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Educational, Scientific
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Energy Agency

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Summer School and Miniconference on
Dynamical Mean-Field Theory for Correlated Electrons:
Applications to Real Materials, Extensions and Perspectives
25 July - 3 August, 2005

Dynamical Mean-Field Theory
I, II & III

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Dynamical mean-field theory

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International Center for Theoretical Physics, Trieste
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Outline

Preamble

- Local-density approximation (LDA)
- Dynamical mean-field theory (DMFT)
- LDA + DMFT

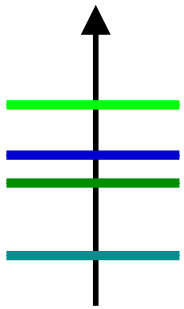
I. Introduction
   - Green functions
   - Useful concepts

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

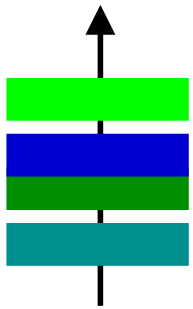
III. Dynamical mean-field theory
   - Mapping onto impurity models
   - A solvable example
   - Impurity solvers
   - Multiband systems

Preamble

condensed matter: electrons in a ionic potential



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



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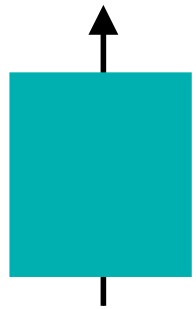
Bloch: $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$
Wannier: $\phi_n(\boldsymbol{r}-\boldsymbol{R})$



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

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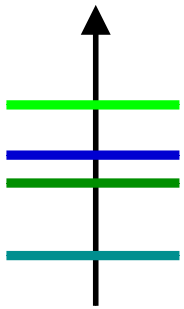

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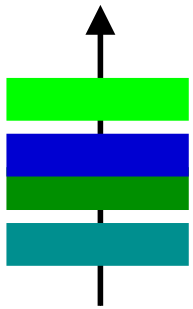

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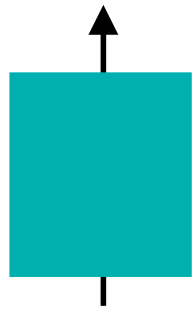

unbound electrons
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Coulomb interaction: $V_{\text{ee}}(\boldsymbol{r}-\boldsymbol{r}') \propto \dfrac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}$

- important for strongly localized 3d, 4d, 4f, ... electrons
  $\Rightarrow$ large overlap $V_{\alpha\beta\gamma\delta} = \langle\alpha\beta|V_{\text{ee}}|\gamma\delta\rangle$
- Bloch theorem applicable, but $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$ unknown
- unsolvable quantum-mechanical many-body problem

Density functional theory

Hohenberg & Kohn ('64):

$$E_0 = E[\rho] = \text{functional of electron density } \rho(\boldsymbol{r})$$

$$= \underbrace{E_{\text{kin}}[\rho] + E_{\text{ion}}[\rho] + E_{\text{Hartree}}[\rho]}_{\text{known contributions}} + \underbrace{E_{\text{xc}}[\rho]}_{\text{unknown}}$$

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Kohn & Sham ('65): $\rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$

$$\left[-\frac{\hbar^2}{2m_e}\Delta + V_{\text{eff}}(\boldsymbol{r}) \right]\varphi_i(\boldsymbol{r}) = \varepsilon_i \varphi_i(\boldsymbol{r}) \qquad \text{Kohn-Sham equations}$$

$$V_{\text{eff}}(\boldsymbol{r}) = V_{\text{ion}}(\boldsymbol{r}) + \int d^3r'\, V_{\text{ee}}(\boldsymbol{r}-\boldsymbol{r'})\rho(\boldsymbol{r'}) + \frac{\delta E_{\text{xc}}[\rho]}{\delta \rho(\boldsymbol{r})}$$

Local Density Approximation

LDA: use $E_{\mathrm{xc}}[\rho]$ of the homogeneous electron gas ($\rho = \text{const}$)

- solve Kohn-Sham equations by iteration

$$\rho(\boldsymbol{r}) \;\Rightarrow\; V_{\mathrm{eff}}(\boldsymbol{r}) \;\Rightarrow\; \{\varepsilon_i,\ \varphi_i(\boldsymbol{r})\} \;\Rightarrow\; \rho(\boldsymbol{r}) \;\Rightarrow\; \ldots$$

- basis-dependent! (LMTO, [F]LAPW, ASW, ...)

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- basis-dependent! (LMTO, [F]LAPW, ASW, ...)

very successful!

- advantages: provides bandstructure, intuitive one-particle picture
- problem: only certain part of V_{ee} taken into account
  $\Rightarrow$ cannot describe strongly correlated systems

Hamilton-Operator:

$$H_{\text{LDA}} = \sum_{ilm,jl'm',\sigma} t_{ilm,jl'm'}\, c^{+}_{ilm\sigma} c_{jl'm'\sigma} \qquad (\ t_{ilm,jl'm'} \leftrightarrow \epsilon_{\boldsymbol{k}lm}\ )$$

Models for correlated electrons

interacting electrons: charge and spin degrees of freedom

$$H = \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta}\, c_{i\alpha\sigma}^{+} c_{j\beta\sigma} + \sum_{\substack{ijkl \\ \alpha\beta\gamma\delta\sigma\sigma'}} V_{ijkl}^{\alpha\beta\gamma\delta}\, c_{i\alpha\sigma}^{+} c_{j\beta\sigma'}^{+} c_{l\delta\sigma'} c_{k\gamma\sigma}$$

$\Rightarrow$ metals, insulators, magnetism, superconductivity, ...

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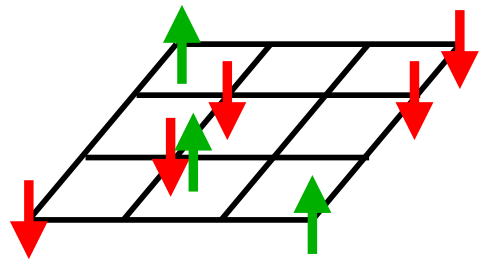
Hubbard model: e.g. 1 band, only

$U = V_{iiii}$

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



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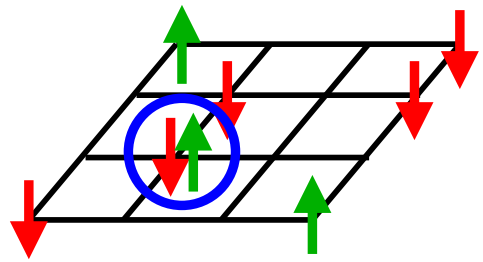

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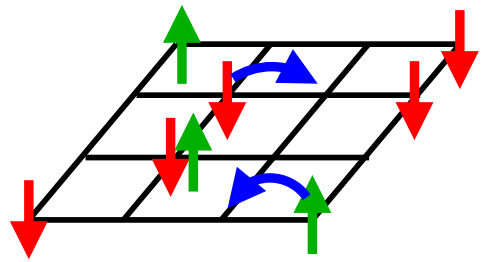

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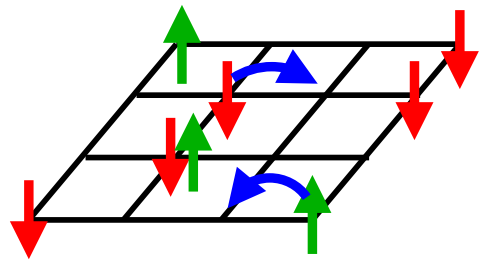

Heisenberg model: $H_{\text{Hubbard}} \overset{U \gg |t_{ij}|}{\longrightarrow} H_{\text{Heisenberg}}$ mit $J_{ij} = \frac{4t_{ij}^2}{U}$

$$H_{\text{Heisenberg}} = \sum_{ij} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

localized q.m. spins

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!

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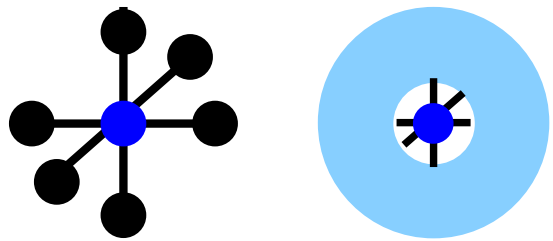
mapping onto single-site problem:



- 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, ...]

LDA + DMFT

DMFT:

- exact for $d = \infty$
- “thermodynamically consistent”, “conserving approximation”
- extensions: many bands, clusters, non-local interactions, ...
- impurity solvers: NRG, QMC, PQMC, ED, NCA... [→ lectures]

LDA + DMFT

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- impurity solvers: NRG, QMC, PQMC, ED, NCA... [→ lectures]

LDA+DMFT: [Anisimov et al. '97; Lichtenstein & Katsnelson '97; Liebsch & Lichtenstein '00; Nekrasov et al. '00; ...]

- use LDA band structure (as input, or self-consistently)
- on-site ("Hund's rule") interactions
- combine with DMFT, cluster extensions, ... [→ lectures]

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 $\alpha\beta(\tau)$:

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

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

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

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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:

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

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

$$= \frac{1}{Z}\sum_{n,m} \langle n|c_\beta^+|m\rangle\langle m|c_\alpha|n\rangle \; (e^{-\beta E_m} - e^{-\beta E_n}) \; \delta(\omega - (E_n - E_m))$$

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local Green function:

$$G_{ii\sigma}(\omega) = G_\sigma(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k}\sigma}(\omega) \qquad (\mathrm{Im}\omega \neq 0)$$

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

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

Free particles

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

$$\Rightarrow \qquad G^{(0)}_{k\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_k}$$

local Green function:

$$G_\sigma(\omega) = \frac{1}{L} \sum_k \frac{1}{\omega + \mu - \epsilon_k} \qquad = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{\omega + \mu - \epsilon}$$

$$S_\sigma(\omega) = \frac{1}{L} \sum_k \delta(\omega + \mu - \epsilon_k) \qquad = \rho(\omega + \mu)$$

with free density of states (which characterizes ϵ_k)

$$\rho(\omega) = \sum_k \delta(\omega - \epsilon_k)$$

Self-energy

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

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

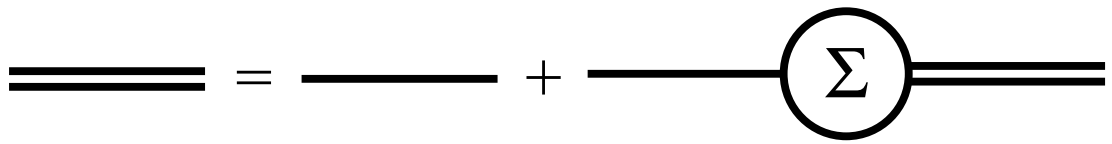
$$G_{\boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_{\boldsymbol{k}\sigma}(\omega)}$$

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

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

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

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]

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imaginary-time-ordered fermionic Green function:

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

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2. Useful concepts
   - Quasiparticles
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2. Useful concepts

if perturbation theory valid (T=0): e.g., for Fermi liquids [Luttinger '60]

$$\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega) \overset{\omega \to 0}{\sim} -\mathrm{sgn}(\omega)\, C_{\boldsymbol{k}}\, \omega^2 \qquad (C_{\boldsymbol{k}} \geq 0)$$

poles in Green function satisfy

$$\omega - (\epsilon_{\boldsymbol{k}} - \mu) - \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega) + i\mathrm{sgn}(\omega)\, C_{\boldsymbol{k}}\, \omega^2 = 0$$

real part vanishes if

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

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

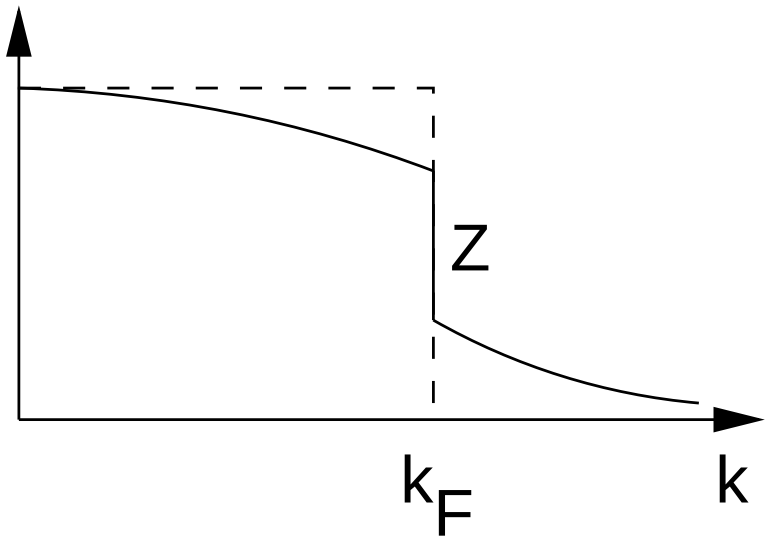
$$G_{\boldsymbol{k}}(\omega) \approx \frac{Z_{\boldsymbol{k}}}{\omega - E_{\boldsymbol{k}} + i\tau_{\boldsymbol{k}}^{-1}}$$

Quasiparticles

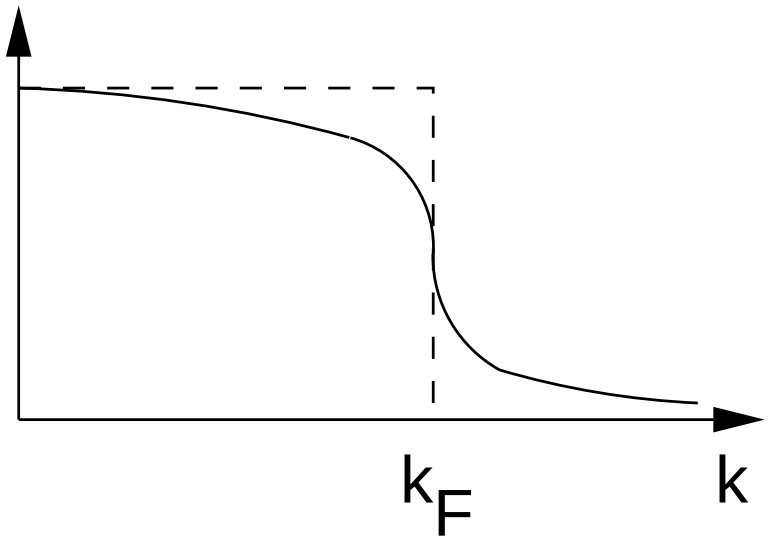
$$Z_{\boldsymbol{k}} = \frac{1}{1 - \mathrm{Re}\Sigma'_{\boldsymbol{k}}(E_{\boldsymbol{k}})}$$ quasiparticle weight

$$\tau_{\boldsymbol{k}} = 1/E^2_{\boldsymbol{k}}$$ quasiparticle lifetime

- quasiparticles stable for $E_{\boldsymbol{k}}$ close enough to Fermi surface
- Fermi energy does not change due to interactions [Luttinger '61]
- Z is related to jump in momentum distribution (absent in $D = 1$)



$D \geq 2$



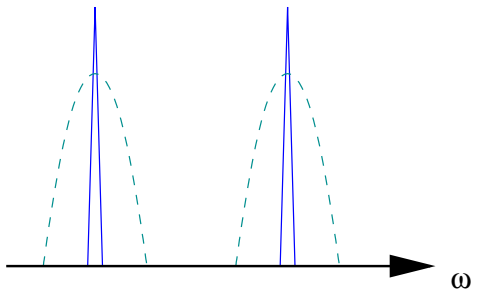
$D = 1$

Hubbard bands, Mott transition

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

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

spectral function:



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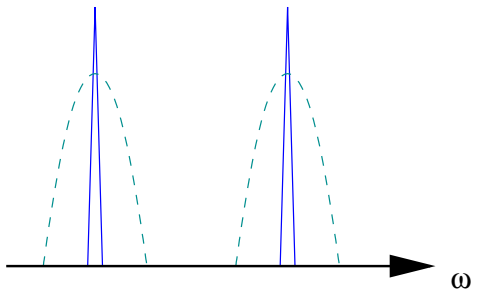


- peaks broaden for $t_{ij} \neq 0 \;\Rightarrow$ Hubbard bands [Hubbard '63]
- Hubbard bands merge for large enough $|t_{ij}|$
- quasiparticle bands develops gaps for large enough U

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

[Mott '46]

Part II
Fermions in infinite dimensions

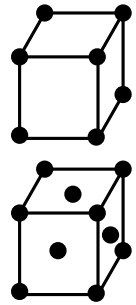
1. Free fermions
   - Scaling of hopping amplitudes
   - Density of states
   - Generalized lattices

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?

