The Foundations of Dynamical Mean-Field Theory

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Autumn School on Correlated Electrons:
DMFT – From Infinite Dimensions to Real Materials
Forschungszentrum Jülich, September 17-21, 2018

Outline

1. **Fermions in high dimensions**
   - Scaling of hopping amplitudes
   - Density of states

2. **Consequences for many-body theory**
   - Green function, Feynman diagrams
   - Self-energy becomes local

3. **Dynamical Mean-Field Theory**
   - Mapping onto single-site problem
   - Solution of effective impurity model

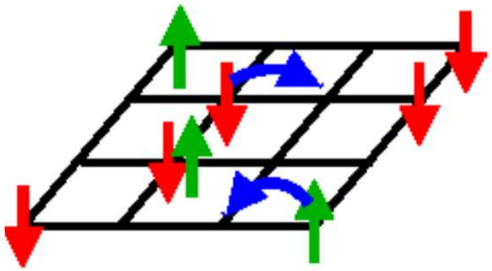
1.
Fermions in high dimensions

Kinetic energy for lattice fermions

- Single-band Hubbard model

$\rightarrow$ **Lecture by D.Vollhardt**

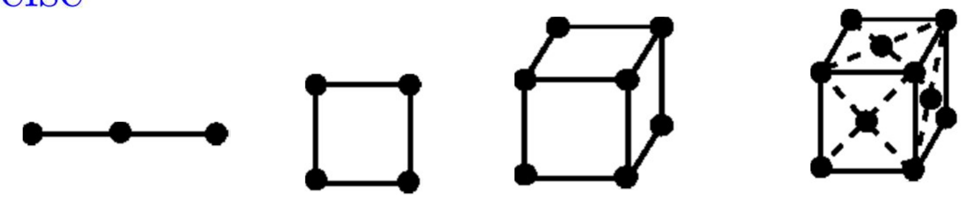
$$H_{\mathrm{Hubbard}} = \underbrace{\sum_{ij\sigma} t_{ij}\, c^+_{i\sigma} c_{j\sigma}}_{= \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}}\, c^+_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



- Nearest-neighbor hopping:

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

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



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

- Nontrivial limit for $d \rightarrow \infty$?

Scaling of hopping amplitudes

- An elegant shortcut: Metzner & Vollhardt 1989
  - consider $k_i \in [-\pi, \pi]$ as independent uniform random variables
  - define $X_i = \sqrt{2}\cos k_i$ (mean 0, variance 1)

    $$X^{(d)} = \frac{1}{\sqrt{d}} \sum_{i=1}^{d} X_i$$ (mean 0, variance 1)
  - central limit theorem for $d \to \infty$: $X^{(d)}$ normal-distributed (Gaussian)
- Density of states = prob. distrib. of $\epsilon_{\boldsymbol{k}}^{(d)} = -2t \sum_{i=1}^{d} \cos k_i = -\underbrace{\sqrt{2d}\, t}_{= t_*} X^{(d)}$

$$\boxed{\rho(\epsilon) = \frac{1}{L} \sum_{\boldsymbol{k}} \delta(\epsilon - \epsilon_{\boldsymbol{k}}) \xrightarrow{d \to \infty} \frac{1}{2\pi |t_*|}\, e^{-\frac{\epsilon^2}{2t_*^2}}}$$

