Nonperturbative conserving approximations and Luttinger’s sum rule

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Luttinger’s sum rule:

the volume in reciprocal space
enclosed by the Fermi surface
equals the average particle number
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conserving approximations:

HF, RPA, FLEX, ...
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conserving approximations:
HF, RPA, FLEX, ...

DMFT-based approximations
dynamical mean-field theory
dynamical cluster approximation
cellular DMFT
...
Nonperturbative conserving approximations and Luttinger’s sum rule

Luttinger’s sum rule:
the volume in reciprocal space enclosed by the Fermi surface equals the average particle number

conserving approximations:
HF, RPA, FLEX, ...

DMFT-based approximations
dynmical mean-field theory
dynamical cluster approximation
cellular DMFT
...

different conserving approximations?
DIA, VCA
(self-energy-functional approach)
non-interacting Fermi gas

Hamiltonian: \( H = \sum_k \sum_{\sigma=\uparrow,\downarrow} \varepsilon(k) c^\dagger_{k\sigma} c_{k\sigma} \)

free dispersion:
\( \varepsilon(k) = \frac{\hbar^2 k^2}{2m} \)

tight-binding dispersion:
\( \varepsilon(k) = -2t(\cos(k_x a) + \cos(k_y a)) \)

Fermi surface: \( \{ k | \varepsilon(k) = \mu \} \)

Fermi-surface volume: \( V_{FS}^{(0)} = 2 \sum_k \Theta(\mu - \varepsilon(k)) \)

\[ V_{FS}^{(0)} = N \]
interacting Fermi system

Hamiltonian: \( H = \sum_{\mathbf{k}} \sum_{\sigma = \uparrow, \downarrow} \varepsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{U}{2L} \sum_{\mathbf{kk}'\mathbf{q}} \sum_{\sigma\sigma'} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'}^{\dagger} c_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'} + q\sigma c_{\mathbf{k}-q\sigma}' \)

Fermi liquid (Landau)

Hamiltonian: \( H_{FL} = \sum_{\mathbf{k}} \sum_{\sigma} \varepsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{2L} \sum_{\mathbf{kk}'\mathbf{\sigma,\sigma'}} F_{\mathbf{kk}'\mathbf{\sigma,\sigma'}}^{\mathbf{\sigma,\sigma'}} n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma'} \)

\( \omega \to 0 \): no phase space for scattering
Fermi-liquid theory:
- there is a Fermi surface
- $V_{FS} = N = V_{FS}^{(0)}$ (Luttinger sum rule)
Hubbard model

\[ H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow} \]

- nearest-neighbor hopping, amplitude: \( t_{ij} \)
- local (on-site) repulsion, strength \( U \)
test of the sum rule

\[ H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_{i=1}^{L} n_{i\uparrow} n_{i\downarrow} \]

- nearest-neighbor hopping, amplitude: \( t_{ij} \)
- local (on-site) repulsion, strength \( U \)

\( t \)-\( J \) model:
expansion up to \( \beta^{12} \), \( J/t = 0.4 \), \( n = 0.8 \), \( T = 0.2J \),
criteria: \( |\nabla n(k)| = \text{max (dotted)}, \frac{dn(k)}{dT} = 0 \) (dashed)

Puttika et al (1998)
Hubbard model:

\[ H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^L n_{i\uparrow} n_{i\downarrow} \]

- nearest-neighbor hopping, amplitude: \( t_{ij} \)
- local (on-site) repulsion, strength \( U \)

Hubbard model:

\( T = 0, U = W \)

ad hoc approximations
Hubbard model

\[ H = H_0 + H_1 = \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i=1}^L n_{i\uparrow} n_{i\downarrow} \]

- nearest-neighbor hopping, amplitude: \( t_{ij} \)
- local (on-site) repulsion, strength \( U \)

**questions:**
- are there violations of Luttinger’s sum rule ?
- how to construct approximations satisfying the sum rule ?
- how to construct approximations not artificially satisfying the sum rule ?
Green's function

one-particle excitation / photoemission:

Green's function: \( G_\mathbf{k}(\omega) = \int dz \frac{A_\mathbf{k}(z)}{\omega - z} \) \( A_\mathbf{k}(\omega) = -\text{Im} \ G(\mathbf{k}, \omega + i0^+)/\pi \)

\[
I(\mathbf{k}, \omega) \propto \sum_m \left| \langle N - 1, m \mid c_\mathbf{k} \mid N, 0 \rangle \right|^2 \delta (\omega - (E_m(N - 1) - E_0(N))) = A_\mathbf{k}(\omega)
\]
Green’s function

one-particle excitation / photoemission:

\[ I(k, \omega) \propto \sum_m \left| \langle N - 1, m | c_k | N, 0 \rangle \right|^2 \delta (\omega - (E_m(N - 1) - E_0(N))) = A_k(\omega) \]

Green’s function:

\[ G_k(\omega) = \int dz \frac{A_k(z)}{\omega - z} \quad A_k(\omega) = -\text{Im} \frac{G(k, \omega + i0^+)}{\pi} \]

→ Luttinger’s sum rule:

\[ N = V_{\text{FS}} \]

\[ N = \sum_k \int_{-\infty}^{0} d\omega \ A_k(\omega) = -\frac{1}{\pi} \text{Im} \sum_k \int_{-\infty}^{0} d\omega \ G_k(\omega + i0^+) \]