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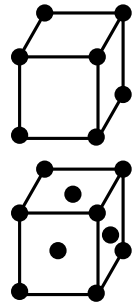
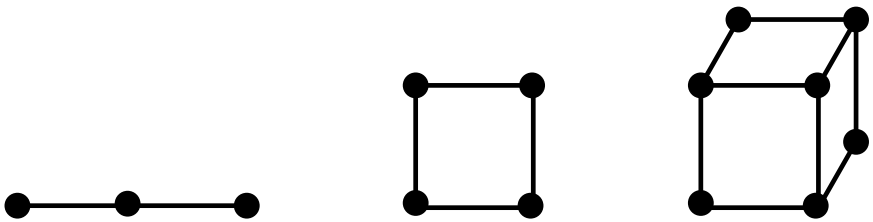


$\Rightarrow$ generalized lattices for any (large) dimension d?

easy for hypercubic lattice:



in d dimensions:

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

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

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

nontrivial limit $d \to \infty$?

density of states:

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

Scaling of hopping amplitudes

elegant answer:

[Metzner & Vollhardt '89]

- $X_d := \sum_{i=1}^{d} \cos k_i$
- random variables $k_i \in [-\pi; \pi]$ (mean=0, variance=1)

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- $X_d := \sum_{i=1}^{d} \cos k_i$
- random variables $k_i \in [-\pi; \pi]$ (mean=0, variance=1)

central limit theorem:

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

density of states:

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

1/d corrections

Fourier transform:

[Müller-Hartmann '89]

$$\Phi(s) = \int_{-\infty}^{\infty} d\epsilon\, e^{is\epsilon}\, \rho(\epsilon) = \int \frac{d^d k}{(2\pi)^d}\, e^{is\epsilon_{\boldsymbol{k}}} \qquad \text{factorizes!}$$

$$= \left[\int_{-\pi}^{\pi} \frac{dk}{2\pi}\, \exp\left(-\frac{2ist_*}{\sqrt{2d}}\, \cos k\right)\right]^d \quad = \quad J_0\left(\frac{2t_*}{\sqrt{2d}}\right)^d$$

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$$= \left[1 - \frac{t_*^2 s^2}{2d} + O\left(\frac{1}{d}\right)\right]^d \quad = \quad \exp\left[-\frac{t_*^2 s^2}{2} + O\left(\frac{1}{d}\right)\right]$$

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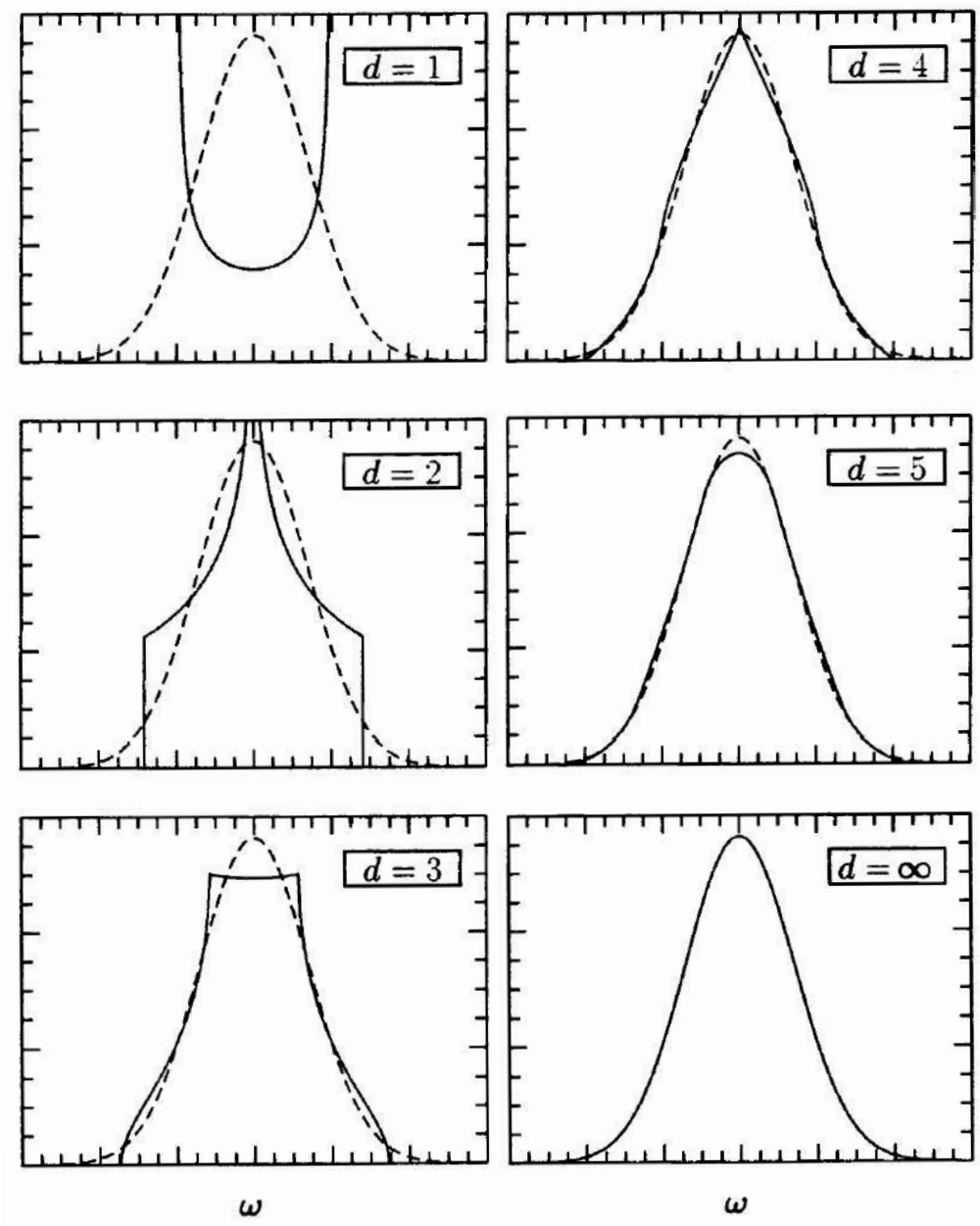
inverse transform:

$$\rho(\epsilon) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi}\, e^{-is\epsilon}\, \Phi(s)$$

$$= \frac{1}{2\pi|t_*|}\, \exp\left[-\frac{\epsilon^2}{2t_*^2} + \frac{1}{16d}\left(3 - \frac{6\epsilon^2}{t_*^2} - \frac{6\epsilon^4}{t_*^4}\right) + O\left(\frac{1}{d^2}\right)\right]$$

Density of states

$\rho(\omega)$



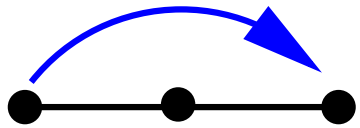
[Vollhardt '93]

Beyond nearest neighbors

[Müller-Hartmann '89]

in general: $t_{ij} \propto \dfrac{1}{\sqrt{\#\text{ sites reached}}}$

hopping along axes: $\epsilon_{\boldsymbol{k}}^{\text{axes}} = \sum_{m \geq 1} \left(\dfrac{-2t_*^{(m)}}{\sqrt{2d}} \right) \sum_i \cos m k_i$



$$\boxed{\rho(\epsilon) \propto \exp\left(-\frac{\epsilon^2}{2t_{\text{eff}}^2} \right)} \quad \text{with} \quad t_{\text{eff}} = \sqrt{t_*^{(1)} + t_*^{(2)} + \ldots}$$

Beyond nearest neighbors

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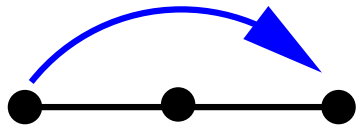

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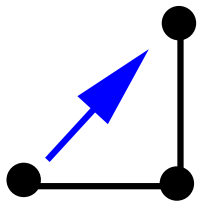
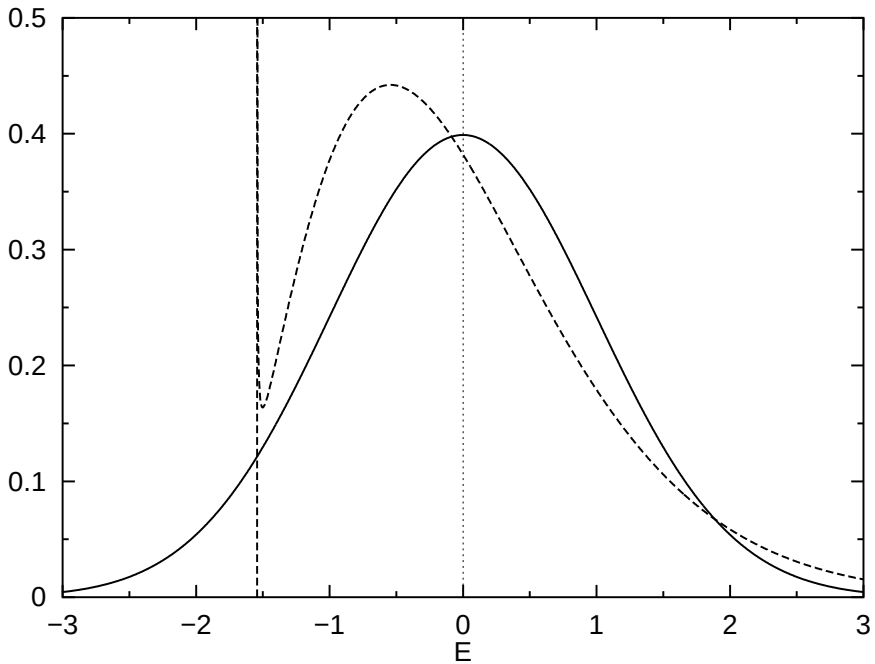
hopping to next-nearest neighbors: $\epsilon_{\boldsymbol{k}}^{\text{NNN}} \sim t' \left(\sum_i \cos k_i \right)^2$



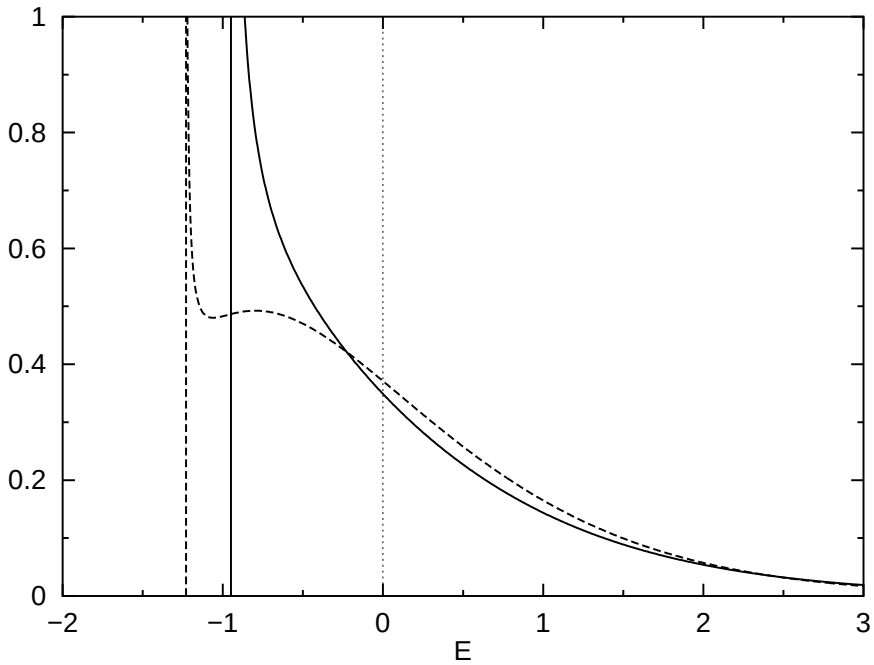
$$\boxed{\rho(\epsilon) \propto \frac{\cosh(E/a^2)\, \exp(-E^2/2a^2)}{E}} \qquad E = \sqrt{1 - 2a\epsilon + a^2}, \qquad a = \frac{\sqrt{2}t'_*}{t_*}$$

Density of states

NN and NNN hopping: $a = 2t'_*/t_*$



$a = 0, a = -0.35$



$a = -0.47, a = -0.71$

[Schlipf '98]

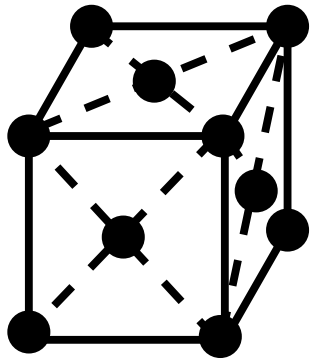
- asymmetric for $t'_* \neq 0$
- square-root singularity at band-edge!

Generalized fcc lattice

NN hopping
on fcc lattice

$\equiv$

NNN hopping
on simple cubic lattice



$$\rho(\epsilon) \propto \frac{e^{-(\epsilon - \epsilon_{\text{min}})/t_*}}{\sqrt{\epsilon - \epsilon_{\text{min}}}} \quad \text{for} \quad \epsilon > \epsilon_{\text{min}} = -\frac{t_*}{\sqrt{2}}$$

- square-root singularity at band-edge
- small energy cost for spin-polarized states

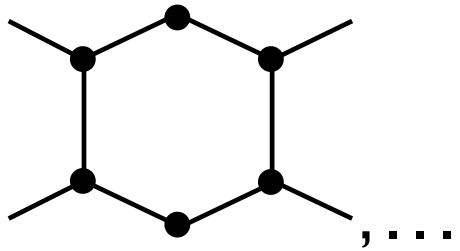
  $\Rightarrow$ favors ferromagnetism

[Müller-Hartmann '91;Ulmke '98; Wahle et al. '98, Vollhardt et al. '99]

Other crystal lattices

honeycomb, diamond, . . . , hyperdiamond lattice: [Sanotoro et al. '93]

$$\rho(\epsilon) \propto |\epsilon| \; e^{-\frac{\epsilon^2}{2t_*^2}}$$



,. . .

- no perfect nesting!
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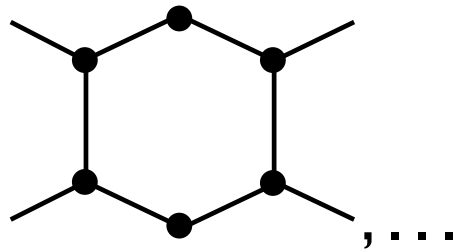

,...

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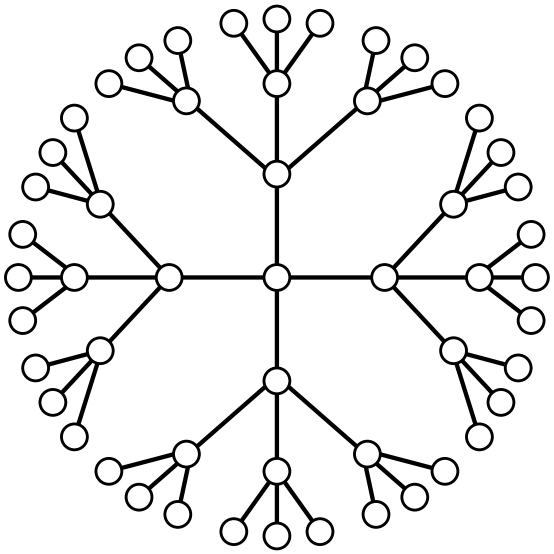
Lorentzian density of states: [Georges et al. '96]

$$\epsilon_{\boldsymbol{k}} = \frac{t_*}{d} \sum_{i=1}^{d} \cot |k_i| \quad \Rightarrow \quad \boxed{\rho(\epsilon) = \frac{1}{\pi} \frac{|t_*|}{t_*^2 + \epsilon^2}}$$

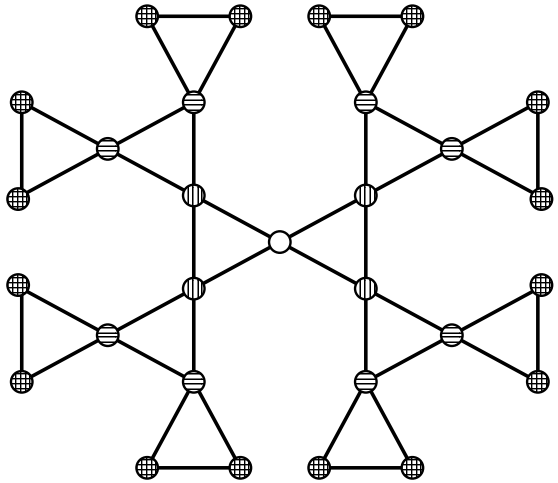
- $E_{\text{kin}} = \int_{-\infty}^{\epsilon_F} d\epsilon\, \rho(\epsilon) = \infty \quad \Rightarrow$ M.-I.-transition at $U_c = \infty$

Recursively defined lattices

Bethe lattice



Husimi cactus



- tree-like structure, Z nearest neighbors
- models for amorphous solids
- no Bloch theorem, no Brillouin zone

- RPE, . . . [Brinkman & Rice '70, Chen et al. '74, Economou '90, Mahan '01]
- algebraic methods [Eckstein et al. '04, Kollar et al. '05]

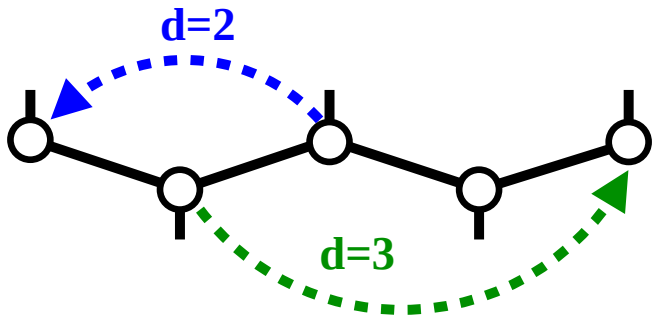
Operator identities

hopping with d steps:

$$H_r = \sum_{d_{ij}=r} c_i^+ c_j$$

$H_1 =$ NN hopping

$$\tilde{H}_r = \frac{H_r}{(Z-1)^{r/2}}, \qquad t_r^* = \frac{t_r^*}{(Z-1)^{r/2}}$$



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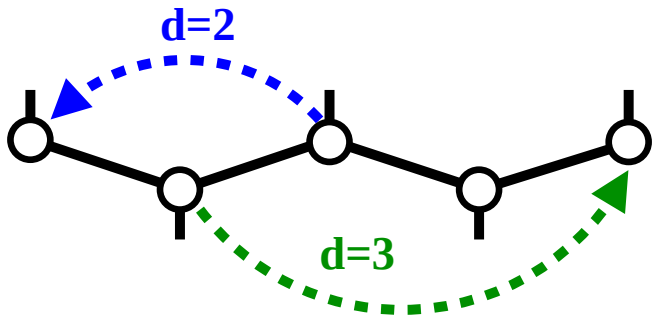


operator identities for Bethe lattice:

$$H_2 = (H_1)^2 - Z, \ \ldots, \qquad \Rightarrow \qquad \boxed{\sum_{r=0}^{\infty} \tilde{H}_r \, x^r = \frac{1 - x^2/(Z-1)}{1 - x\tilde{H}_1 + x^2}}$$

- $H_{\text{kin}} = \epsilon(\tilde{H}_1) \quad \Rightarrow \quad H_{\text{kin}}|\lambda\rangle = \epsilon(\lambda)|\lambda\rangle$
- $\epsilon(\lambda)$ = "dispersion" on interval $-2 \le \lambda \le 2$

NN and NNN hopping

for NN hopping ($Z = \infty$):

$$\rho_1(\lambda) = \frac{1}{2\pi}\sqrt{4-\lambda^2}$$

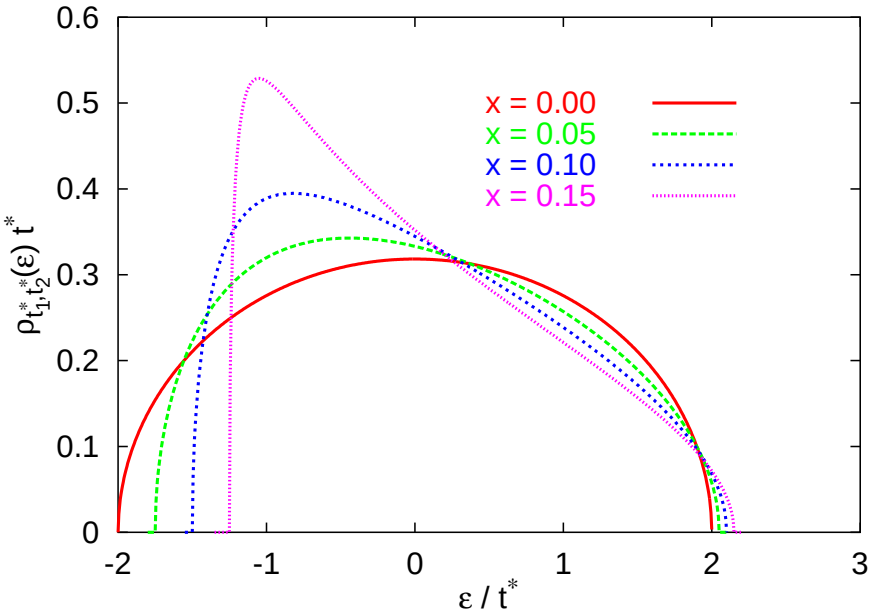
for any $H_{\text{kin}} = \epsilon(\tilde{H}_1)$:

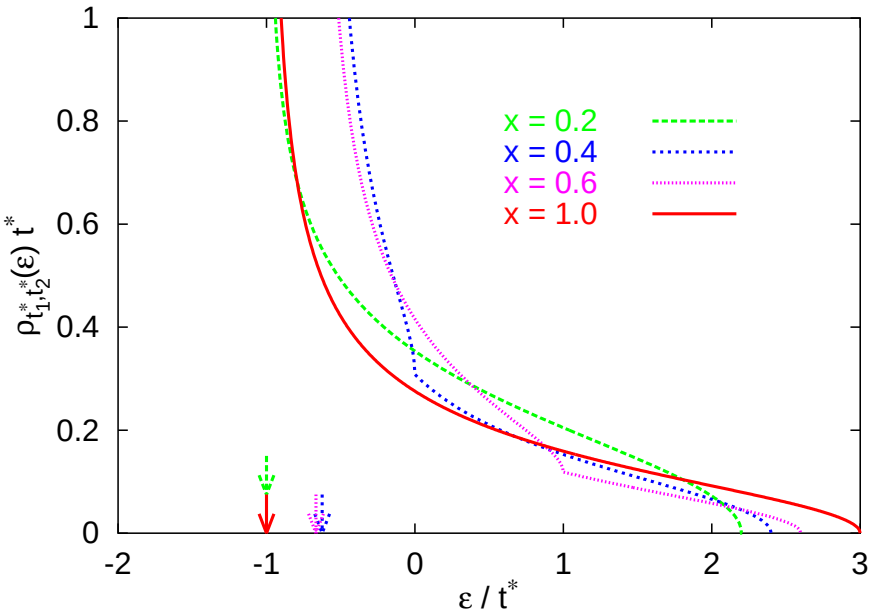
$$\rho(\epsilon) = \int_{-2}^{2} d\lambda\, \rho_1(\lambda)\, \delta(\epsilon - \epsilon(\lambda))$$

for NN and NNN hopping:

$$\epsilon(\lambda) = \text{const} + t_1^*\lambda + t_2^*\lambda^2$$

$$x = \frac{t_2^*}{|t_1^*|+|t_2^*|}$$





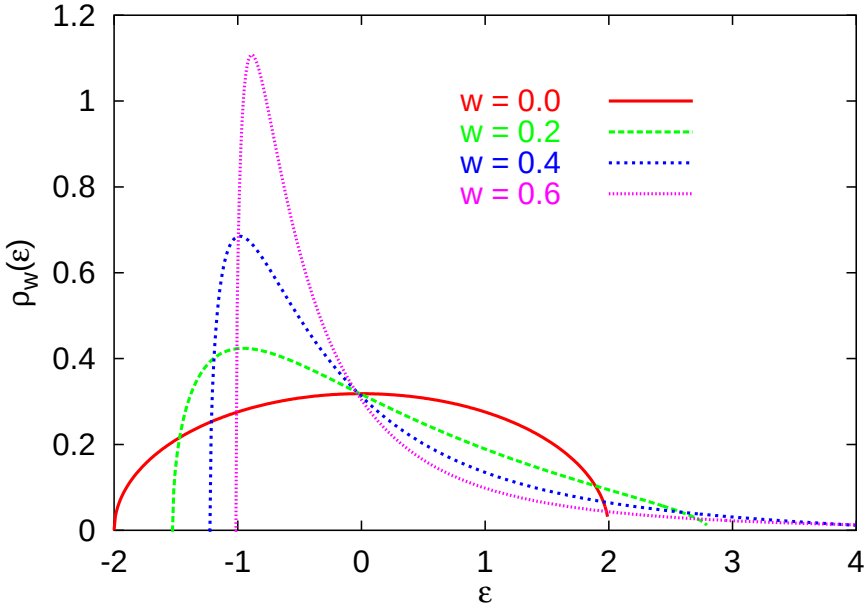
DOS for long-range hopping

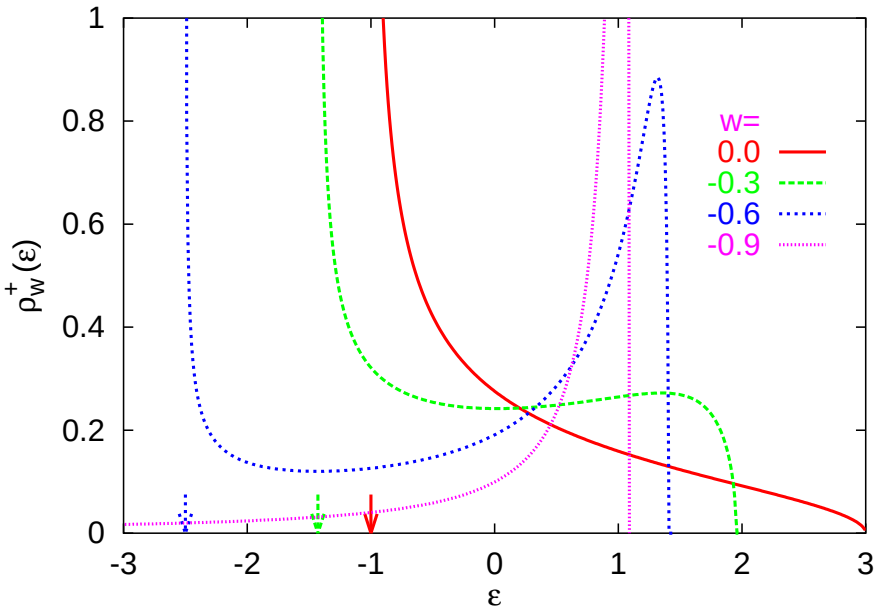
$$t_r^* \propto \exp(-\text{const} \cdot d)$$

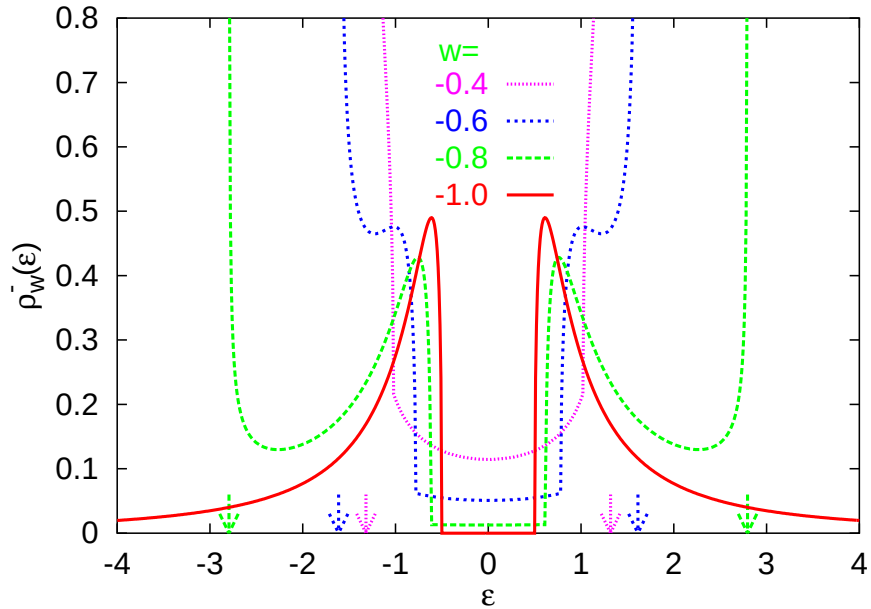
$$H_w = \sum_r w^{r-1} \tilde{H}_r$$

$$H_w^+ = \sum_r w^{r-1} \tilde{H}_{2r}$$

$$H_w^- = \sum_r w^{r-1} \tilde{H}_{2r-1}$$







Lattice representation of density of states

1-particle quantities:

- e.g., thermodynamics, Green function, ...
- in $d = \infty$ only $\rho(\epsilon)$ enters (instead of $\epsilon_{\boldsymbol{k}}$)
- simply use $\rho(\epsilon)$ of finite-d system (e.g., LDA)

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- in $d = \infty$ only $\rho(\epsilon)$ enters (instead of $\epsilon_{\boldsymbol{k}}$)
- simply use $\rho(\epsilon)$ of finite-d system (e.g., LDA)

2-particle quantities, ...:

- e.g., correlation functions, symmetry-broken phases, ...
- need lattice with hopping amplitudes t_r^*
- any $\rho(\epsilon)$ can be represented for $Z \to \infty$
  - on hypercubic lattice [Blümer '02]
  - on Bethe lattice [Eckstein et al. '04]

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Fermions in infinite dimensions

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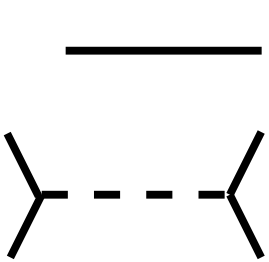
2. Many-body theory

Feynman diagrams for Green functions:

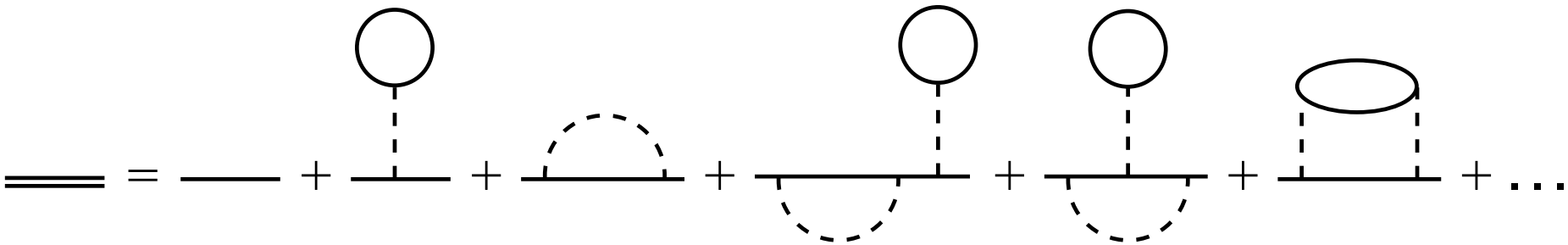


= non-interacting Green function line $\boldsymbol{G}^{(0)}$

= interaction vertex

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

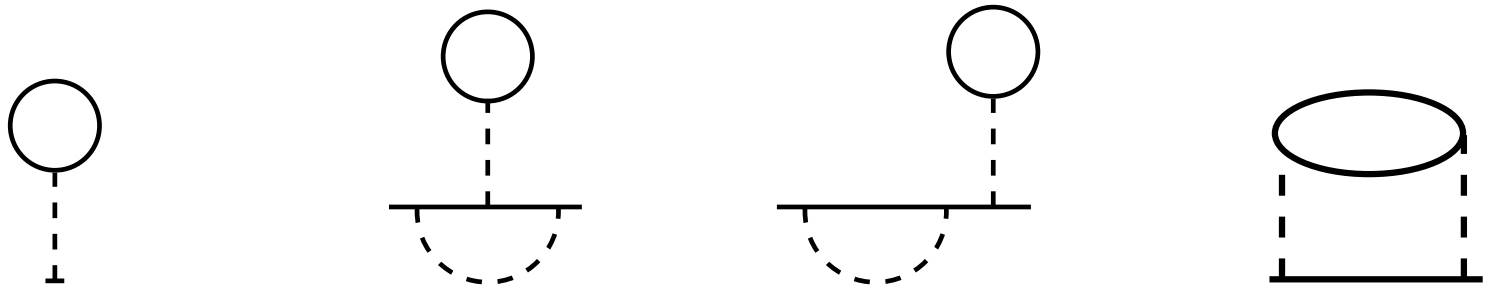
perturbation expansion:



Self-energy

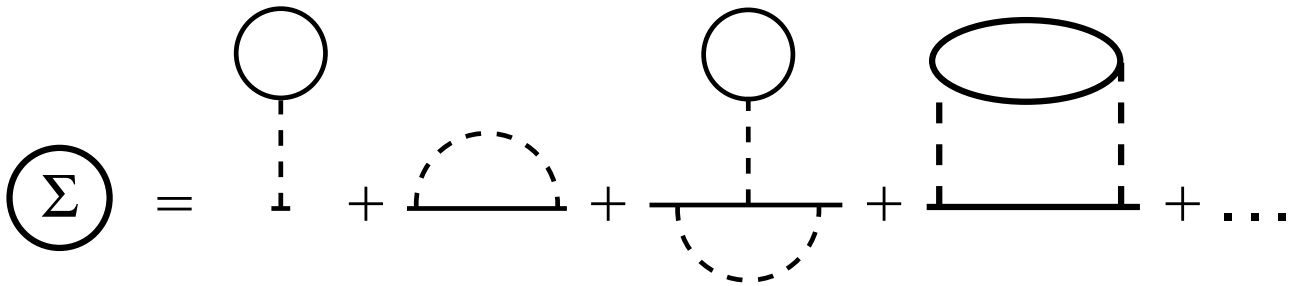
proper self-energy diagrams:

- external vertex amputated
- cannot be cut in two pieces



proper proper not proper proper

self-energy:

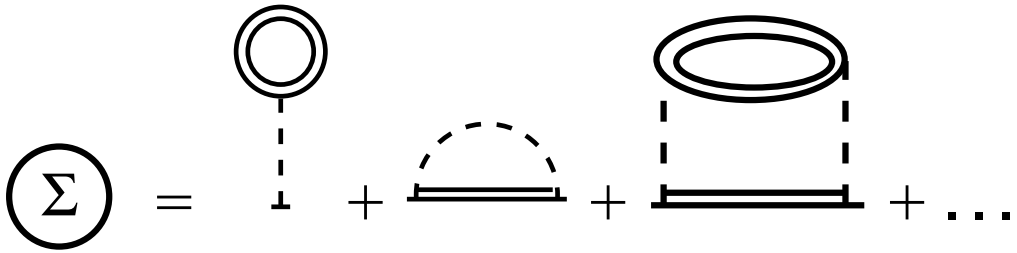


Skeleton expansion

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: $t_{ij} = t^*_{ij}\, d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||}$

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:

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

Power counting in 1/d

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

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

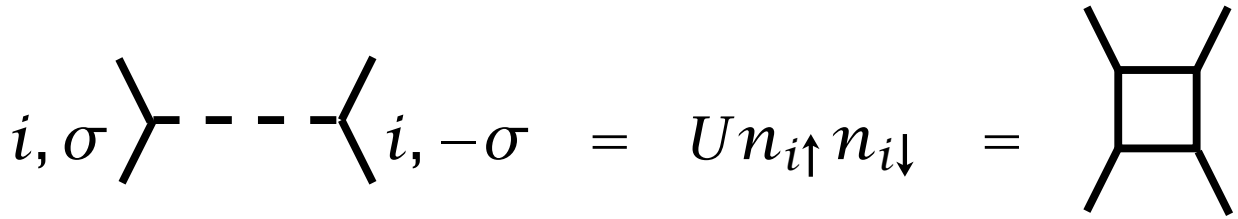
Green function:

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

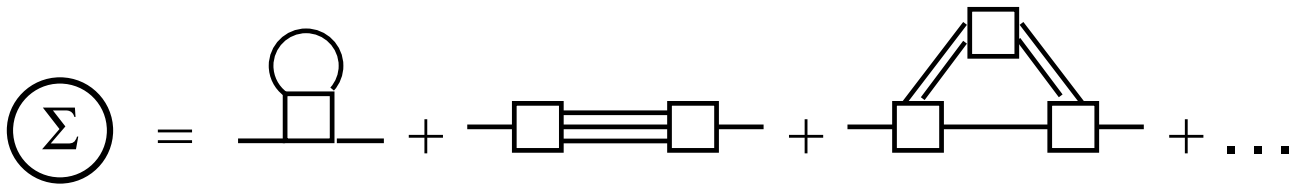
$\Rightarrow$ simplifications for Feynman diagrams!

Diagrammatic simplifications

Hugenholtz diagrams: (Hubbard model: no exchange diagrams)

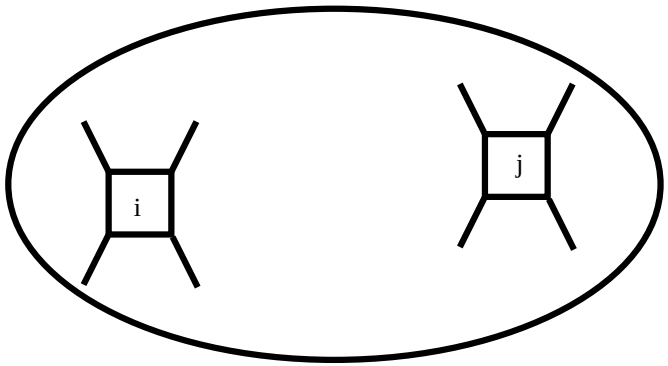


Skeleton expansion:



(0)

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

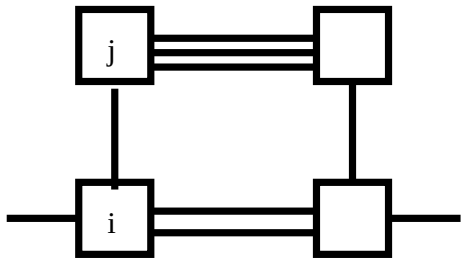


Collapse of position space diagrams

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



not skeleton

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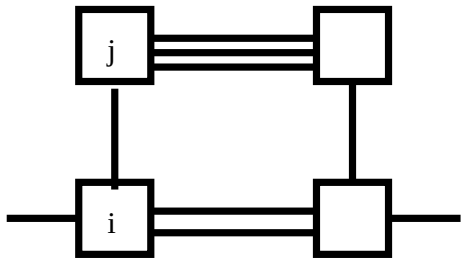

not skeleton

in $d = \infty$:

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

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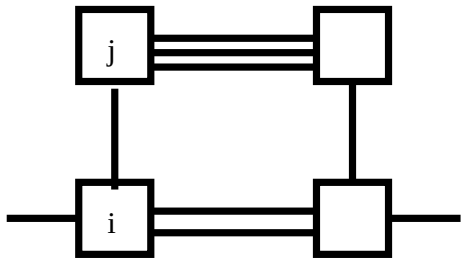

not skeleton

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:

$$G_{\boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(\omega)} = G^{(0)}_{\boldsymbol{k}\sigma}(\omega - \Sigma_\sigma(\omega))$$

- local Green function:

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

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

(later: “self-consistency equation”)

Pinning of DOS at Fermi surface

Volume of Fermi sea: unchanged by interactions [Luttinger '60, '61]

$d = 3$:

$$n = 2 \int \frac{d^d k}{(2\pi)^d} \, \Theta(\mu^{(0)} - \epsilon_{\boldsymbol{k}})$$

$$= 2 \int \frac{d^d k}{(2\pi)^d} \, \Theta(\mu - \Sigma_{\boldsymbol{k}}(0) - \epsilon_{\boldsymbol{k}})$$

shape of Fermi surface may change

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shape of Fermi surface may change

$d = \infty$: shape unchanged, $\mu = \mu^{(0)} + \Sigma(0)$

$$S(\omega) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega \, \frac{\rho(\epsilon)}{\omega + i0 + \mu - \Sigma_\sigma(\omega + i0) - \epsilon} \quad \Rightarrow \quad S(0) = \rho(\mu^{(0)})$$

spectral function is pinned at Fermi energy

[Müller-Hartmann 1989]

Non-local interactions

Coulomb interaction terms between different sites: e.g.,

$$H_{\text{density}} = \frac{V_*}{d} \sum_{\langle ij \rangle} n_i n_j$$

$$H_{\text{exchange}} = \frac{F_*}{d} \sum_{\langle ij \rangle \sigma \sigma'} c^+_{i\sigma} c^+_{j\sigma'} c_{i\sigma'} c_{j\sigma} = -\frac{2F_*}{d} \sum_{\langle ij \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \tfrac{1}{4} n_i n_j)$$

$$\text{interaction lines} \propto \frac{1}{d} \Rightarrow \text{only Hartree diagram survives}$$

[Müller-Hartmann 1989]

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[Müller-Hartmann 1989]

"Extended DMFT"

- consider quantum fluctuations of H_{density}
- $H_{\text{density}} - \langle H_{\text{density}} \rangle = O(d^{-\frac{1}{2}})$

[Si et al. '96,...]