with

$$\boxed{t = \frac{t_*}{\sqrt{2d}}}$$

Scaling of hopping amplitudes

➤ Alternative: Fourier transformation

Müller-Hartmann 1989

$$\boxed{t = \frac{t_*}{\sqrt{2d}}}$$

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

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

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

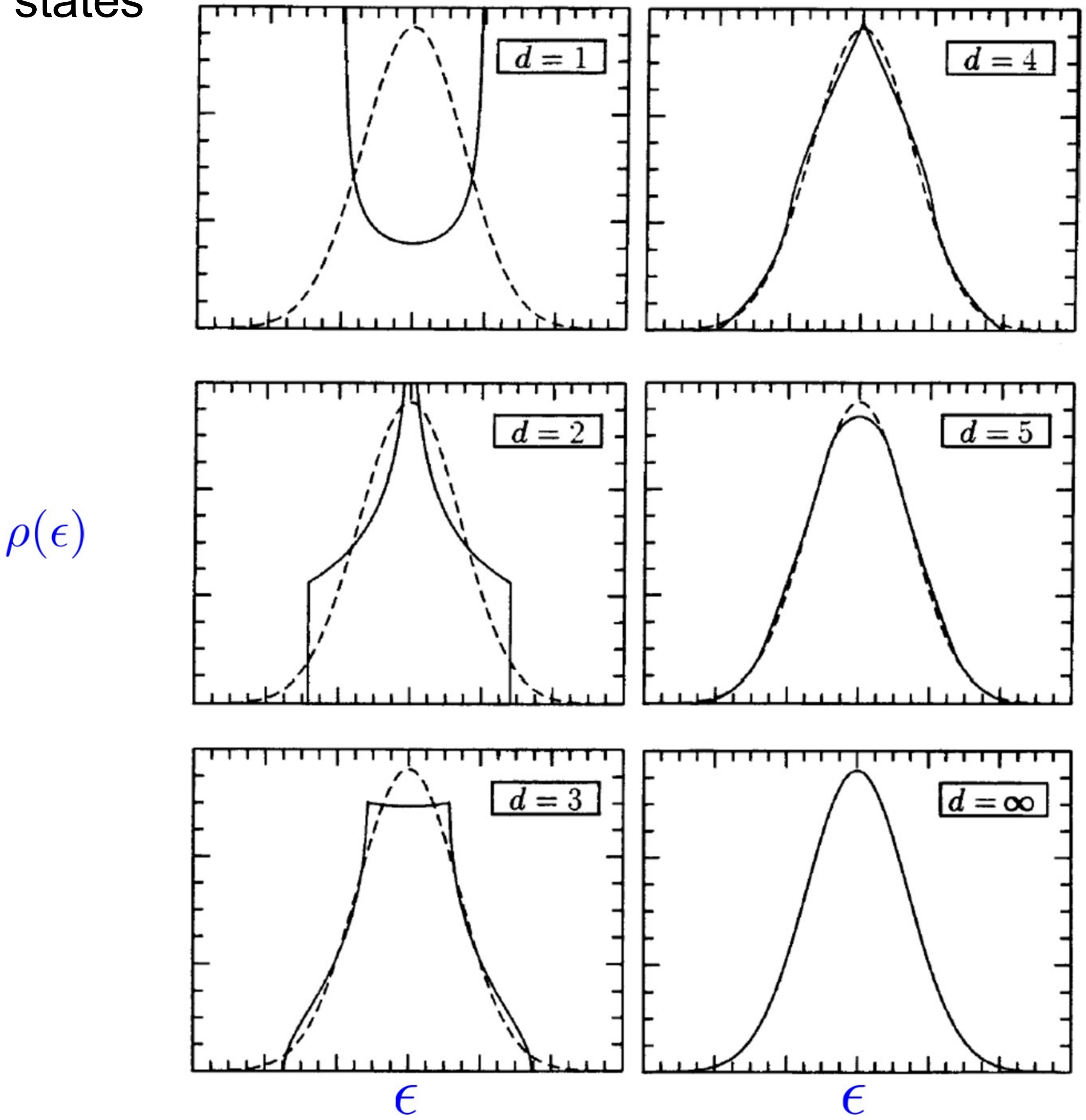
➤ Back transformation:

$$\rho(\epsilon) = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \; e^{-is\epsilon} \; \Phi(s) = \boxed{\frac{1}{2\pi |t_*|} \; \exp\left[-\frac{\epsilon^2}{2t_*^2} + O\left(\frac{1}{d} \right) \right]}$$

