G_{ii\sigma}(i\omega_n) = G_{\sigma}(i\omega_n) = \frac{1}{L} \sum_k G_{k\sigma}(i\omega_n)
\]

\[
A_{ii\sigma}(\omega) = A_{\sigma}(\omega) = -\frac{1}{\pi} \text{Im} \frac{1}{L} \sum_k G_{k\sigma}(\omega + i0)
\]

= interacting density of states
Free particles

**Free particles:**  \[ H - \mu N = \sum_{k \sigma} (\epsilon_k - \mu) \ c_k^\dagger c_k \]

\[ \Rightarrow \quad G_{k\sigma}^{(0)}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k} \]

**Local Green function:**

\[ G_\sigma(i\omega_n) = \frac{1}{L} \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k} = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{i\omega_n + \mu - \epsilon} \]

\[ A_\sigma(\omega) = \frac{1}{L} \sum_k \delta(\omega + \mu - \epsilon_k) = \rho(\omega + \mu) \]

with **free density of states**  (which characterizes \( \epsilon_k \))

\[ \rho(\omega) = \sum_k \delta(\omega - \epsilon_k) \]
Self-energy

self-energy $\Sigma_k(i\omega_n)$:

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

$$G_{k\sigma}(i\omega_n)^{-1} = G_{k\sigma}^{(0)}(i\omega_n)^{-1} - \Sigma_{k\sigma}(i\omega_n)$$

Dyson equation

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

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

or

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

diagrammatic notation:
Path-integral formulation

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

$$Z = \text{Tr} e^{-\beta(H-\mu N)} = \int \mathcal{D}(\phi^*_\alpha(\tau), \phi_\alpha(\tau)) \exp(\mathcal{A})$$

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

action:

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

imaginary-time-ordered fermionic Green function:

$$G_{\alpha\beta}(\tau) = \frac{1}{Z} \int \mathcal{D}(\phi^*\phi) \phi_\alpha(\tau)\phi^*_\beta(0) \exp(\mathcal{A})$$

e.g., Negele & Orland
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

\[ A_k(\omega) = \frac{1}{\pi} \frac{\text{Im}\Sigma_k(\omega)}{[\omega - \epsilon_k + \mu - \text{Re}\Sigma_k(\omega)]^2 + [\text{Im}\Sigma_k(\omega)]^2} \]

real part vanishes if

\[ \omega = \epsilon_k - \mu + \text{Re}\Sigma_k(\omega) \Rightarrow \text{solutions } \omega = E_k \]
2. Useful concepts. Quasiparticles

**Spectral function**: describes single-particle excitations

\[ A_k(\omega) = \frac{1}{\pi} \frac{\text{Im}\Sigma_k(\omega)}{[\omega - \epsilon_k + \mu - \text{Re}\Sigma_k(\omega)]^2 + [\text{Im}\Sigma_k(\omega)]^2} \]

Real part vanishes if

\[ \omega = \epsilon_k - \mu + \text{Re}\Sigma_k(\omega) \Rightarrow \text{solutions } \omega = E_k \]

For \( \omega \approx E_k \):

\[ G_k(\omega) \approx \frac{Z_k(E_k)}{\omega - E_k + i\tau_k(E_k)^{-1}} \]

\[ Z_k(\omega) = 1/[1 - \frac{\partial}{\partial \omega}\text{Re}\Sigma_k(\omega)] \]

\[ \tau_k(\omega) = 1/[ -Z_k\text{Im}\Sigma(\omega)] \]

Fermi liquid: coherent quasiparticles for sufficiently small \( \omega \)
Hubbard bands, Mott transition

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

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

spectral function:

- peaks broaden for \( t_{ij} \neq 0 \) \( \Rightarrow \) Hubbard bands
- Hubbard bands merge for large enough \( |t_{ij}| \)
- quasiparticle bands develops gaps for large enough \( U \)

\[ \Rightarrow \text{(non-magnetic) Mott-Hubbard transition at } U = U_c \text{ and } n = 1 \]
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:

$e_1 = (1, 0, 0, \ldots)$
$e_2 = (0, 1, 0, \ldots)$
$\ldots = \ldots$
$e_d = (0, 0, 0, \ldots, 1)$
Next-neighbor hopping

**kinetic energy:** \[ H_{\text{kin}} = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^+ c_{j\sigma} = \sum_{k,\sigma} \epsilon_k c_{k\sigma}^+ c_{k\sigma} \]

**NN hopping:** \[ t_{ij} = t(R_i - R_j) = \begin{cases} -t & \text{if } R_i - R_j = \pm e_n \\ 0 & \text{else} \end{cases} \]