Part III
Dynamical mean-field theory

1. Mapping onto impurity models
2. A solvable example
3. Impurity solvers
4. Multi-band systems

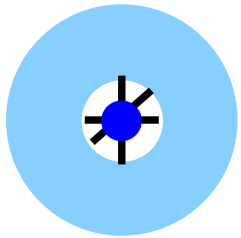
1. Mapping onto impurity models

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

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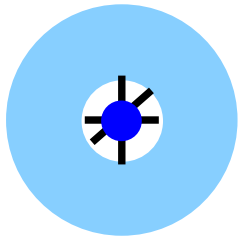

$$\mathcal{A}_2 = -U \int_0^\beta d\tau\; c_\uparrow^*(\tau) c_\uparrow(\tau) c_\downarrow^*(\tau) c_\downarrow(\tau)$$ local Hubbard interaction

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 $\mathcal{G}^{-1} = \partial_\tau - \mu$

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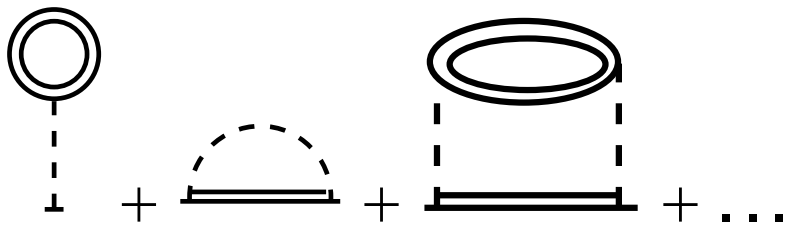
impurity Dyson equation

- skeleton expansion:

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

one site only!

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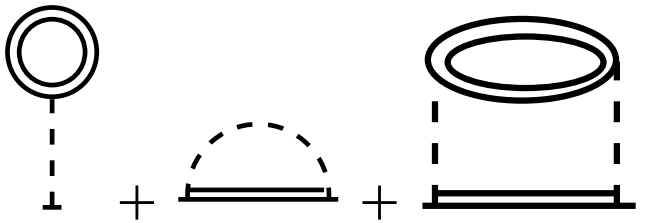
$$\tilde{\boldsymbol{\Sigma}}[\boldsymbol{G}] =$$  $$+ \ldots$$ one site only!

$$= \boldsymbol{\Sigma}[\boldsymbol{G}]$$ same as for Hubbard model in $d = \infty$!

Dynamical mean-field equations

lattice Dyson equation:

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

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

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together with

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

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

$$\Rightarrow \quad \boxed{\text{three equations for unknowns } \boldsymbol{G},\ \boldsymbol{\mathcal{G}},\ \boldsymbol{\widetilde{\Sigma}}}$$

Some simple limits

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

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

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

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

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

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

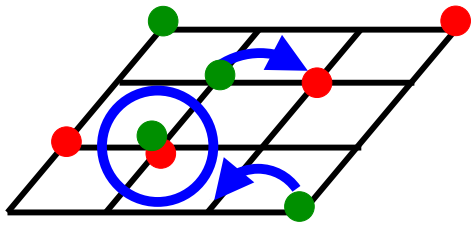
$$\Rightarrow \qquad \mathcal{G}^{-1}_\sigma(\tau) = \partial_\tau - \mu \qquad \Rightarrow \quad (3) \quad \checkmark$$

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 $T > T_c > 0$ [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:

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

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

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 $\rho_d(\epsilon)$

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skeleton functional $\Sigma_d[G_d]$:

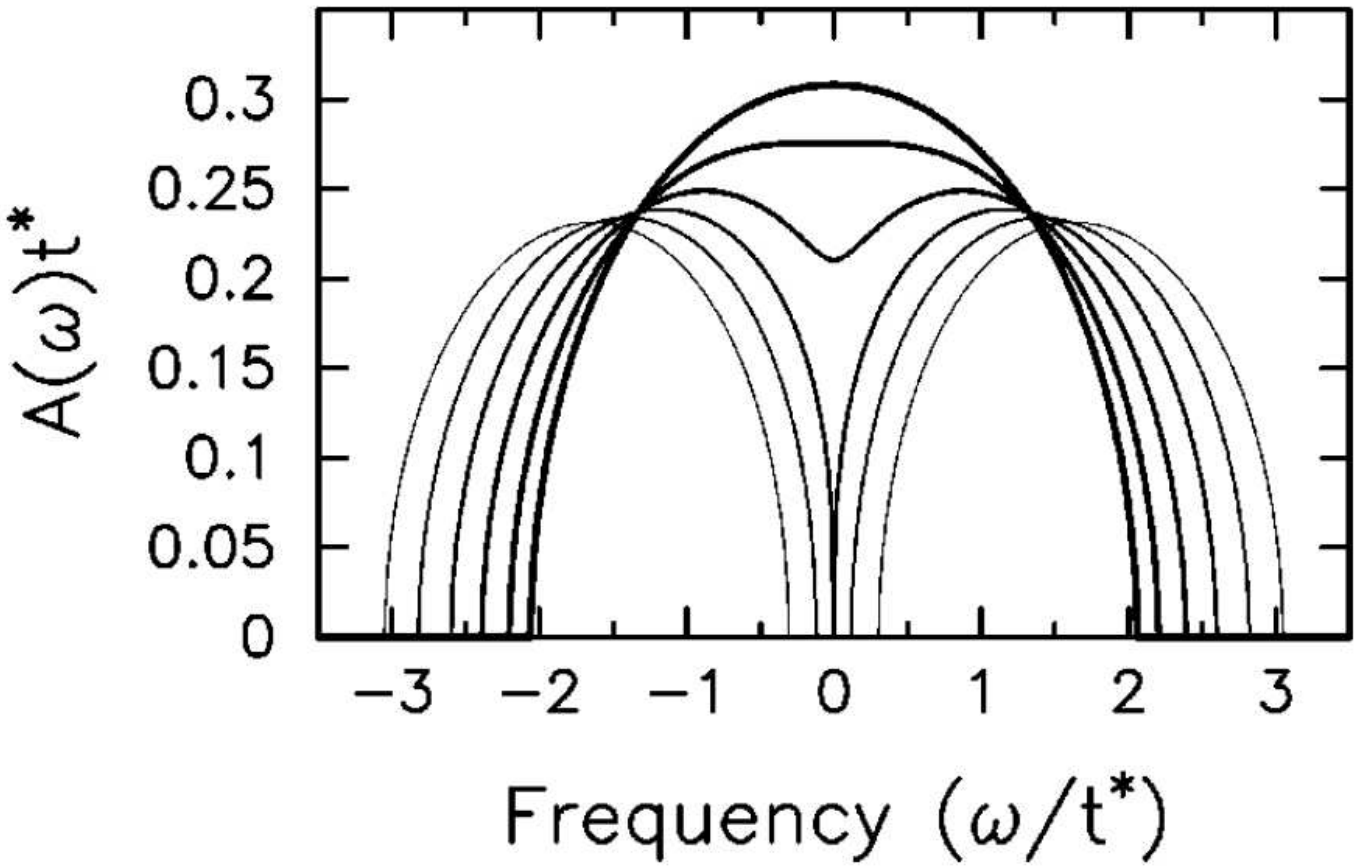
$$\Sigma_d(i\omega_n) = \frac{U}{2} - \frac{1}{2G_d(i\omega_n)} \pm \sqrt{\left(\frac{U}{2} - \frac{1}{2G_d(i\omega_n)}\right)^2 + \frac{Un_f}{G_d(i\omega_n)}}$$

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:

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

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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

QMC

Trotter decomposition of imaginary-time action, T not too small

PQMC

projection onto ground state, $T = 0$ only

NRG

logarithmic discretization of host spectrum, sites added successively

NCA

summation of a subset of Feynman diagrams

ED

exact diagonalization for small number of host sites

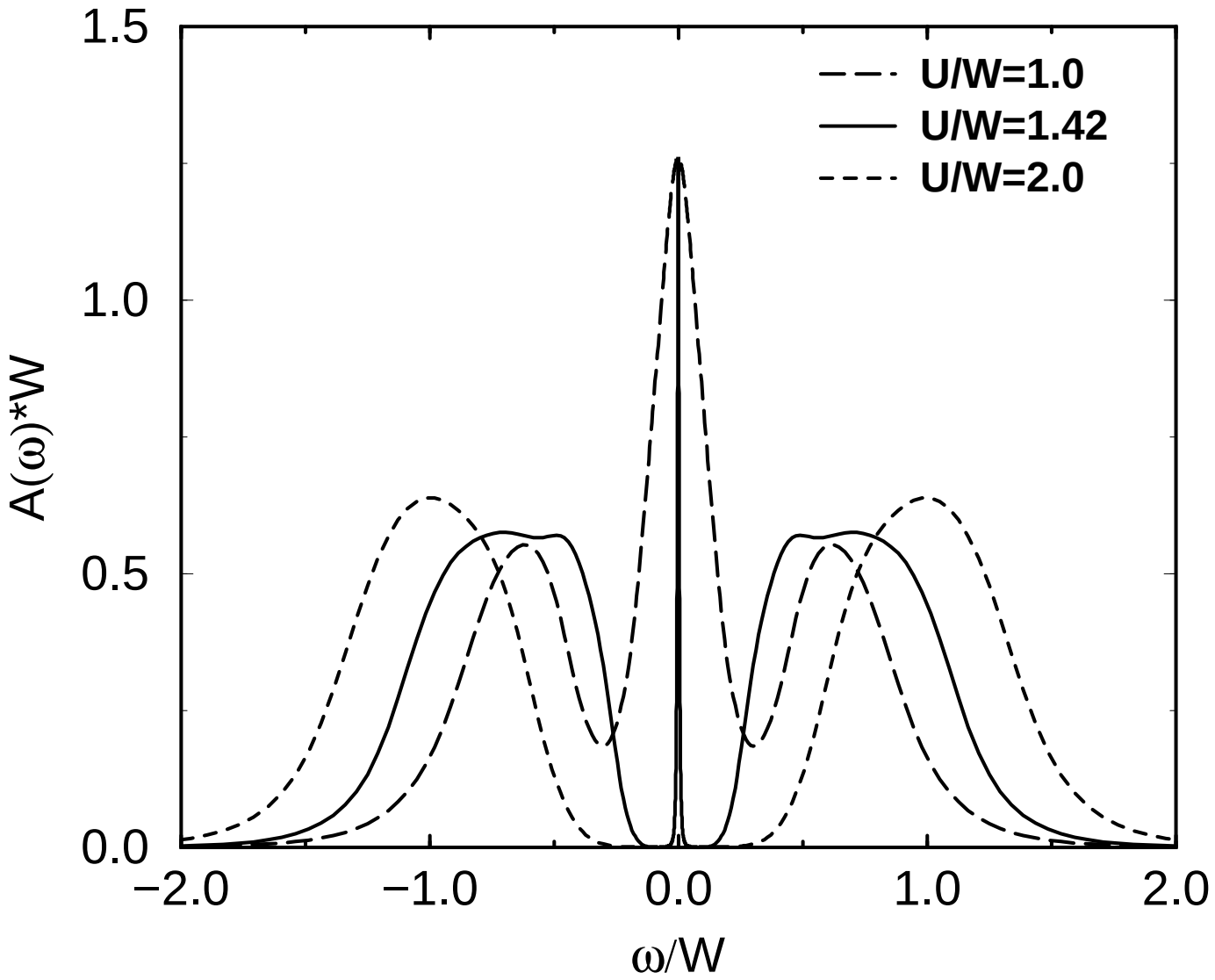
DMRG

blocks with varying number of sites, dynamical quantities available

[→ lectures]

Metal-insulator transition

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

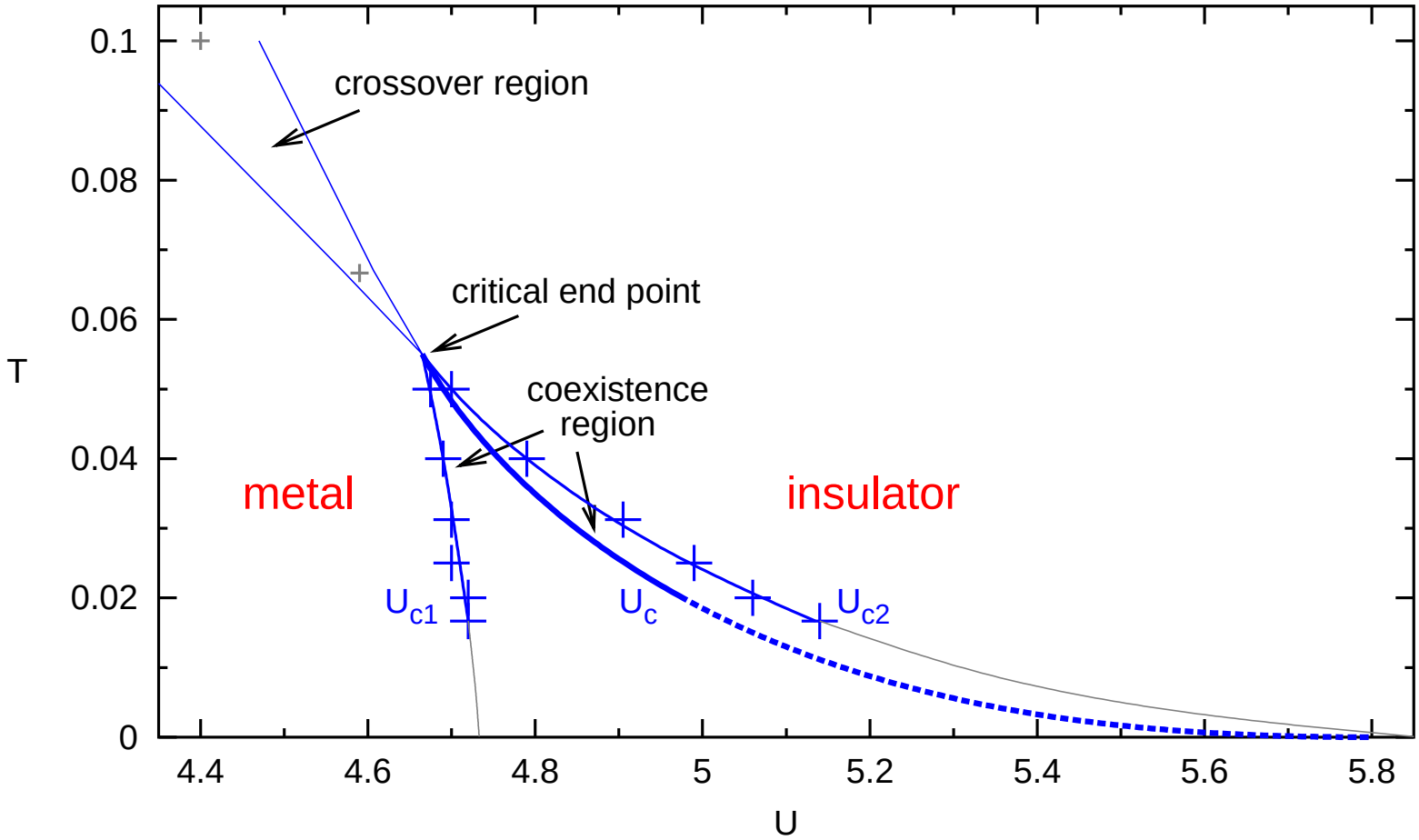


[Bulla '99]

Phase diagram

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

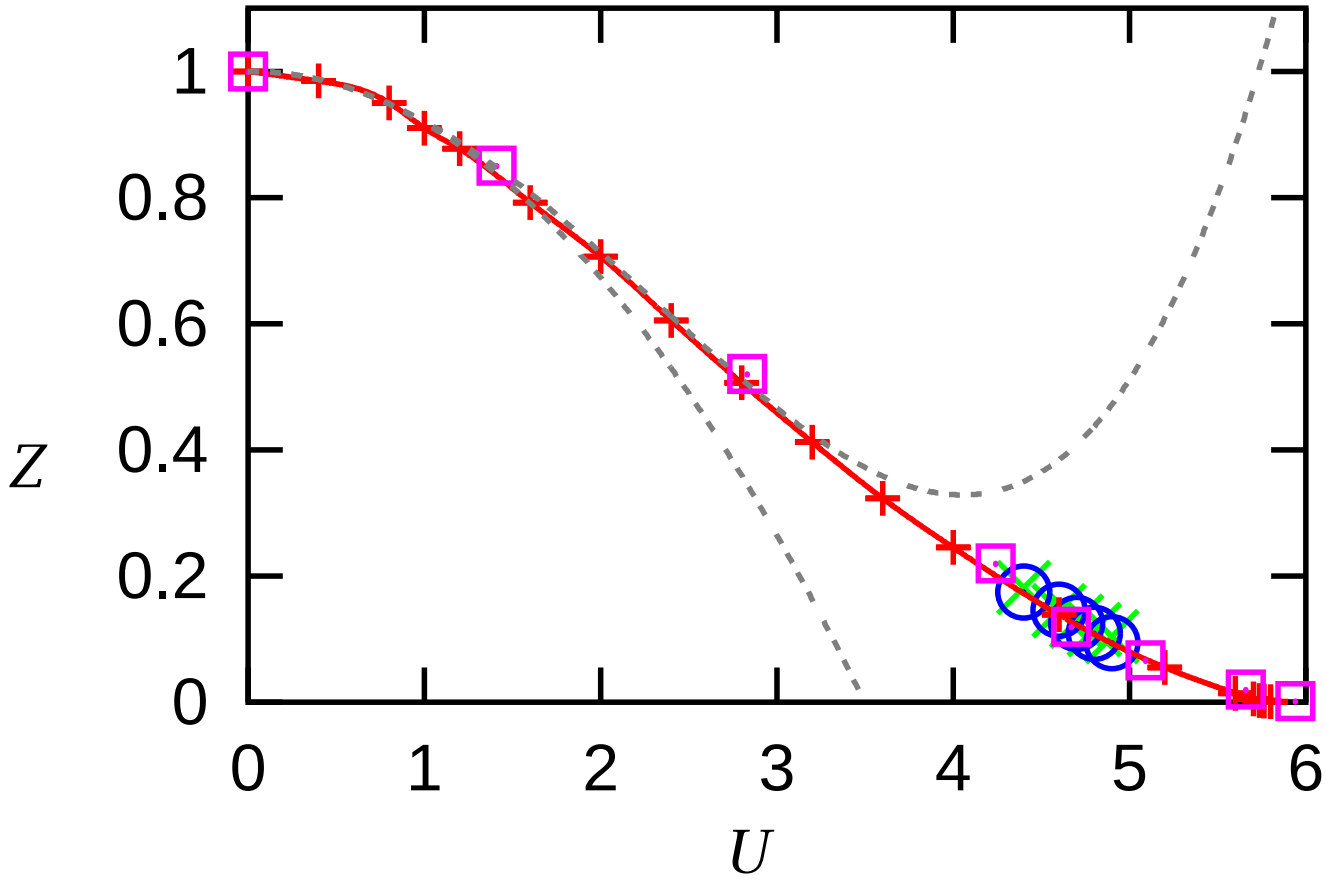
[Blümer '02]



- coexistence region $[U_{c1}; U_{c2}]$, first-order transition
- crossover above critical region

Quasiparticle weight

Hubbard model, Bethe lattice, $n = 1$, DMFT(NRG/QMC/...)