➤ Higher-order corrections, generalizations, representations, …

Hypercubic lattice in *d* dimensions

➤ Density of states



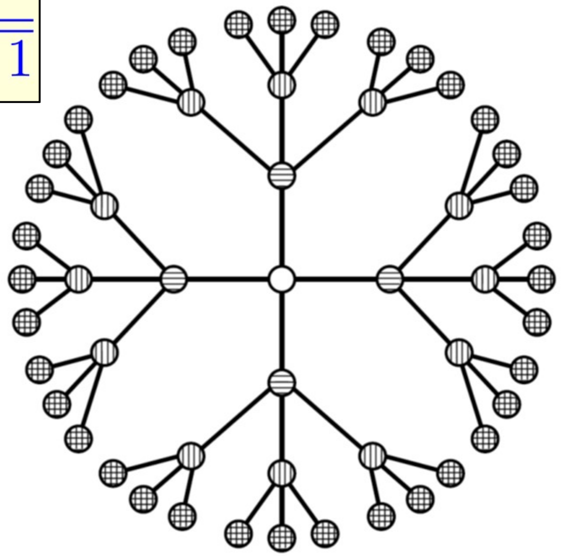
Vollhardt 1993

Bethe lattice with Z nearest neighbors

- Bethe lattice is recursively defined; not a Bravais lattice

e.g. Mahan 2001
Eckstein et al. 2004

$$\boxed{t = \frac{t_*}{\sqrt{Z-1}}}$$

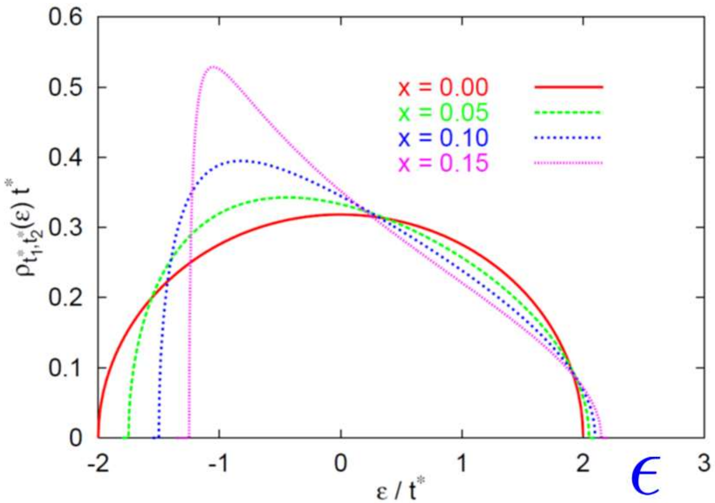


$$\rho(\epsilon) = \frac{\sqrt{4t_*^2 - \epsilon^2}}{2\pi t_*^2} \Big/ \left[\frac{Z}{Z-1} - \frac{\epsilon^2}{Z\,t_*^2}\right] \longrightarrow \boxed{\frac{\sqrt{4t_*^2 - \epsilon^2}}{2\pi t_*^2}}$$

- d.o.s. with finite band-width
- also for additional NNN hopping

$$x = t_*/t'_*$$

$\rho(\epsilon)$



2.
Consequences for many-body theory

Green functions

- Imaginary-time-ordered fermionic Green function

e.g. Negele & Orland

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

$$= -G_{\alpha\beta}(\tau+\beta) \qquad (-\beta < \tau < 0)$$

in terms of imaginary-time Heisenberg operators $X(\tau) = e^{H\tau} X e^{-H\tau}$

- Matsubara Green function

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

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

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

Spectral representations

- Spectral decomposition

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

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

spectral function

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

Lehmann representation

- Local Green function and local spectral function

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

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

~ interacting d.o.s.

Free fermions

- Free Green function in absence of interactions:

$$H_0 - \mu N = \sum_{\boldsymbol{k}\sigma} (\epsilon_{\boldsymbol{k}} - \mu)\, c^{+}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \qquad \Rightarrow \qquad G^{(0)}_{\boldsymbol{k}\sigma}(i\omega_n) = \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}}}$$

- Free local Green function / spectral function

$$G^{(0)}_{\sigma}(i\omega_n) = \frac{1}{L} \sum_{\boldsymbol{k}} \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}}} \qquad = \qquad \int_{-\infty}^{\infty} d\epsilon \, \frac{\rho(\epsilon)}{i\omega_n + \mu - \epsilon}$$

$$A^{(0)}_{\sigma}(\omega) = \frac{1}{L} \sum_{\boldsymbol{k}} \delta(\omega + \mu - \epsilon_{\boldsymbol{k}}) \qquad = \qquad \rho(\omega + \mu)$$

free density of states $\rho(\omega) = \sum_{\boldsymbol{k}} \delta(\omega - \epsilon_{\boldsymbol{k}})$

Self-energy

- Self-energy $\Sigma_{\boldsymbol{k}\sigma}(i\omega_n)$ characterizes effect of interactions

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

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

Dyson equation

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

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

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

- Feynman diagrams:

Quasiparticles

- Spectral function describes single-particle excitations

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

real part vanishes if

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

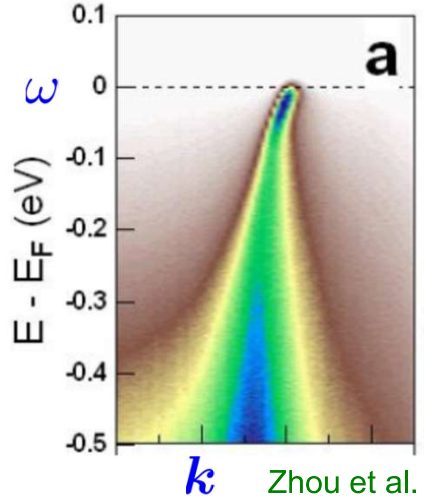
- For $\omega \approx E_{\boldsymbol{k}}$:

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

$$Z_{\boldsymbol{k}}(\omega) = [1 - \mathrm{Re}\Sigma'_{\boldsymbol{k}}(\omega)]^{-1}$$

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

ARPES on LSCO



Zhou et al. 2006

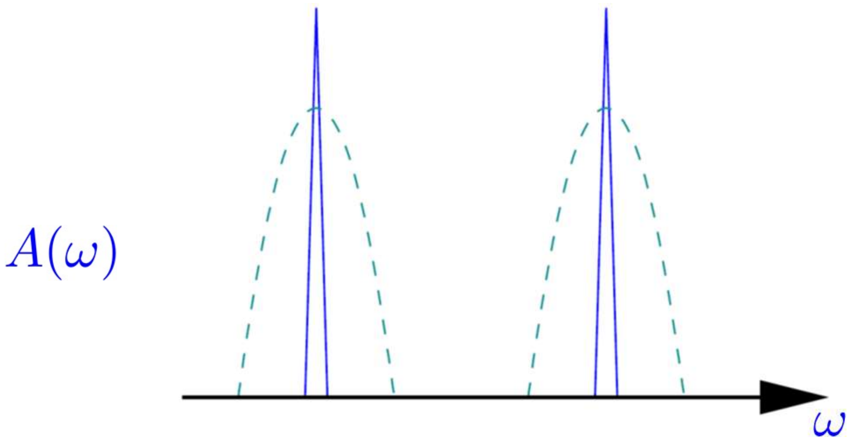
- <u>Fermi liquid:</u> coherent quasiparticles for sufficiently small ω

Hubbard bands and Mott-Hubbard transition

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

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

- Local spectral function:



  - Delta peaks become broad for $t_{ij} \neq 0$: Hubbard bands
  - Hubbard bands merge for large enough $|t_{ij}|$
  - *nonmagnetic* Mott-Hubbard transition occurs at $U = U_c$

Mott 1946, Hubbard 1963

Green function diagrams

- Feynman diagrams for Green function:

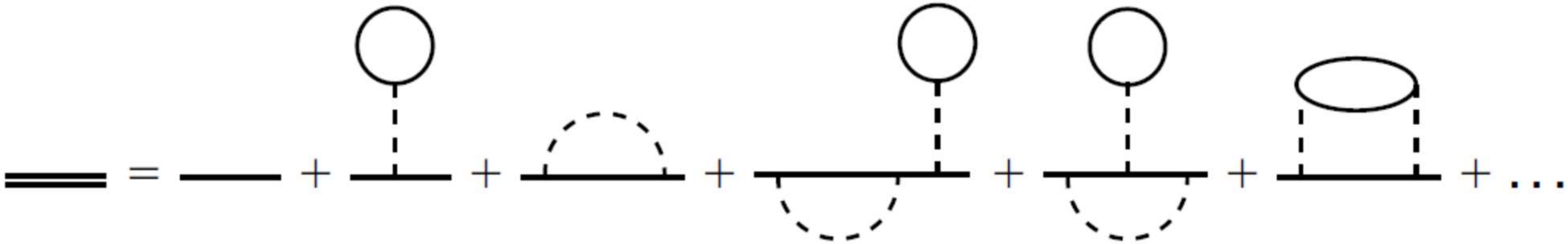
e.g. Negele & Orland

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

= interaction vertex

= full (interacting) Green function line G

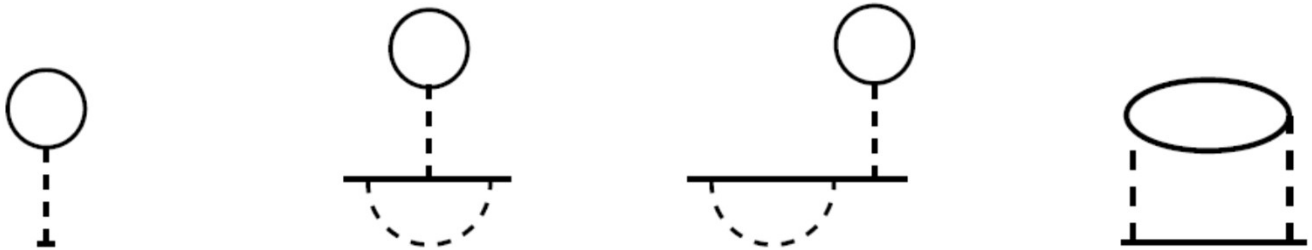
- Perturbation expansion:



- Evaluate with diagram rules (trace over internal degrees of freedom, etc.)

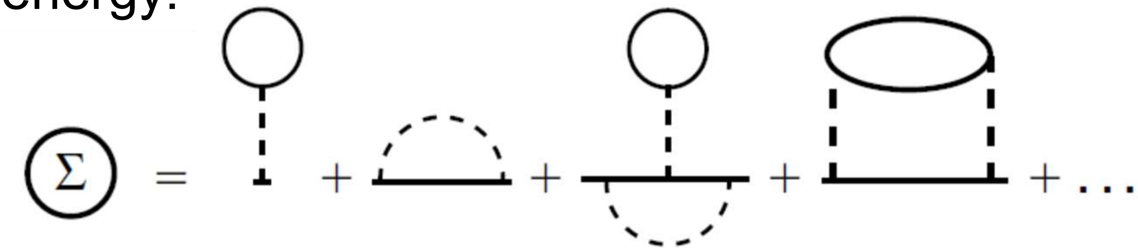
Self-energy diagrams

- Proper self-energy diagrams:
  - have amputated external vertex
  - cannot be cut in two pieces *(1-particle irreducible)*



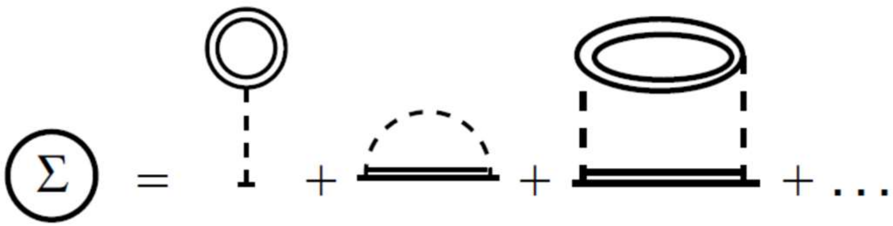
proper proper not proper proper

- Self-energy:



Skeleton expansion

- $\mathbf{\Sigma}[G^{(0)}]$ = self-energy in terms of free Green functions
- Next step: omit self-energy insertions such as  etc.
- $\mathbf{\Sigma}[G]$ = skeleton expansion



  - must avoid double counting
  - bare and skeleton expansion contain the same (perturbative) diagrams
  - convergence & uniqueness of skeleton expansion is not guaranteed

Many-body theory for infinite dimensions

- Power counting in $1/d$ for $G_{ij\sigma}(\omega)$

- Hopping amplitudes:

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

- Kinetic energy:

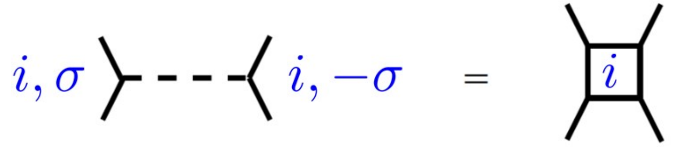
$$E_{\mathrm{kin},\sigma} = \sum_{ij} t_{ij} \langle c_{i\sigma}^{+} c_{j\sigma} \rangle = \underbrace{\sum_{ij}}_{O(d^{||\boldsymbol{R}_i - \boldsymbol{R}_j||})} t_{ij} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i}\, G_{ij\sigma}(\omega)\, e^{i\omega 0^{+}} = O(d^{0})$$

- Green function:

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

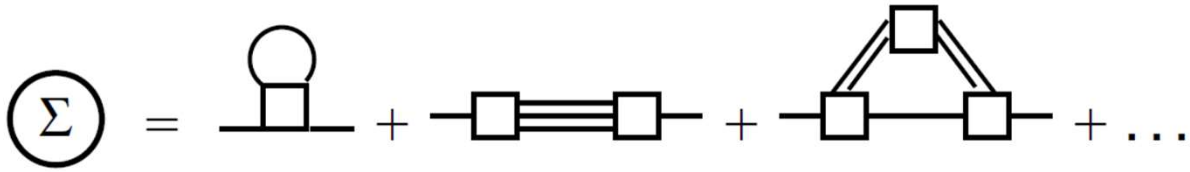
→ Simplifications for Feynman diagrams?