**dispersion:** \[ \epsilon_k = -2t \sum_{i=1}^{d} \cos k_i \]

**density of states:**

\[ \rho(\epsilon) = \frac{1}{L} \sum_k \delta(\epsilon - \epsilon_k) \quad L \to \infty \quad \int \frac{d^d k}{(2\pi)^d} \delta(\epsilon - \epsilon_k) \]

**nontrivial limit** \( d \to \infty ? \)
Scaling of hopping amplitudes

**elegant answer:**

- 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 $\sqrt{2dt}X_d$

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

\[ \rho(\omega) \]

\( d = 1 \quad d = 2 \quad d = 3 \quad d = 4 \quad d = 5 \quad d = \infty \)

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:

- \( G^{(0)} \) = non-interacting Green function line
- Interaction vertex
- \( G \) = full (interacting) Green function line

perturbation expansion:
Self-energy

proper self-energy diagrams:

- external vertex amputated
- cannot be cut in two pieces

\[
\Sigma = \quad \text{proper} \quad + \quad \text{proper} \quad + \quad \text{not proper} \quad + \quad \text{proper} \quad + \ldots
\]
Skeleton expansion

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

now: omit self-energy insertions, etc.

$\Rightarrow$ skeleton expansion $\Sigma[G]$

$\Sigma = \circ + \text{dashed} + \text{solid} + ...$

- 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:

$$t_{ij} = t_{ij}^{*} d^{-\frac{1}{2}} ||R_i - R_j||$$

kinetic energy:

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

Green function:

$$G_{ij\sigma}(\omega) = O(d^{-\frac{1}{2}} ||R_i - R_j||) , \quad G_{ii\sigma}(\omega) = O(d^0)$$

$\Rightarrow$ simplifications for Feynman diagrams!
Diagrammatic simplifications

Hugenholtz diagrams: (Hubbard model: no exchange diagrams)

\[ i, \sigma \overset{\text{---}}{\longrightarrow} i, -\sigma = Un_i^{\uparrow} n_i^{\downarrow} \]

skeleton expansion:

\[ \Sigma = \quad + \quad + \quad + \ldots \]  \hspace{1cm} (1)

consider fixed \( i \): compare \( j \neq i \) with \( j = i \)
Collapse of position space diagrams

skeleton expansion: \( \geq 3 \) independent paths from \( i \) to \( j \)

- Green function lines: \( O(d^{-\frac{3}{2}}||R_i-R_j||) \)
- summation over \( j \): \( O(d||R_i-R_j||) \)

\( \Rightarrow \) skeleton diagram is \( O(d^{-\frac{1}{2}}||R_i-R_j||) \)

in \( d = \infty \):

all vertices in \( \Sigma[G] \) have the same site label!

self-energy is local!

\[
\Sigma_{ij\sigma}(\omega) = \delta_{ij} \Sigma_{i\sigma}(\omega) = \delta_{ij} \Sigma_{\sigma}(\omega) \\
\Sigma_{k\sigma}(\omega) = \Sigma_{\sigma}(\omega) \quad \text{independent of } k!
\]
Consequences of local self-energy

**simple \( k \) dependence:**

\[
G_{k\sigma}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma}(i\omega_n)}
\]

**local Green function:**

\[
G_{\sigma}(i\omega_n) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma}(i\omega_n)}
\]

- **Dyson equation**
- **Hilbert transform**

\[
= \int_{-\infty}^{\infty} d\epsilon \ \frac{\rho(\epsilon)}{i\omega_n + \mu - \Sigma_{\sigma}(i\omega_n) - \epsilon}
\]

(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: $\mathcal{A} = \mathcal{A}_1 + \mathcal{A}_2$

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

\[= \sum_{n,\sigma} c^*_\sigma(i\omega_n) G_\sigma(i\omega_n)^{-1} c_\sigma(i\omega_n)\]

\[\mathcal{A}_2 = -U \int_0^\beta d\tau \; c^*_\uparrow(\tau)c^*_\downarrow(\tau)c_\uparrow(\tau)c_\downarrow(\tau)\]  

local Hubbard interaction

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

Green function: $G_\sigma(i\omega_n) = \langle c_\sigma(i\omega_n)c^*_\sigma(i\omega_n)\rangle_{\mathcal{A}[\mathcal{G}]}$
Dynamical mean-field theory