[Bulla '99, Fig. from Blümer '02]

red +: NRG

blue ∘: QMC

pink □: ED

grey line: perturbation theory

4. Multi-band systems: LDA+DMFT

LDA: Hartree-Term + ?

LDA+DMFT: include Coulomb interaction for correlated orbitals

[Anisimov et al. '97; Lichtenstein & Katsnelson '97; Liebsch & Lichtenstein '00; Nekrasov et al. '00; ...]

$$H_{\text{int}} = \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'\sigma'}}' U^{\sigma\sigma'}_{mm'} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}$$
$$- \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'}}' J_{mm'} \hat{c}^{\dagger}_{ilm\sigma} \hat{c}^{\dagger}_{ilm'\bar{\sigma}} \hat{c}_{ilm'\sigma} \hat{c}_{ilm\bar{\sigma}}$$

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$$H = H_{\mathrm{LDA}} + H_{\mathrm{int}} - H^{U}_{\mathrm{LDA}}$$

$$H_{\mathrm{int}} = \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'\sigma'}}' U^{\sigma\sigma'}_{mm'} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}$$

$$- \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'}}' J_{mm'} \hat{c}^{\dagger}_{ilm\sigma} \hat{c}^{\dagger}_{ilm'\bar{\sigma}} \hat{c}_{ilm'\sigma} \hat{c}_{ilm\bar{\sigma}}$$

H^{U}_{LDA} = already contained in LDA;
determine from *constrained LDA*

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[Anisimov et al. '97; Lichtenstein & Katsnelson '97; Liebsch & Lichtenstein '00; Nekrasov et al. '00; ...]

$$H = H_{\text{LDA}} + H_{\text{int}} - H^{U}_{\text{LDA}} = H^{0}_{\text{LDA}} + H_{\text{int}}$$

$$H_{\text{int}} = \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'\sigma'}}' U^{\sigma\sigma'}_{mm'} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}$$

$$- \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'}}' J_{mm'} \hat{c}^{\dagger}_{ilm\sigma} \hat{c}^{\dagger}_{ilm'\bar{\sigma}} \hat{c}_{ilm'\sigma} \hat{c}_{ilm\bar{\sigma}}$$

H^{U}_{LDA} = already contained in LDA;
determine from *constrained LDA*

$$H^{0}_{\text{LDA}} = \sum_{ilm, jl'm', \sigma} t^{0}_{ilm, jl'm'} \, c^{+}_{ilm\sigma} c_{jl'm'\sigma}$$

Summary

DMFT:

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

[→ lectures, talks]

Extensions: (numerical effort increases ...)

- multiband systems
- spatial fluctuations, clusters
- coupling to bosonic baths

[→ lectures, talks]

Dynamical mean-field theory

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Summer School on
Dynamical Mean Field Theory for Correlated Electrons:
Applications to Real Materials, Extensions and Perspectives

International Center for Theoretical Physics, Trieste
July 25 – August 3, 2005

Outline

Preamble

- Local-density approximation (LDA)
- Dynamical mean-field theory (DMFT)
- LDA + DMFT

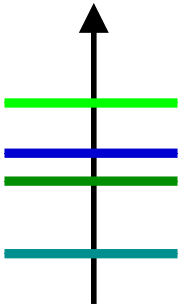
I. Introduction
   - Green functions
   - Useful concepts

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

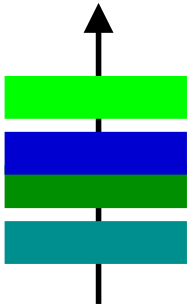
III. Dynamical mean-field theory
   - Mapping onto impurity models
   - A solvable example
   - Impurity solvers
   - Multiband systems

Preamble

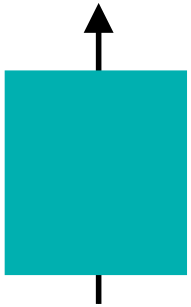
condensed matter: electrons in a ionic potential



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

- important for strongly localized 3d, 4d, 4f, ... electrons
  $\Rightarrow$ large overlap $V_{\alpha\beta\gamma\delta} = \langle\alpha\beta|V_{\text{ee}}|\gamma\delta\rangle$
- Bloch theorem applicable, but $\psi_{n\boldsymbol{k}}(\boldsymbol{r})$ unknown
- unsolvable quantum-mechanical many-body problem

Density functional theory

Hohenberg & Kohn ('64):

$$E_0 = E[\rho] = \text{functional of electron density } \rho(\boldsymbol{r})$$

$$= \underbrace{E_{\text{kin}}[\rho] + E_{\text{ion}}[\rho] + E_{\text{Hartree}}[\rho]}_{\text{known contributions}} + \underbrace{E_{\text{xc}}[\rho]}_{\text{unknown}}$$

Kohn & Sham ('65): $\rho(\boldsymbol{r}) = \sum_i |\varphi_i(\boldsymbol{r})|^2$

$$\Big[-\frac{\hbar^2}{2m_e}\Delta + V_{\text{eff}}(\boldsymbol{r}) \Big]\varphi_i(\boldsymbol{r}) = \varepsilon_i \varphi_i(\boldsymbol{r}) \qquad \text{Kohn-Sham equations}$$

$$V_{\text{eff}}(\boldsymbol{r}) = V_{\text{ion}}(\boldsymbol{r}) + \int d^3r'\, V_{\text{ee}}(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}') + \frac{\delta E_{\text{xc}}[\rho]}{\delta \rho(\boldsymbol{r})}$$

Local Density Approximation

LDA: use $E_{\mathrm{xc}}[\rho]$ of the homogeneous electron gas ($\rho = \text{const}$)

- solve Kohn-Sham equations by iteration

$$\rho(\boldsymbol{r}) \;\Rightarrow\; V_{\mathrm{eff}}(\boldsymbol{r}) \;\Rightarrow\; \{\varepsilon_i,\ \varphi_i(\boldsymbol{r})\} \;\Rightarrow\; \rho(\boldsymbol{r}) \;\Rightarrow\; \ldots$$

- basis-dependent! (LMTO, [F]LAPW, ASW, ...)

very successful!

- advantages: provides bandstructure, intuitive one-particle picture
- problem: only certain part of V_{ee} taken into account
  $\Rightarrow$ cannot describe strongly correlated systems

Hamilton-Operator:

$$H_{\mathrm{LDA}} = \sum_{ilm,jl'm',\sigma} t_{ilm,jl'm'}\, c^{+}_{ilm\sigma} c_{jl'm'\sigma} \qquad (\ t_{ilm,jl'm'} \leftrightarrow \epsilon_{\boldsymbol{k}lm}\ )$$

Models for correlated electrons

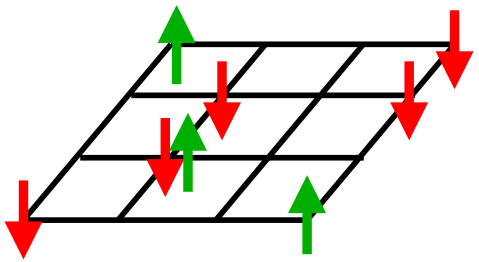
interacting electrons: charge and spin degrees of freedom

$$H = \sum_{ij\alpha\beta\sigma} t_{ij}^{\alpha\beta}\, c^{+}_{i\alpha\sigma} c_{j\beta\sigma} \;+\; \sum_{\substack{ijkl \\ \alpha\beta\gamma\delta\sigma\sigma'}} V_{ijkl}^{\alpha\beta\gamma\delta}\, c^{+}_{i\alpha\sigma} c^{+}_{j\beta\sigma'} c_{l\delta\sigma'} c_{k\gamma\sigma}$$

$\Rightarrow$ metals, insulators, magnetism, superconductivity, ...

Hubbard model: e.g. 1 band, only

$U = V_{iiii}$



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

Heisenberg model: $H_{\text{Hubbard}} \overset{U \gg |t_{ij}|}{\longrightarrow} H_{\text{Heisenberg}}$ mit $J_{ij} = \frac{4t_{ij}^2}{U}$

$$H_{\text{Heisenberg}} = \sum_{ij} J_{ij}\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

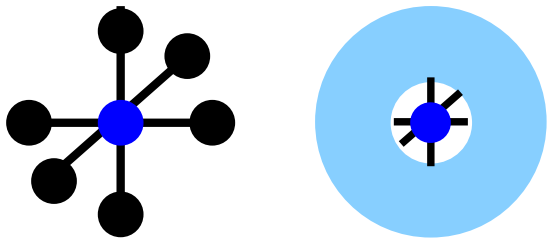
localized q.m. spins

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, ...]

LDA + DMFT

DMFT:

- exact for $d = \infty$
- "thermodynamically consistent", "conserving approximation"
- extensions: many bands, clusters, non-local interactions, ...
- impurity solvers: NRG, QMC, PQMC, ED, NCA... [→ lectures]

LDA+DMFT: [Anisimov et al. '97; Lichtenstein & Katsnelson '97; Liebsch & Lichtenstein '00; Nekrasov et al. '00; ...]

- use LDA band structure (as input, or self-consistently)
- on-site ("Hund's rule") interactions
- combine with DMFT, cluster extensions, ... [→ lectures]

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 $\alpha\beta(\tau)$:

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

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:

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

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

$$= \frac{1}{Z}\sum_{n,m} \langle n|c_\beta^+|m\rangle\langle m|c_\alpha|n\rangle \ (e^{-\beta E_m} - e^{-\beta E_n})\ \delta(\omega - (E_n - E_m))$$

local Green function:

$$G_{ii\sigma}(\omega) = G_\sigma(\omega) = \frac{1}{L}\sum_{\boldsymbol{k}} G_{\boldsymbol{k}\sigma}(\omega) \qquad (\mathrm{Im}\omega \neq 0)$$

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

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

Free particles

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

$$\Rightarrow \qquad G^{(0)}_{k\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_k}$$

local Green function:

$$G_\sigma(\omega) = \frac{1}{L} \sum_k \frac{1}{\omega + \mu - \epsilon_k} \qquad = \int_{-\infty}^{\infty} d\epsilon \frac{\rho(\epsilon)}{\omega + \mu - \epsilon}$$

$$S_\sigma(\omega) = \frac{1}{L} \sum_k \delta(\omega + \mu - \epsilon_k) \qquad = \rho(\omega + \mu)$$

with free density of states (which characterizes ϵ_k)

$$\rho(\omega) = \sum_k \delta(\omega - \epsilon_k)$$

Self-energy

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

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

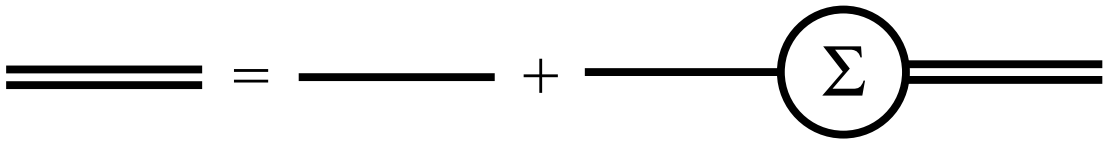
$$G_{\boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_{\boldsymbol{k}\sigma}(\omega)}$$

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

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

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

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:

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

2. Useful concepts

if perturbation theory valid (T=0): e.g., for Fermi liquids [Luttinger '60]

$$\mathrm{Im}\Sigma_{\boldsymbol{k}}(\omega) \overset{\omega \to 0}{\sim} -\mathrm{sgn}(\omega)\, C_{\boldsymbol{k}}\, \omega^2 \qquad (C_{\boldsymbol{k}} \geq 0)$$

poles in Green function satisfy

$$\omega - (\epsilon_{\boldsymbol{k}} - \mu) - \mathrm{Re}\Sigma_{\boldsymbol{k}}(\omega) + i\mathrm{sgn}(\omega)\, C_{\boldsymbol{k}}\, \omega^2 = 0$$

real part vanishes if

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

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

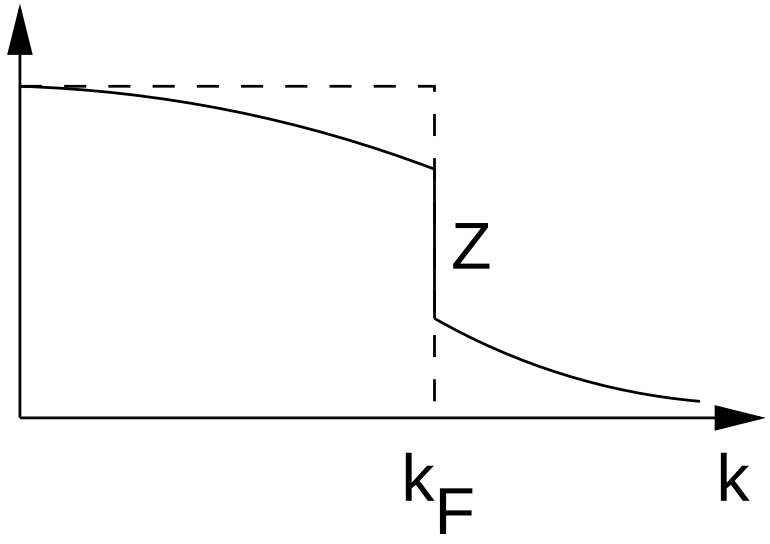
$$G_{\boldsymbol{k}}(\omega) \approx \frac{Z_{\boldsymbol{k}}}{\omega - E_{\boldsymbol{k}} + i\tau_{\boldsymbol{k}}^{-1}}$$

Quasiparticles

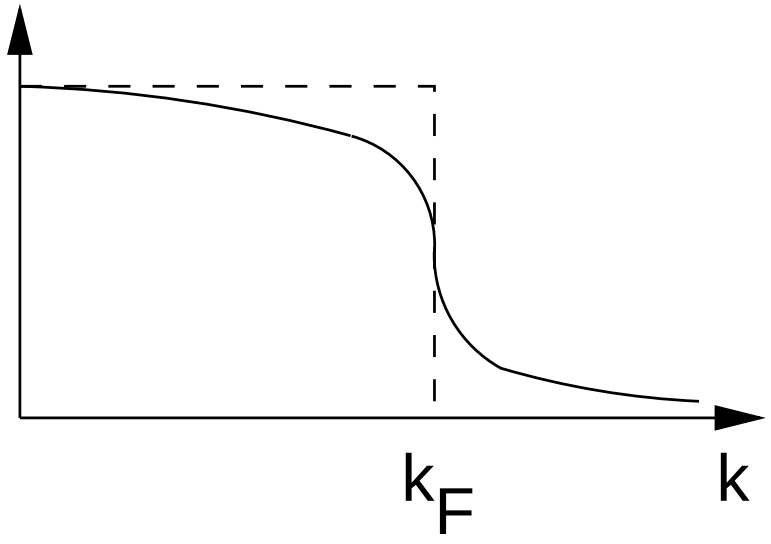
$$Z_{\boldsymbol{k}} = \frac{1}{1 - \mathrm{Re}\Sigma'_{\boldsymbol{k}}(E_{\boldsymbol{k}})}$$ quasiparticle weight

$$\tau_{\boldsymbol{k}} = 1/E^2_{\boldsymbol{k}}$$ quasiparticle lifetime

- quasiparticles stable for $E_{\boldsymbol{k}}$ close enough to Fermi surface
- Fermi energy does not change due to interactions [Luttinger '61]
- Z is related to jump in momentum distribution (absent in $D = 1$)



$D \geq 2$



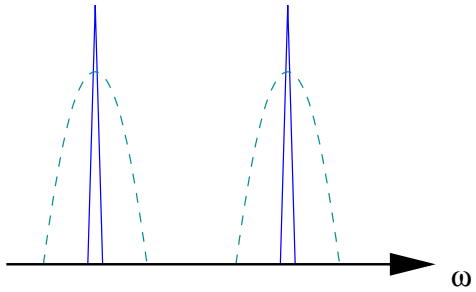
$D = 1$

Hubbard bands, Mott transition

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

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

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

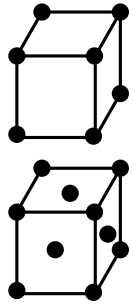
1. Free fermions
   - Scaling of hopping amplitudes
   - Density of states
   - Generalized lattices

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

1. Free fermions

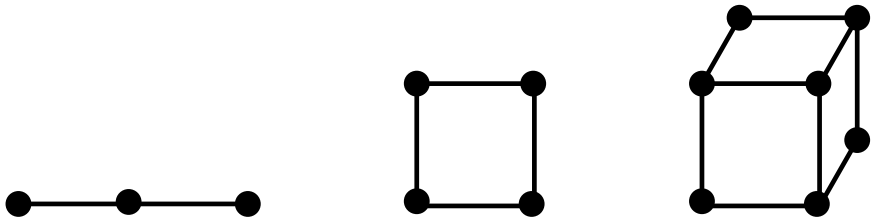
crystal lattices in $d = 3$:

- 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:

$$\boldsymbol{e}_1 = (1, 0, 0, \dots \quad)$$
$$\boldsymbol{e}_2 = (0, 1, 0, \dots \quad)$$
$$\dots = \dots$$
$$\boldsymbol{e}_d = (0, 0, 0, \dots, 1)$$

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:

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

Scaling of hopping amplitudes

elegant answer: [Metzner & Vollhardt '89]

- $X_d := \sum_{i=1}^{d} \cos k_i$
- random variables $k_i \in [-\pi; \pi]$ (mean=0, variance=1)

central limit theorem:

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

density of states:

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

1/d corrections

Fourier transform:

[Müller-Hartmann '89]

$$\Phi(s) = \int_{-\infty}^{\infty} d\epsilon\, e^{is\epsilon}\, \rho(\epsilon) = \int \frac{d^d k}{(2\pi)^d}\, e^{is\epsilon_{\boldsymbol{k}}} \qquad \text{factorizes!}$$

$$= \left[\int_{-\pi}^{\pi} \frac{dk}{2\pi}\, \exp\left(-\frac{2ist_*}{\sqrt{2d}}\, \cos k\right)\right]^d = J_0\left(\frac{2t_*}{\sqrt{2d}}\right)^d$$

$$= \left[1 - \frac{t_*^2 s^2}{2d} + O\left(\frac{1}{d}\right)\right]^d = \exp\left[-\frac{t_*^2 s^2}{2} + O\left(\frac{1}{d}\right)\right]$$

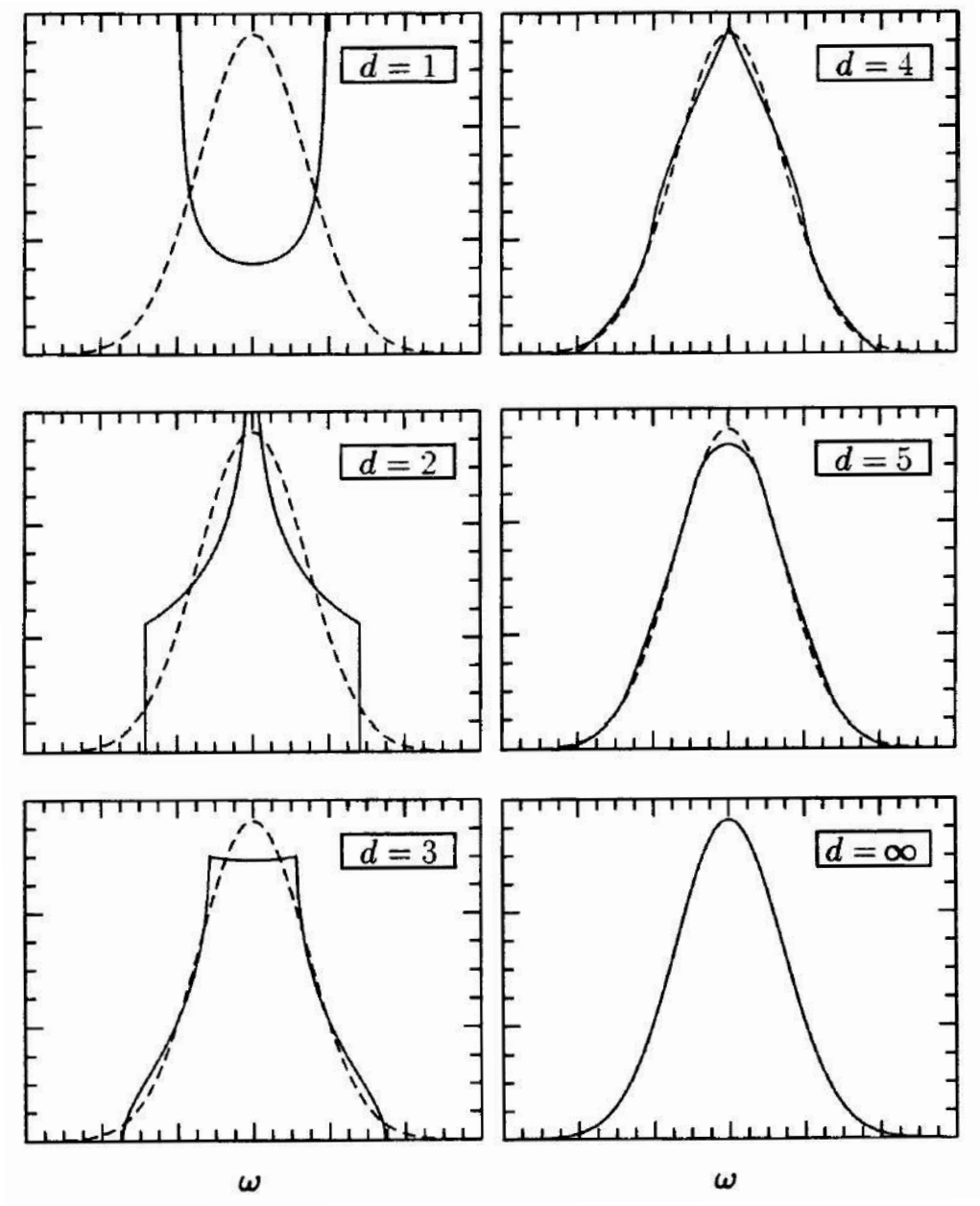
inverse transform:

$$\rho(\epsilon) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi}\, e^{-is\epsilon}\, \Phi(s)$$

$$= \frac{1}{2\pi|t_*|}\, \exp\left[-\frac{\epsilon^2}{2t_*^2} + \frac{1}{16d}\left(3 - \frac{6\epsilon^2}{t_*^2} - \frac{6\epsilon^4}{t_*^4}\right) + O\left(\frac{1}{d^2}\right)\right]$$

Density of states

$\rho(\omega)$



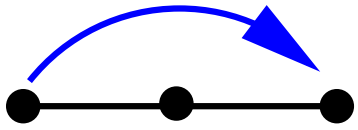
[Vollhardt '93]

Beyond nearest neighbors

[Müller-Hartmann '89]

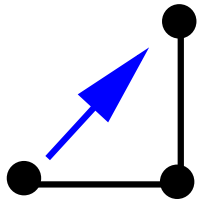
in general: $t_{ij} \propto \dfrac{1}{\sqrt{\#\text{ sites reached}}}$

hopping along axes: $\epsilon_{\boldsymbol{k}}^{\text{axes}} = \sum_{m \geq 1} \left(\dfrac{-2t_*^{(m)}}{\sqrt{2d}} \right) \sum_i \cos m k_i$



$$\boxed{\rho(\epsilon) \propto \exp\left(-\frac{\epsilon^2}{2t_{\text{eff}}^2} \right)} \qquad \text{with} \quad t_{\text{eff}} = \sqrt{t_*^{(1)} + t_*^{(2)} + \ldots}$$

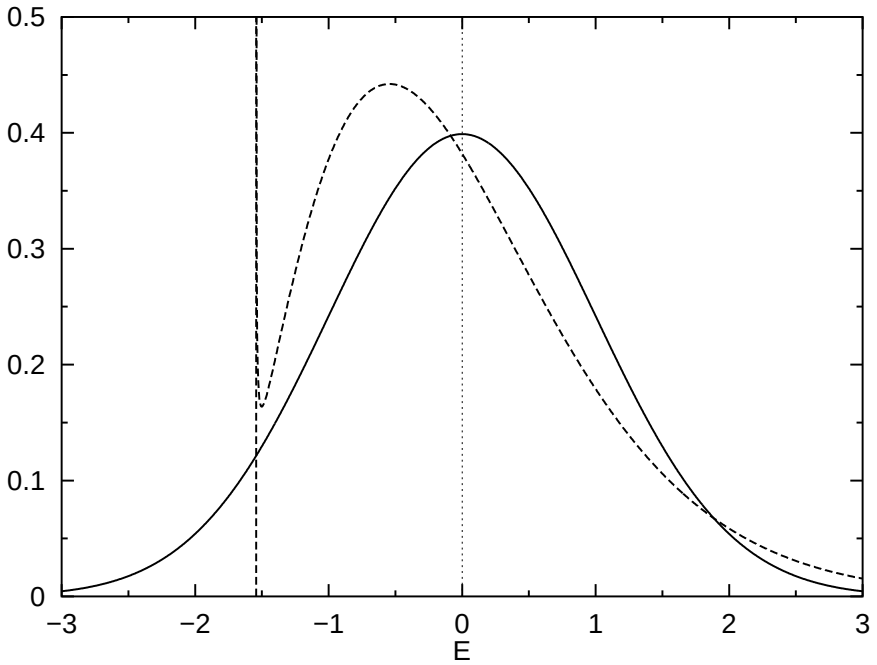
hopping to next-nearest neighbors: $\epsilon_{\boldsymbol{k}}^{\text{NNN}} \sim t' \left(\sum_i \cos k_i \right)^2$



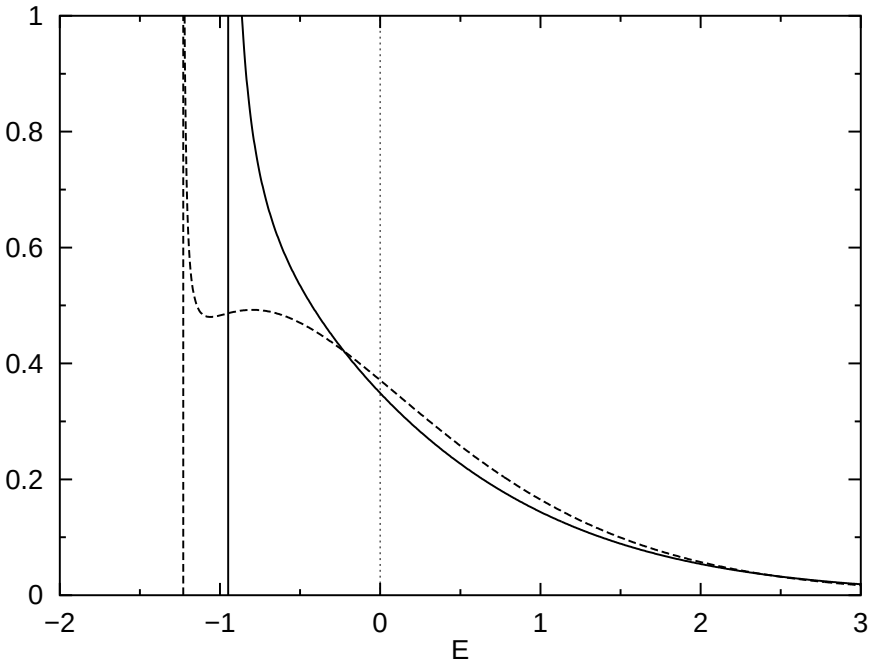
$$\boxed{\rho(\epsilon) \propto \frac{\cosh(E/a^2)\, \exp(-E^2/2a^2)}{E}} \qquad E = \sqrt{1 - 2a\epsilon + a^2}, \qquad a = \frac{\sqrt{2}t'_*}{t_*}$$

Density of states

NN and NNN hopping: $a = 2t'_*/t_*$



$a = 0, a = -0.35$



$a = -0.47, a = -0.71$

[Schlipf '98]

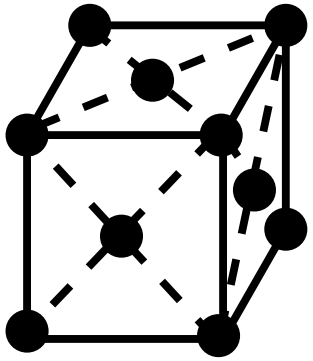
- asymmetric for $t'_* \neq 0$
- square-root singularity at band-edge!

Generalized fcc lattice

NN hopping
on fcc lattice

$\equiv$

NNN hopping
on simple cubic lattice



$$\rho(\epsilon) \propto \frac{e^{-(\epsilon - \epsilon_{\text{min}})/t_*}}{\sqrt{\epsilon - \epsilon_{\text{min}}}} \quad \text{for} \quad \epsilon > \epsilon_{\text{min}} = -\frac{t_*}{\sqrt{2}}$$

- square-root singularity at band-edge
- small energy cost for spin-polarized states

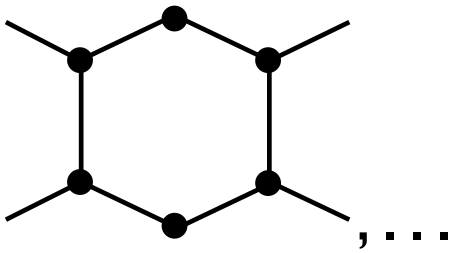
  $\Rightarrow$ favors ferromagnetism

[Müller-Hartmann '91;Ulmke '98; Wahle et al. '98, Vollhardt et al. '99]

Other crystal lattices

honeycomb, diamond, . . . , hyperdiamond lattice: [Sanotoro et al. '93]

$$\rho(\epsilon) \propto |\epsilon|\, e^{-\frac{\epsilon^2}{2t_*^2}}$$



,...

- no perfect nesting!
- antiferromagnetism suppressed

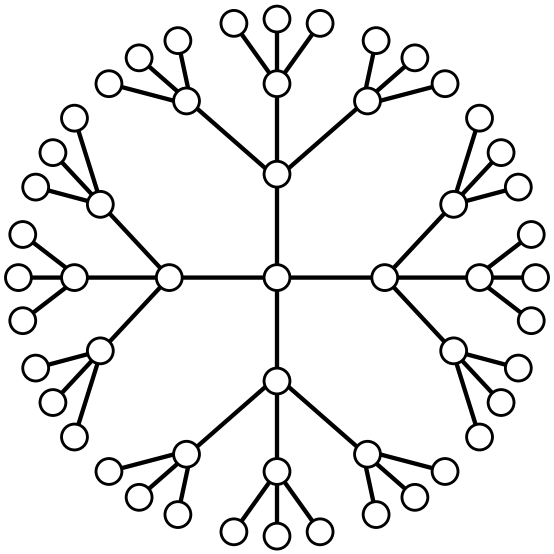
Lorentzian density of states: [Georges et al. '96]

$$\epsilon_{\boldsymbol{k}} = \frac{t_*}{d} \sum_{i=1}^{d} \cot |k_i| \quad \Rightarrow \quad \boxed{\rho(\epsilon) = \frac{1}{\pi} \frac{|t_*|}{t_*^2 + \epsilon^2}}$$

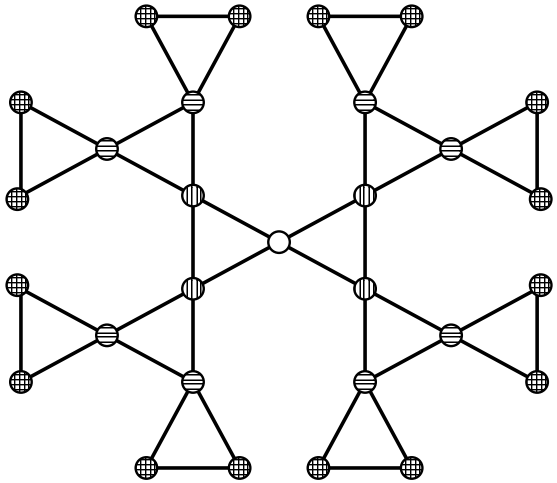
- $E_{\text{kin}} = \int_{-\infty}^{\epsilon_F} d\epsilon\, \rho(\epsilon) = \infty \quad \Rightarrow$ M.-I.-transition at $U_c = \infty$

Recursively defined lattices

Bethe lattice



Husimi cactus



- tree-like structure, Z nearest neighbors
- models for amorphous solids
- no Bloch theorem, no Brillouin zone

- RPE, . . . [Brinkman & Rice '70, Chen et al. '74, Economou '90, Mahan '01]
- algebraic methods [Eckstein et al. '04, Kollar et al. '05]

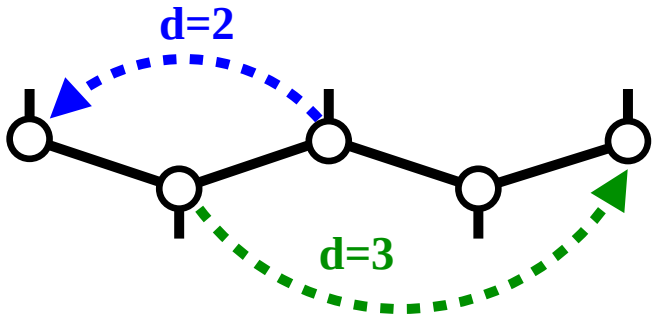
Operator identities

hopping with d steps:

$$H_r = \sum_{d_{ij}=r} c_i^+ c_j$$

$H_1 =$ NN hopping

$$\tilde{H}_r = \frac{H_r}{(Z-1)^{r/2}}, \qquad t_r^* = \frac{t_r^*}{(Z-1)^{r/2}}$$



operator identities for Bethe lattice:

$$H_2 = (H_1)^2 - Z, \ \ldots, \qquad \Rightarrow \qquad \boxed{\sum_{r=0}^{\infty} \tilde{H}_r \, x^r = \frac{1 - x^2/(Z-1)}{1 - x\tilde{H}_1 + x^2}}$$

- $H_{\text{kin}} = \epsilon(\tilde{H}_1) \quad \Rightarrow \quad H_{\text{kin}}|\lambda\rangle = \epsilon(\lambda)|\lambda\rangle$
- $\epsilon(\lambda)$ = "dispersion" on interval $-2 \le \lambda \le 2$

NN and NNN hopping

for NN hopping ($Z = \infty$):

$$\rho_1(\lambda) = \frac{1}{2\pi}\sqrt{4-\lambda^2}$$

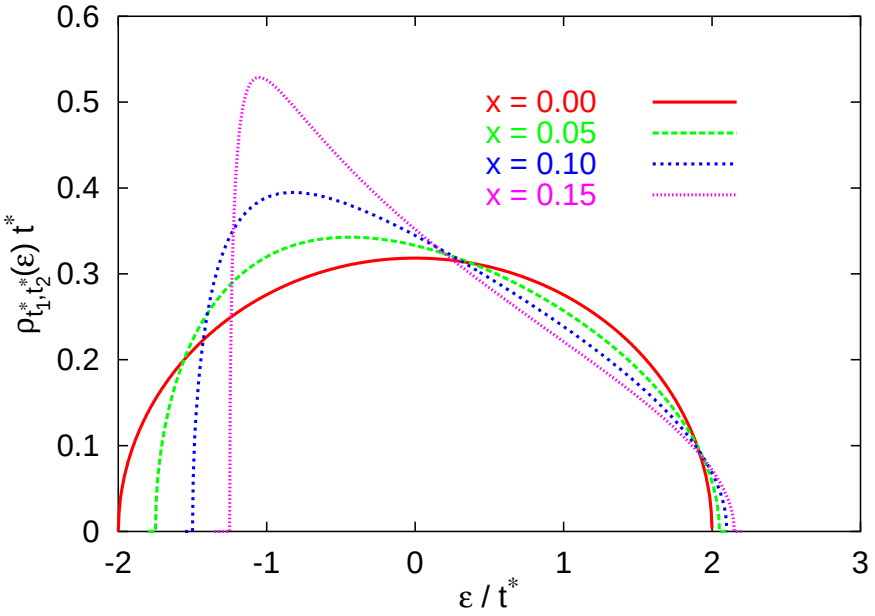
for any $H_{\text{kin}} = \epsilon(\tilde{H}_1)$:

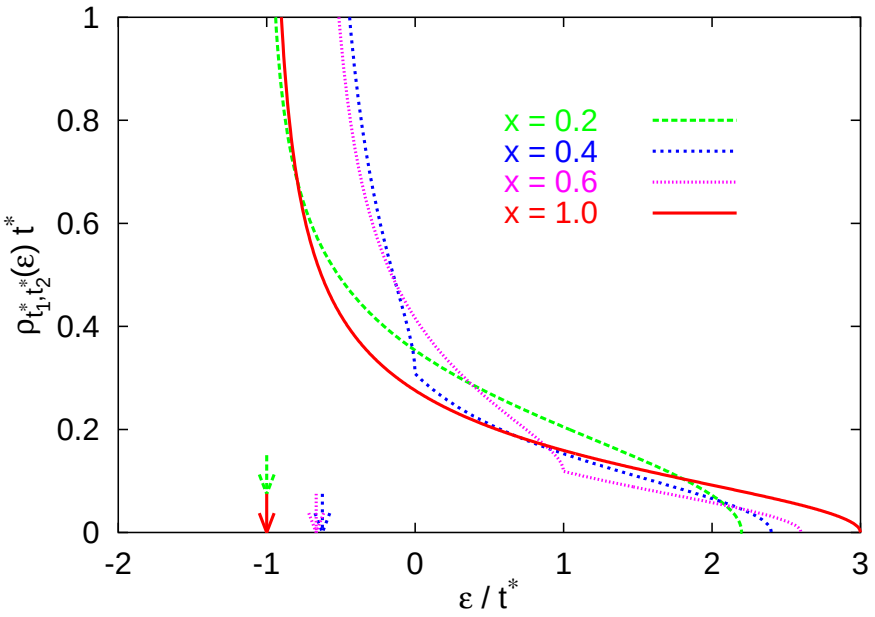
$$\rho(\epsilon) = \int_{-2}^{2} d\lambda\, \rho_1(\lambda)\, \delta(\epsilon - \epsilon(\lambda))$$

for NN and NNN hopping:

$$\epsilon(\lambda) = \text{const} + t_1^*\lambda + t_2^*\lambda^2$$

$$x = \frac{t_2^*}{|t_1^*|+|t_2^*|}$$





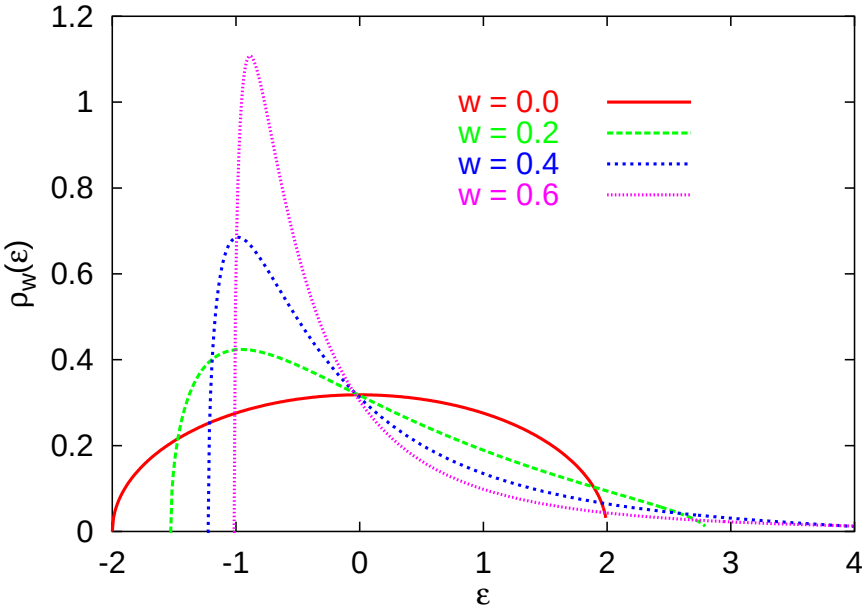
DOS for long-range hopping

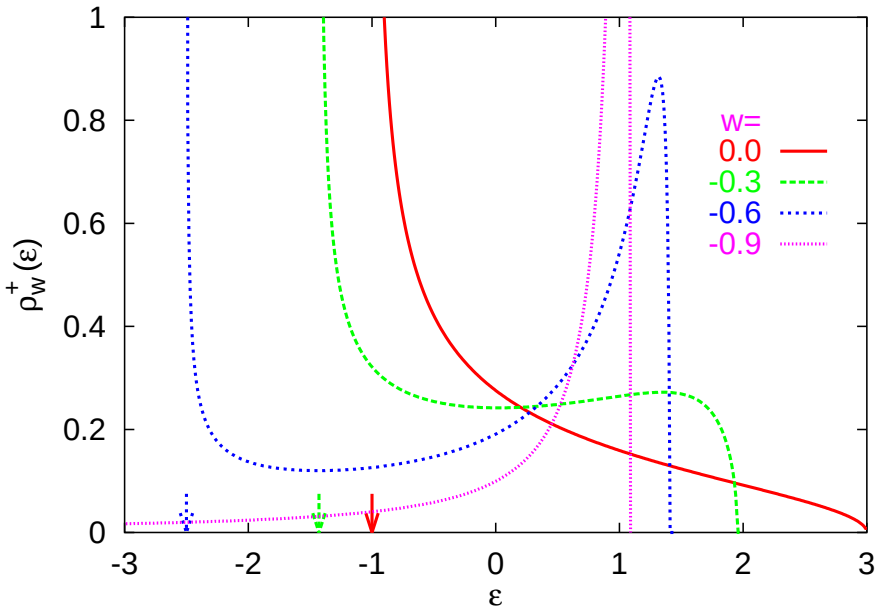
$$t_r^* \propto \exp(-\text{const} \cdot d)$$

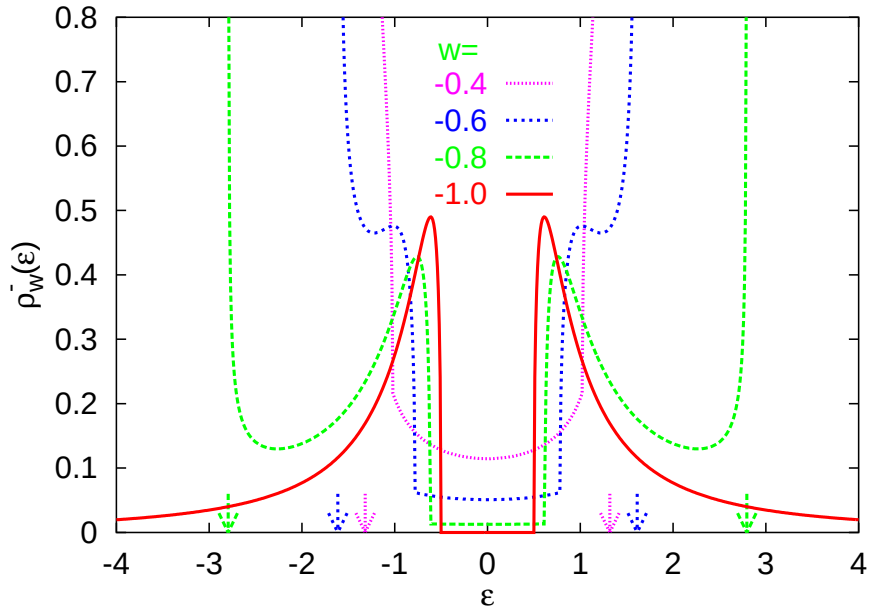
$$H_w = \sum_r w^{r-1} \tilde{H}_r$$

$$H_w^+ = \sum_r w^{r-1} \tilde{H}_{2r}$$

$$H_w^- = \sum_r w^{r-1} \tilde{H}_{2r-1}$$







Lattice representation of density of states

1-particle quantities:

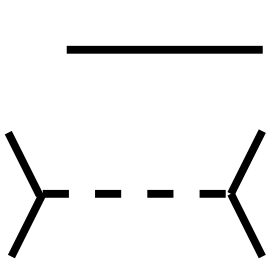
- e.g., thermodynamics, Green function, ...
- in $d = \infty$ only $\rho(\epsilon)$ enters (instead of $\epsilon_{\boldsymbol{k}}$)
- simply use $\rho(\epsilon)$ of finite-d system (e.g., LDA)

2-particle quantities, ...:

- e.g., correlation functions, symmetry-broken phases, ...
- need lattice with hopping amplitudes t_r^*
- any $\rho(\epsilon)$ can be represented for $Z \to \infty$
  - on hypercubic lattice [Blümer '02]
  - on Bethe lattice [Eckstein et al. '04]

2. Many-body theory

Feynman diagrams for Green functions:

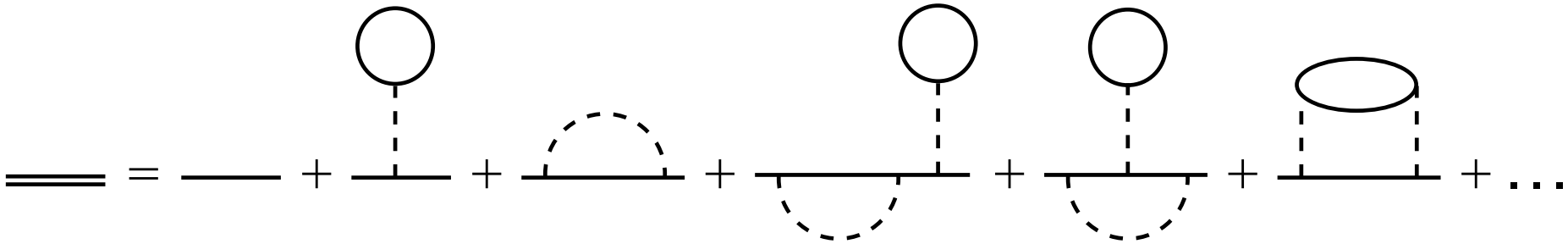


= non-interacting Green function line $\boldsymbol{G}^{(0)}$

= interaction vertex

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

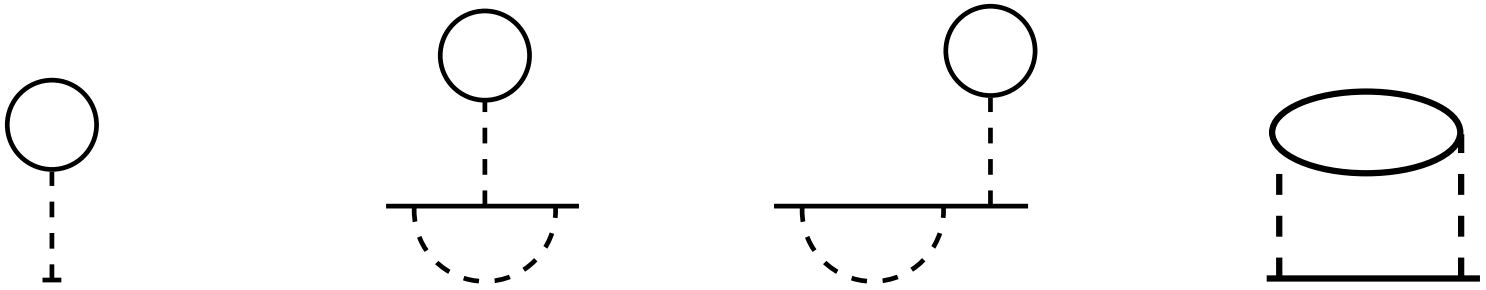
perturbation expansion:



Self-energy

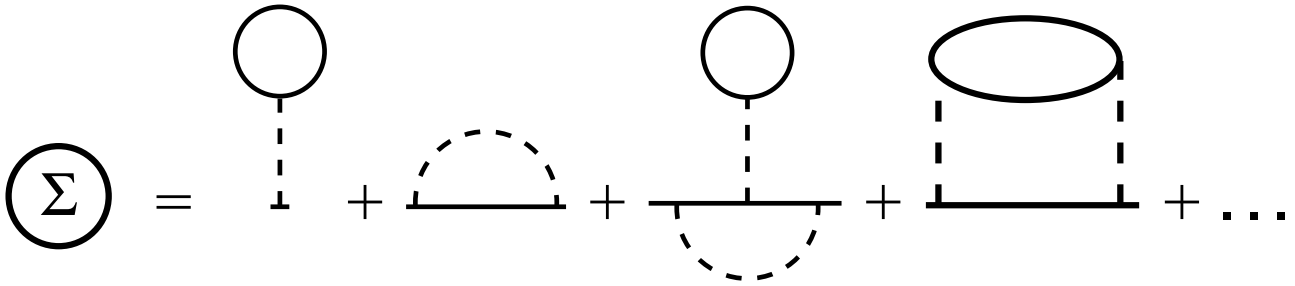
proper self-energy diagrams:

- external vertex amputated
- cannot be cut in two pieces



proper proper not proper proper

self-energy:

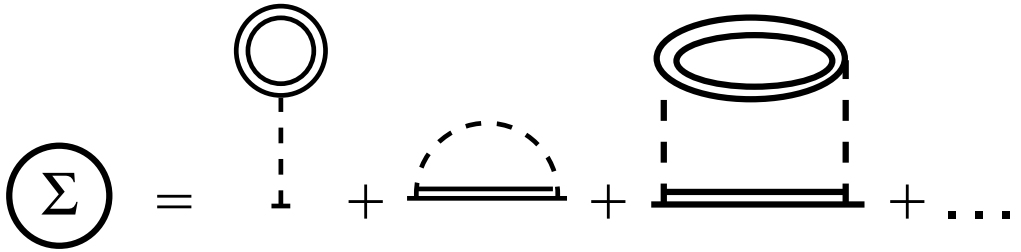


Skeleton expansion

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:

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

Green function:

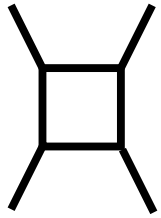
$$G_{ij\sigma}(\omega) = O(d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||}), \qquad G_{ii\sigma}(\omega) = O(d^0)$$

$\Rightarrow$ simplifications for Feynman diagrams!

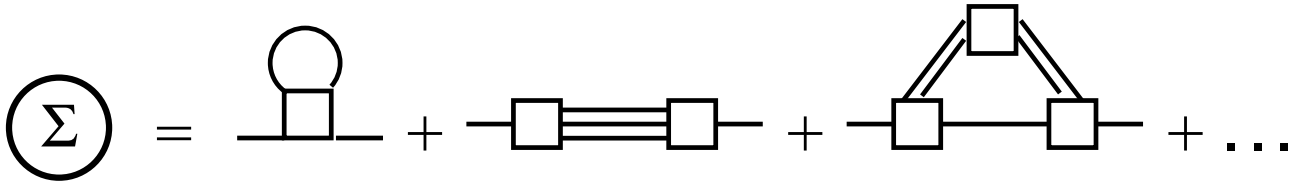
Diagrammatic simplifications

Hugenholtz diagrams: (Hubbard model: no exchange diagrams)

$$i,\sigma \;\rangle\!\!-\!\!-\!\!-\!\!\langle\; i,-\sigma \;=\; U n_{i\uparrow} n_{i\downarrow} \;=$$

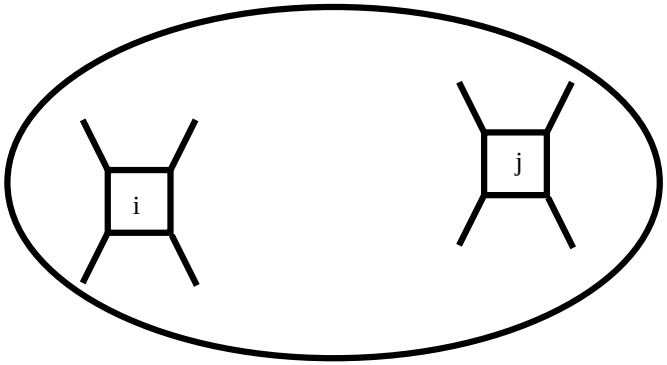


Skeleton expansion:



(1)

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

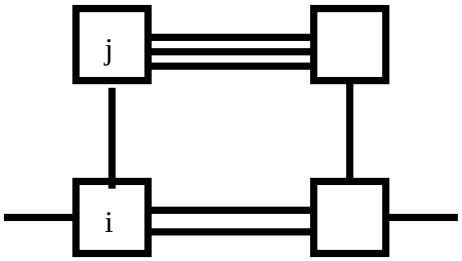


Collapse of position space diagrams

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



not skeleton

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:

$$G_{\boldsymbol{k}\sigma}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(\omega)} = G^{(0)}_{\boldsymbol{k}\sigma}(\omega - \Sigma_\sigma(\omega))$$

- local Green function:

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

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

(later: “self-consistency equation”)

Pinning of DOS at Fermi surface

Volume of Fermi sea: unchanged by interactions [Luttinger '60, '61]

$d = 3$:

$$n = 2 \int \frac{d^d k}{(2\pi)^d} \, \Theta(\mu^{(0)} - \epsilon_{\boldsymbol{k}})$$

$$= 2 \int \frac{d^d k}{(2\pi)^d} \, \Theta(\mu - \Sigma_{\boldsymbol{k}}(0) - \epsilon_{\boldsymbol{k}})$$

shape of Fermi surface may change

$d = \infty$: shape unchanged, $\mu = \mu^{(0)} + \Sigma(0)$

$$S(\omega) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega \, \frac{\rho(\epsilon)}{\omega + i0 + \mu - \Sigma_\sigma(\omega + i0) - \epsilon} \quad \Rightarrow \quad S(0) = \rho(\mu^{(0)})$$

spectral function is pinned at Fermi energy

[Müller-Hartmann 1989]

Non-local interactions

Coulomb interaction terms between different sites: e.g.,

$$H_{\text{density}} = \frac{V_*}{d} \sum_{\langle ij \rangle} n_i n_j$$

$$H_{\text{exchange}} = \frac{F_*}{d} \sum_{\langle ij \rangle \sigma \sigma'} c^+_{i\sigma} c^+_{j\sigma'} c_{i\sigma'} c_{j\sigma} = -\frac{2F_*}{d} \sum_{\langle ij \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \tfrac{1}{4} n_i n_j)$$

$$\text{interaction lines} \propto \frac{1}{d} \Rightarrow \text{only Hartree diagram survives}$$

[Müller-Hartmann 1989]

"Extended DMFT"

- consider quantum fluctuations of H_{density}
- $H_{\text{density}} - \langle H_{\text{density}} \rangle = O(d^{-\frac{1}{2}})$

[Si et al. '96,...]