Diagrammatic simplifications

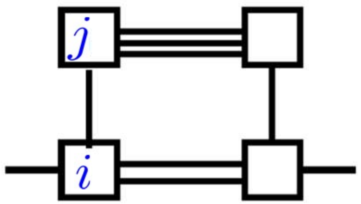
- Hugenholtz diagrams: 

$= U \sum_i n_{i\uparrow} n_{i\downarrow}$

- Skeleton expansion: <u>at least 3 independent paths</u> between i and j



- Power counting in $1/d$:



  - Green function lines: $O(d^{-\frac{3}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||})$
  - Summation over j : $O(d^{||\boldsymbol{R}_i - \boldsymbol{R}_j||})$
  - Skeleton diagram is $O(d^{-\frac{1}{2}||\boldsymbol{R}_i - \boldsymbol{R}_j||})$

- All vertices in $\boldsymbol{\Sigma}[\boldsymbol{G}]$ have the same label in $d \to \infty$

- The self-energy becomes local!

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

Müller-Hartmann 1989

Local self-energy

- Simple momentum dependence:

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

$$\Sigma_{\boldsymbol{k}\sigma}(\omega) = \Sigma_{\sigma}(\omega)$$

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

- Local Green function:

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

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

3.
Dynamical mean-field theory

Path integral representation

Negele & Orland

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

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

- Functional integral over Grassmann variables $\phi_\alpha^*(\tau),\phi_\alpha(\tau)$ with action

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

- Imaginary-time-ordered Green function:

$$G_{\alpha\beta}(\tau) = \frac{1}{Z}\int\limits_{\mathrm{APBC}} \mathcal{D}(\phi^*\phi) \quad \phi_\alpha(\tau)\phi_\beta^*(0) \quad \exp(\mathcal{S})$$

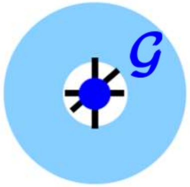
Mapping onto single-site models

Kotliar & Georges 1992
Jarrell 1992

➤ Consider an effective single-site action $\mathcal{S} = \mathcal{S}_1 + \mathcal{S}_2$

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

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



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

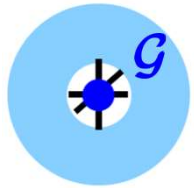
local Hubbard interaction

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

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

Dynamical mean-field theory

- Quadratic action $\mathcal{S}_1$ does not correspond to single-site Hamiltonian
  - $\mathcal{G}$ represents a dynamical mean field
  - from single-site Hamiltonian only in atomic limit

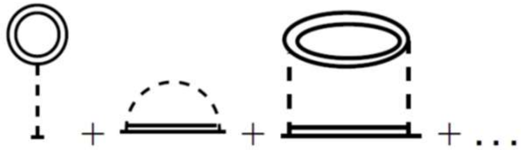


- Define impurity self-energy $\widetilde{\boldsymbol{\Sigma}}$

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

impurity Dyson equation

- Skeleton expansion:

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

involves only one site!

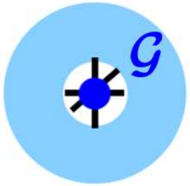
$= \boldsymbol{\Sigma}[\boldsymbol{G}]$ same diagrams as for inf.-dim. Hubbard model!

Dynamical mean-field equations

➤ Single-impurity problem:

$$G_\sigma(i\omega_n) = \langle c_\sigma(i\omega_n) c^*_\sigma(i\omega_n)\rangle_{\mathcal{S}[\mathcal{G}]}$$

(solve numerically)



➤ Impurity Dyson equation:

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

➤ Lattice Dyson equation:

$$\begin{aligned} G_\sigma(i\omega_n) &= \int \frac{d^d k}{(2\pi)^d} \frac{1}{i\omega_n + \mu - \epsilon_{\boldsymbol{k}} - \Sigma_\sigma(i\omega_n)} \\ &= \int_{-\infty}^{\infty} d\epsilon\, \frac{\rho(\epsilon)}{i\omega_n + \mu - \Sigma_\sigma(i\omega_n) - \epsilon} \end{aligned}$$