- in general $A_1$ is not due to a single-site Hamiltonian
  - $\mathcal{G}$ is a dynamical mean field
  - only single-site Hamiltonian $H^{\mathrm{at}}$ for $\mathcal{G}^{-1} = -\partial_\tau + \mu$

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

\[
G = \left( \mathcal{G}^{-1} - \tilde{\Sigma} \right)^{-1}
\]

impurity Dyson equation

- skeleton expansion:

\[
\tilde{\Sigma}[G] = \ldots + \ldots + \ldots + \ldots
\]

one site only!

\[
= \Sigma[G]
\]

same as for Hubbard model in $d = \infty$!
Dynamical mean-field equations

lattice Dyson equation:

\[ G_\sigma(i\omega_n) = \int \frac{d^d k}{(2\pi)^d} \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_\sigma(i\omega_n)} \]

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

together with

\[ G_\sigma(i\omega_n) = \left[ G_\sigma(i\omega_n)^{-1} - \Sigma_\sigma(i\omega_n) \right]^{-1} \quad (2) \]

\[ G_\sigma(i\omega_n) = \langle c_\sigma(i\omega_n)c^{*}_\sigma(i\omega_n) \rangle_A[G] \quad \text{(solve numerically)} \quad (3) \]

⇒ three equations for unknowns \( G, G, \Sigma \)
Some simple limits

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

(1) $\Rightarrow$ $G_\sigma(i\omega_n) = G_\sigma^{(0)}(i\omega_n) = \frac{1}{L} \sum_k G_k^{(0)}(i\omega_n)$

(2) $\Rightarrow$ $G_\sigma(i\omega_n) = G_\sigma(i\omega_n)$ $\Rightarrow$ (3) ✔

atomic limit, $t_{ij} = 0$, $\epsilon_k = 0$: $\rho(\epsilon) = \delta(\epsilon)$

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

(2) $\Rightarrow$ $G_\sigma(i\omega_n)^{-1} = i\omega_n + \mu$

$\Rightarrow$ $G_\sigma^{-1}(\tau) = -\partial_\tau + \mu$ $\Rightarrow$ (3) ✔
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: $G_f^{-1} = -\partial_\tau + \mu$

DMFT action:

$$\mathcal{A} = \int_0^\beta d\tau \int_0^\beta d\tau' d^*(\tau) G_d^{-1}(\tau, \tau') d(\tau')$$

$$+ \int_0^\beta d\tau f^*(\tau)(\partial_\tau - \mu + E_f) f(\tau) - U \int_0^\beta d\tau d^*(\tau) d(\tau) f^*(\tau) f(\tau)$$

integrate out $f$ electrons: (atomic limit!)

$$G_d(i\omega_n) = \langle d(i\omega_n)d^*(i\omega_n) \rangle_\mathcal{A}$$

$$= \frac{n_f}{G_d(i\omega_n)^{-1} - U} + \frac{1 - n_f}{G_d(i\omega_n)^{-1}}$$
DMFT solution

self-consistency equations:

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

\[
G_d(i\omega_n)^{-1} = G_d(i\omega_n)^{-1} - \Sigma_d(i\omega_n)
\]

⇒ 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, $n_d = n_f = \frac{1}{2}$, $U = 0.5, 1.0, \ldots, 3.0$

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

Freericks & Zlatic '03
3. Impurity solvers

representation of $G$ 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

$$G_{\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{\ell} \frac{V_{\ell}^2}{i\omega_n - \epsilon_{\ell}}$$

$$= i\omega_n + \mu - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\Delta(\omega)}{i\omega_n - \omega}$$

$$\Delta(\omega) = \pi \sum_{\ell} V_{\ell}^2 \delta(\omega - \epsilon_{\ell}) \quad \text{hybridization function}$$
3. Impurity solvers

representation of \( G \) 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

\[
G_{\sigma}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{\ell} \frac{V_{\ell}^2}{i\omega_n - \epsilon_{\ell}}
\]

\[
= i\omega_n + \mu - \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\Delta(\omega)}{i\omega_n - \omega}
\]

\[
\Delta(\omega) = \pi \sum_{\ell} V_{\ell}^2 \delta(\omega - \epsilon_{\ell}) \quad \text{hybridization function}
\]
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)

![Graph showing A(ω)W vs. ω/W for different values of U/W: U/W=1.0, U/W=1.42, U/W=2.0. The graph illustrates the behavior of the system across different interaction strengths.]

Bulla '99
Summary

DMFT:

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

Outlook:

- multiband systems, real materials, LDA+DMFT
- numerical methods
- spatial fluctuations: cluster theories, dual fermions, \( \Delta \Gamma \), . . .