Part III
Dynamical mean-field theory

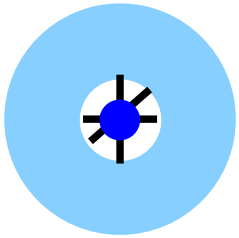
1. Mapping onto impurity models
2. A solvable example
3. Impurity solvers
4. Multi-band systems

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

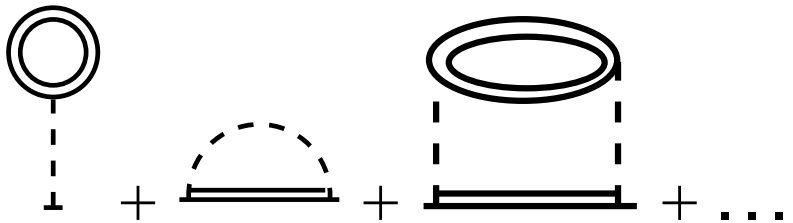
- in general $\mathcal{A}_1$ is not due to a single-site Hamiltonian
  - $\mathcal{G}$ is a dynamical mean field
  - only single-site Hamiltonian H^{at} for $\mathcal{G}^{-1} = \partial_\tau - \mu$

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

$$\boldsymbol{G} = \left[\mathcal{G}^{-1} - \tilde{\boldsymbol{\Sigma}}\right]^{-1} \qquad \text{impurity Dyson equation}$$

- skeleton expansion:

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



$$+ \ldots \qquad \text{one site only!}$$

$$= \boldsymbol{\Sigma}[\boldsymbol{G}] \qquad \boxed{\text{same as for Hubbard model in } d = \infty!}$$

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

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

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

$\Rightarrow$ three equations for unknowns G, $\mathcal{G}$, $\widetilde{\boldsymbol{\Sigma}}$

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

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

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

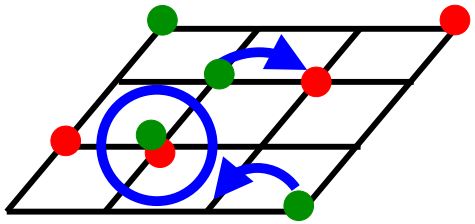
$$\Rightarrow \qquad \mathcal{G}^{-1}_\sigma(\tau) = \partial_\tau - \mu \qquad \Rightarrow \quad (3) \quad \checkmark$$

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 $T > T_c > 0$ [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 $\Sigma_d[G_d]$:

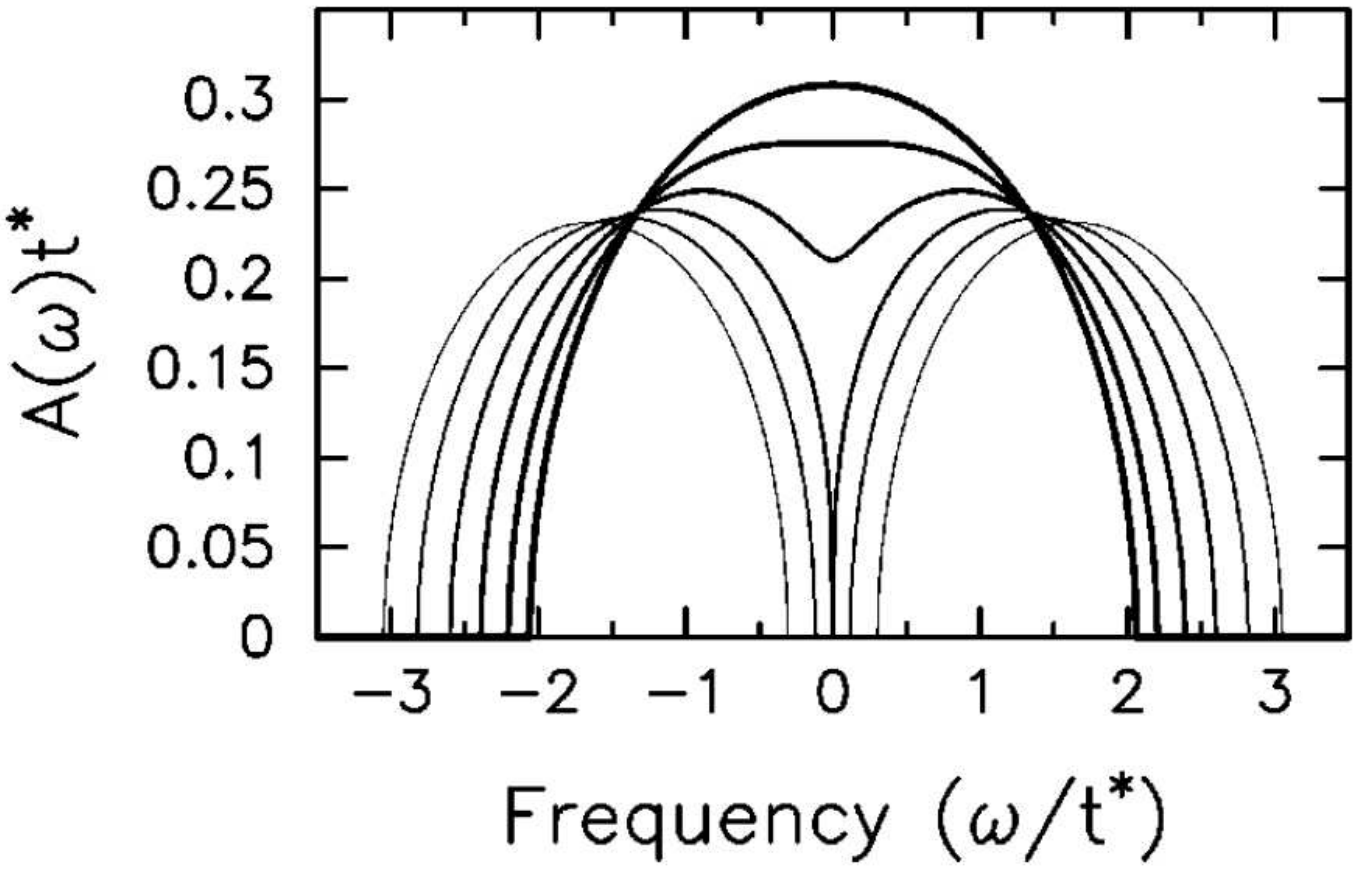
$$\Sigma_d(i\omega_n) = \frac{U}{2} - \frac{1}{2G_d(i\omega_n)} \pm \sqrt{\left(\frac{U}{2} - \frac{1}{2G_d(i\omega_n)}\right)^2 + \frac{Un_f}{G_d(i\omega_n)}}$$

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

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

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

Numerical methods

QMC

Trotter decomposition of imaginary-time action, T not too small

PQMC

projection onto ground state, $T = 0$ only

NRG

logarithmic discretization of host spectrum, sites added successively

NCA

summation of a subset of Feynman diagrams

ED

exact diagonalization for small number of host sites

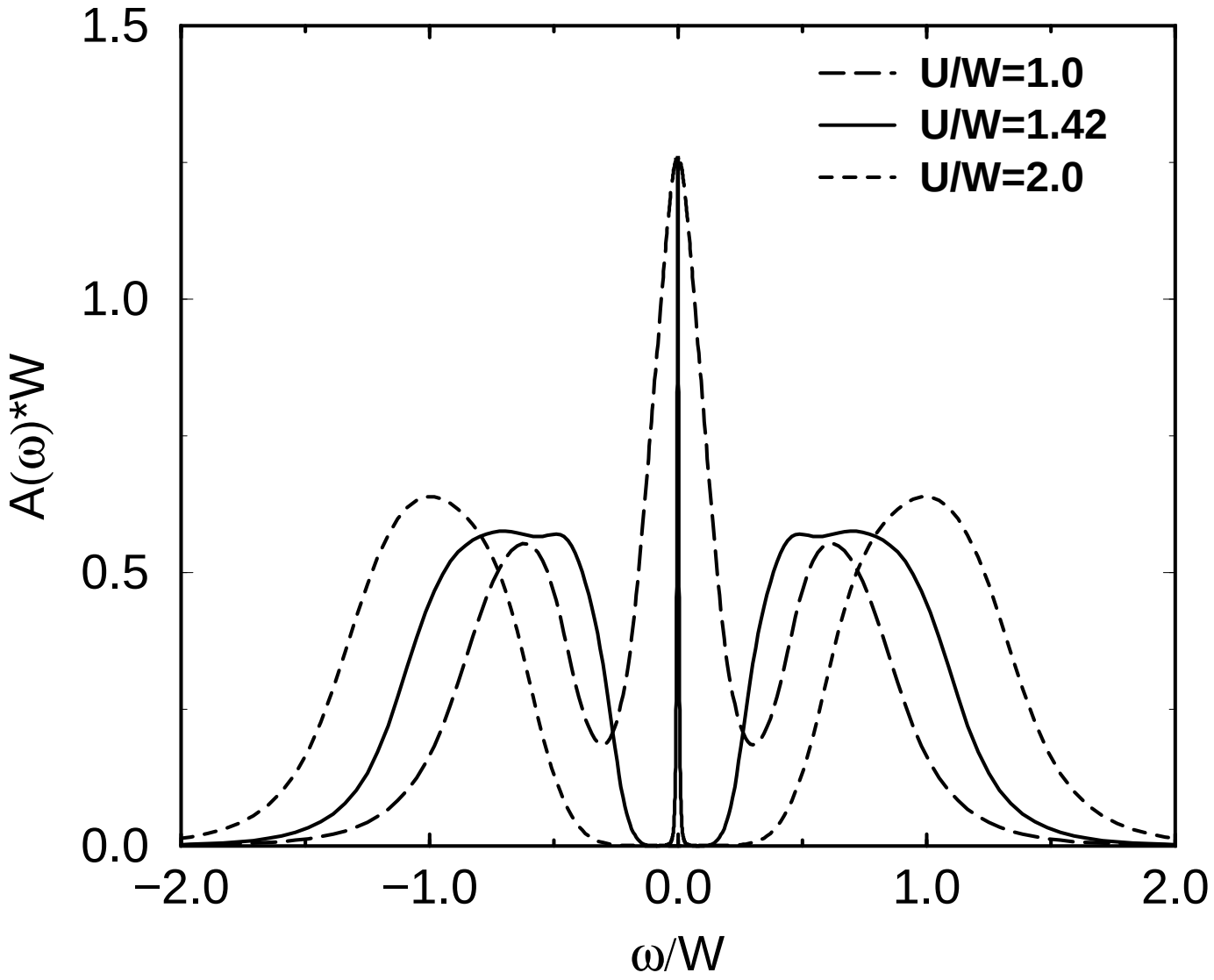
DMRG

blocks with varying number of sites, dynamical quantities available

[→ lectures]

Metal-insulator transition

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

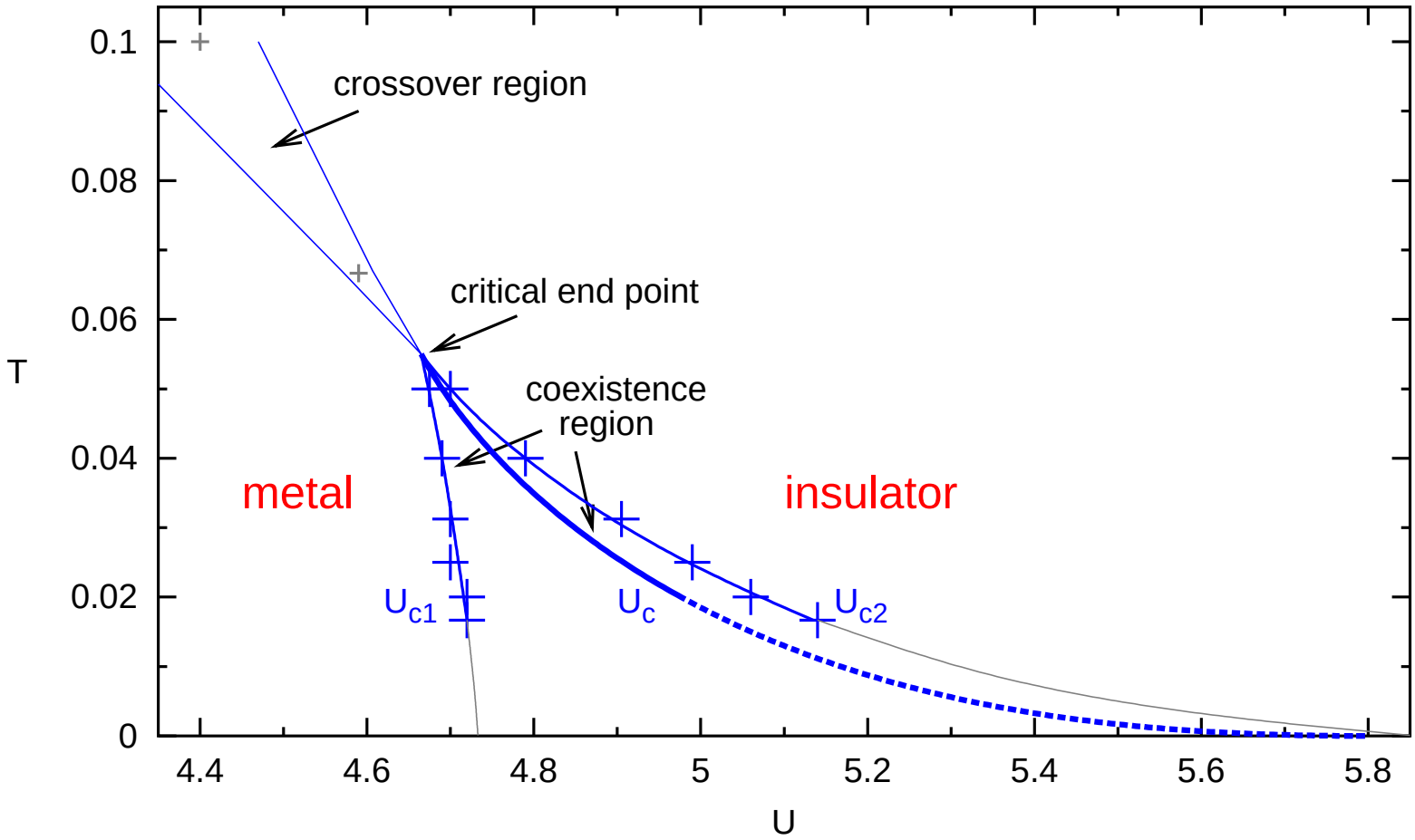


[Bulla '99]

Phase diagram

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

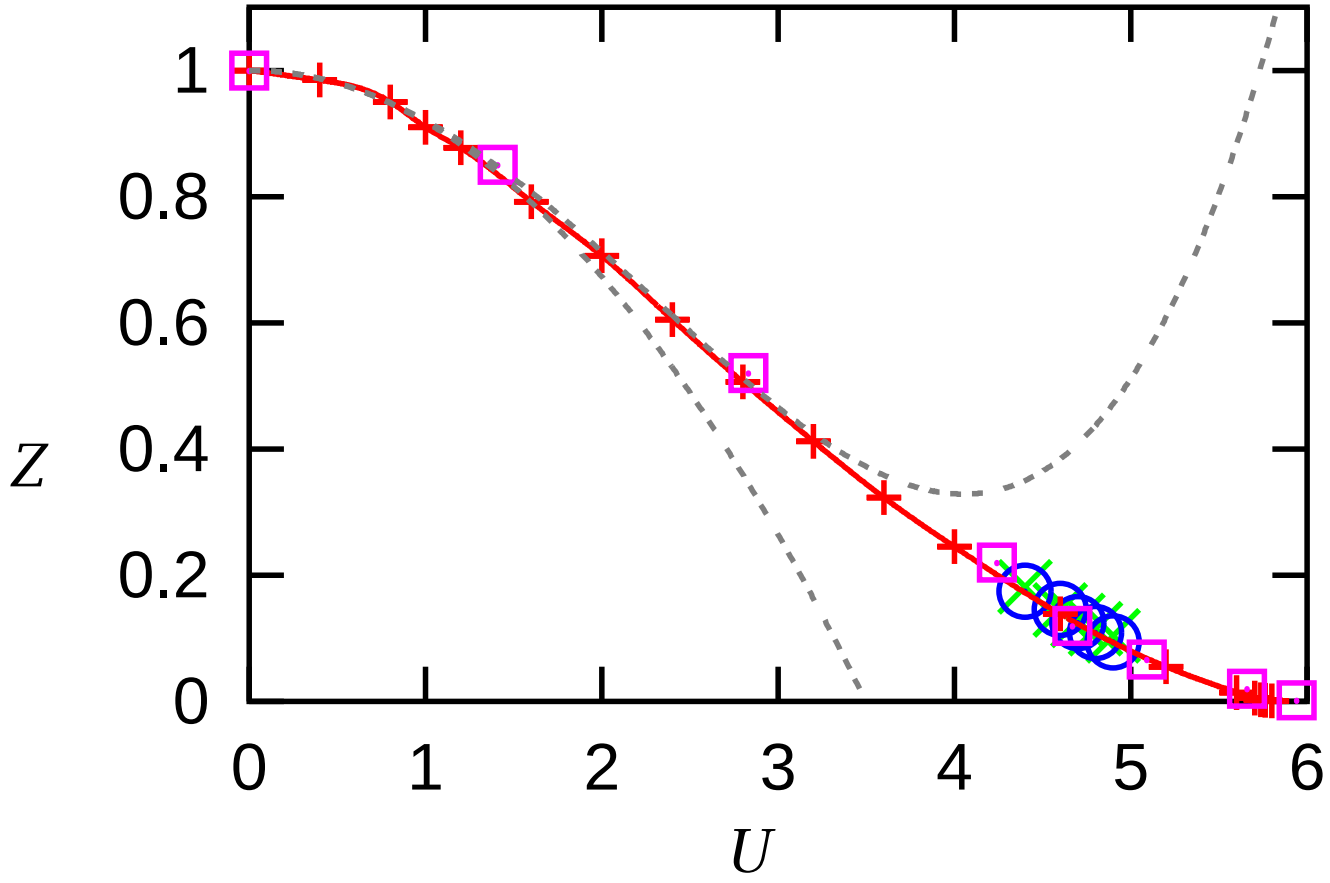
[Blümer '02]



- coexistence region $[U_{c1}; U_{c2}]$, first-order transition
- crossover above critical region

Quasiparticle weight

Hubbard model, Bethe lattice, $n = 1$, DMFT(NRG/QMC/...)



[Bulla '99, Fig. from Blümer '02]

red +: NRG

blue ∘: QMC

pink □: ED

grey line: perturbation theory

4. Multi-band systems: LDA+DMFT

LDA: Hartree-Term + ?

LDA+DMFT: include Coulomb interaction for correlated orbitals

[Anisimov et al. '97; Lichtenstein & Katsnelson '97; Liebsch & Lichtenstein '00; Nekrasov et al. '00; ...]

$$H = H_{\text{LDA}} + H_{\text{int}} - H^{U}_{\text{LDA}} = H^{0}_{\text{LDA}} + H_{\text{int}}$$

$$H_{\text{int}} = \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'\sigma'}}' U^{\sigma\sigma'}_{mm'} \hat{n}_{ilm\sigma} \hat{n}_{ilm'\sigma'}$$

$$- \frac{1}{2} \sum_{i=i_d, l=l_d} {\sum_{m\sigma, m'}}' J_{mm'} \hat{c}^{\dagger}_{ilm\sigma} \hat{c}^{\dagger}_{ilm'\bar{\sigma}} \hat{c}_{ilm'\sigma} \hat{c}_{ilm\bar{\sigma}}$$

H^{U}_{LDA} = already contained in LDA;
determine from *constrained LDA*

$$H^{0}_{\text{LDA}} = \sum_{ilm, jl'm', \sigma} t^{0}_{ilm, jl'm'} \, c^{+}_{ilm\sigma} c_{jl'm'\sigma}$$

Summary

DMFT:

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

[→ lectures, talks]

Extensions: (numerical effort increases ...)

- multiband systems
- spatial fluctuations, clusters
- coupling to bosonic baths

[→ lectures, talks]