(self-consistency)

→ three equations for three unknowns $G,\ \mathcal{G},\ \Sigma$

Free and atomic limit

➤ Non-interacting case, $U = 0$:

$$\Sigma_\sigma(i\omega_n) = 0$$

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

$$\mathcal{G}_\sigma(i\omega_n) = G_\sigma(i\omega_n)$$

✔

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

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

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

$$\mathcal{G}_\sigma^{-1}(\tau) = -\partial_\tau + \mu$$

✔

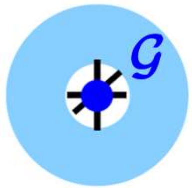
Hamiltonian representation as SIAM

➤ Representation by single-impurity 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 to obtain action $\mathcal{S}$ with

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



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

➤ Hamiltonian representation of Weiss field through additional particles

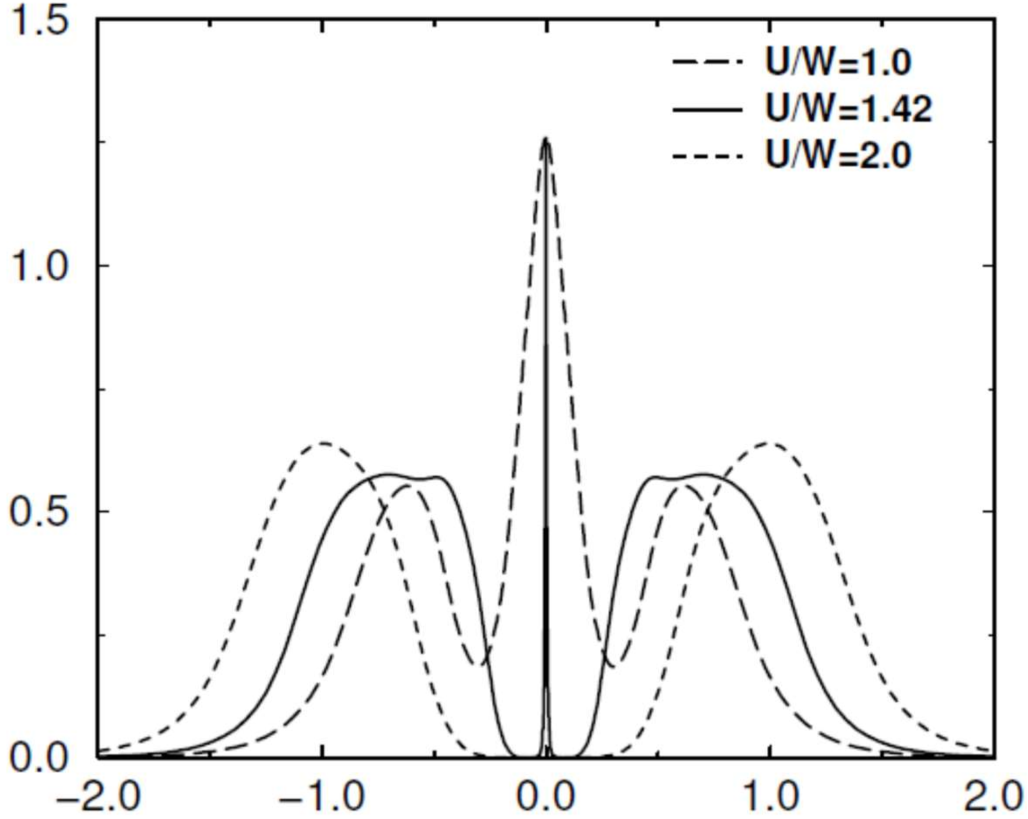
Impurity solvers

- Perturbation theory / Iterated Perturbation Theory (IPT)
  - inexpensive
  - works on real frequency axis
- Quantum Monte Carlo (QMC)
  - works directly with action (in continuous time, CT-QMC)
  - requires analytical continuation from Matsubara frequencies → **Lecture by E. Koch**
- Exact Diagonalization (ED)
  - requires discretization
  - works on real frequency axis
- Numerical Renormalization Group (NRG)
  - logarithmic discretization, resolution best near Fermi surface
  - works on real frequency axis
- Density-Matrix Renormalization Group (DMRG)

  → **Lectures by H. G. Evertz**

Results for the Hubbard model

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



$A(\omega)W$

ω/W

Bulla 1999

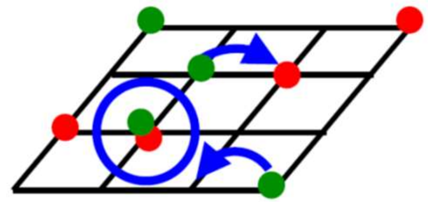
A solvable case: the Falicov Kimball model

Brandt & Mielsch 1989
van Dongen 1990
Si et al. 1992
Freericks & Zlatic 2003

- Falicov-Kimball model: hopping only for one 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 move with background of f electrons
  f configuration optimizes free energy



- DMFT action:

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

- 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:

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

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

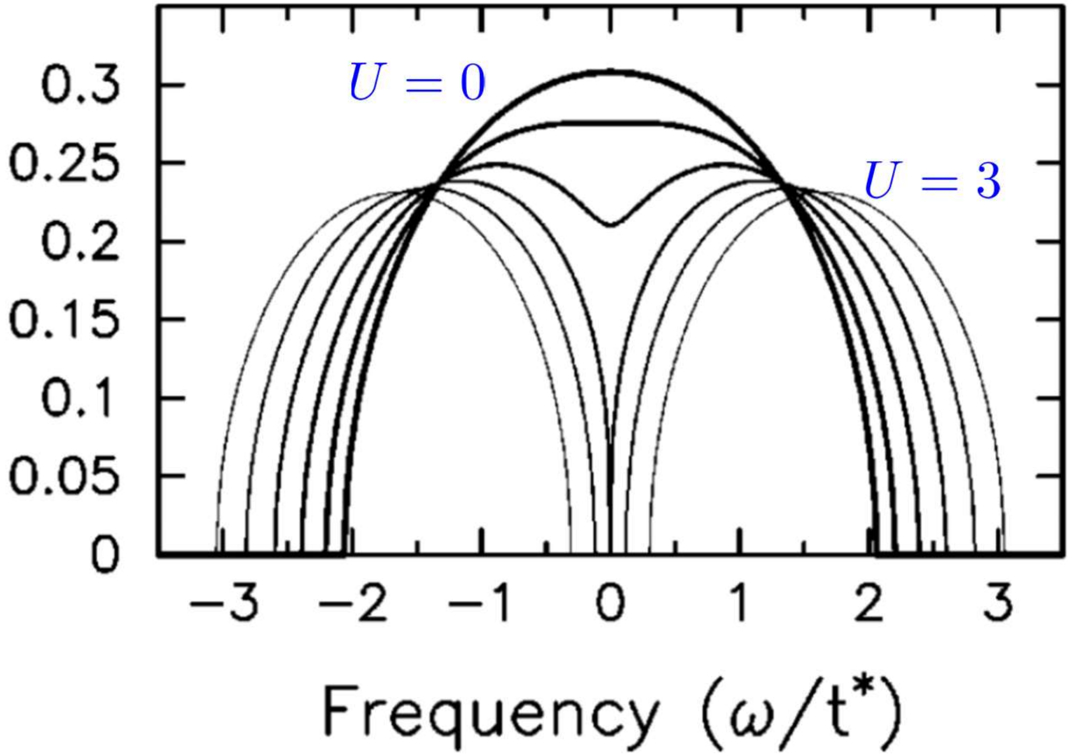
$\rightarrow$ determines $G_d(i\omega_n)$ for a given density of states

- Skeleton self-energy:

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

A solvable case: the Falicov Kimball model

- Falicov-Kimball model, Bethe lattice, homog. phase, DMFT, $n_d = n_f = \frac{1}{2}$



- Non-Fermi liquid ,Mott metal-insulator transition at $U = 2t_*$
- Temperature-independent spectrum in homogeneous phase

Freericks & Zlatic 2003

Generalizations and Perspectives

Generalizations and Perspectives

- **Here: one band, infinite dimensions, thermal equilibrium**

- **Realistic multiband systems:**
  - On-site interactions, Hund‘s rules, multiplets
  - Connection with density-functional theory
  - Multiband impurity solvers

→ **Lectures by O. Andersen, F. Aryasetiawan, F. Lechermann, E. Pavarini, H. G. Evertz**

- **Finite dimensions:**
  - Cluster expansions
  - Dual fermions
  - Diagrammatic approaches

→ **Lectures by M. Potthoff, H. Hafermann, K. Held**

- **Real-time dynamics in nonequilibrium**

→ **Lecture by M. Eckstein**