→ FS: \[ G_k(\omega = 0)^{-1} = 0 \quad V_{\text{FS}} = \sum_k \Theta(G_k(\omega = 0)^{-1}) \]
perturbation theory

\[ H = H_0 \rightarrow G_k^{(0)}(\omega) \] (free system)

\[ H = H_0 + H_1 \rightarrow G_k(\omega) \] (interacting system)

\[ \Sigma_k(\omega) : \text{self-energy} \]

\[ G_k(\omega) = G_k^{(0)}(\omega) + G_k^{(0)}(\omega)\Sigma_k(\omega)G_k(\omega) \] (Dyson’s equation)
proof of the sum rule

expansion of the self-energy:

\[ \Sigma = \quad + \quad + \quad + \ldots \]

define Luttinger-Ward functional:

\[ \Phi = \quad + \quad + \quad + \ldots \]

hence:

\[ \Sigma[G] = \frac{\delta \Phi[G]}{\delta G} \]

consider shift transformation

\[ G(\omega) \rightarrow G(\omega + \nu) \equiv G_\nu(\omega) \]

exploiting the invariance:

\[ 0 = \frac{d}{d\nu} \Phi[G_\nu]\bigg|_{\nu=0} = \int d\omega \frac{\delta \Phi}{\delta G} \frac{\partial G}{\partial \omega} = \text{Tr} \left( \Sigma \frac{\partial G}{\partial \omega} \right) \]

some algebra:

\[ N = \text{Tr} G = \text{Tr} \left( G \frac{\partial G^{(0)^{-1}}}{\partial \omega} \right) = \text{Tr} \left( G \frac{\partial}{\partial \omega} (G^{-1} + \Sigma) \right) \]

\[ = \text{Tr} \left( \frac{\partial}{\partial \omega} \ln G^{-1} \right) - \text{Tr} \left( \Sigma \frac{\partial G}{\partial \omega} \right) = V_{FS} \]

*Luttinger, Ward (1963)*
conserving approximations

recipe:

– write down a truncated Luttinger-Ward functional: \( \Phi[G] \mapsto \Phi_{\text{trunc}}[G] \)

\[ \Phi_{\text{HF}} = \begin{array}{c}
\begin{array}{c}
\text{circ}
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\text{dashed}
\end{array}
\end{array} \]

e.g. Hartree-Fock approximation:

– derive self-energy: ("\( \Phi \) derivable")

\[ \Sigma[G] = \frac{\delta \Phi[G]}{\delta G} \]

– use Dyson’s equation

\[ G = \frac{1}{G^{(0)}^{-1} - \Sigma} \]

result:

Baym, Kadanoff (1961)

– macroscopic conservations laws respected (energy, momentum, spin, ...)

– thermodynamical consistency

– Luttinger’s sum rule satisfied

\[ \rightarrow \text{non-perturbative conserving approximations?} \]
non-perturbative construction of $\Phi$

$$\Omega_{U}[G_{0}^{-1}] = -T \ln \int D[c^{*}, c] \ e^{-S_{U}[G_{0}^{-1}]}$$

$$G[G_{0}^{-1}] = - \frac{1}{T} \frac{\delta \Omega_{U}[G_{0}^{-1}]}{\delta G_{0}^{-1}} \quad \text{(one-to-one)}$$

$$\Phi_{U}[G] = \Omega_{U}[G_{0}^{-1}, U[G]] + \text{Tr}(GG_{0, U}^{-1}[G]) - \text{Tr} \ln G$$

$\rightarrow$ Luttinger-Ward functional, universal

$\Lambda_{U}[\Sigma]$: Legendre transform of $\Phi_{U}[G]$

$$\Omega_{t, U}[\Sigma] = \text{Tr} \ln \frac{1}{G_{0, t}^{-1} - \Sigma} + \Lambda_{U}[\Sigma]$$

$$\delta \Omega_{t, U}[\Sigma] = 0 \iff \frac{-1}{G_{0, t}^{-1} - \Sigma} = \frac{\delta \Lambda_{U}[\Sigma]}{\delta \Sigma}$$

$\delta \Omega[\Sigma] = 0$

$\Omega = \Omega[\Sigma]$

self-energy-functional theory (SFT)
\[ \Omega U[G_0^{-1}] = -T \ln \int D[c^*, c] e^{-S_U[G_0^{-1}]} \]

\[ G[G_0^{-1}] = -\frac{1}{T} \frac{\delta \Omega U[G_0^{-1}]}{\delta G_0^{-1}} \] (one-to-one)

\[ \Phi_U[G] = \Omega U[G_0^{-1}, U[G]] + \text{Tr}(GG_0^{-1}U[G]) \]
\[-\text{Tr} \ln G \]

→ Luttinger-Ward functional, universal

\[ \Lambda_U[\Sigma]: \text{Legendre transform of } \Phi_U[G] \]

\[ \Omega_{t, U}[\Sigma] = \text{Tr} \ln \frac{1}{G_{0,t}^{-1} - \Sigma} + \Lambda_U[\Sigma] \]

\[ \delta \Omega_{t, U}[\Sigma] = 0 \iff \frac{-1}{G_{0,t}^{-1} - \Sigma} = \frac{\delta \Lambda_U[\Sigma]}{\delta \Sigma} \]

→ \( \Omega[\Sigma] \) stationary at physical self-energy

→ \( \Lambda_U[\Sigma] \) constructed formally, but unknown

|         | SFT          | DFT          |
|---------|--------------|--------------|
| \( \delta \Omega[\Sigma] \) | 0            | \( \delta \Omega[n] \) = 0 |

- p.10
Rayleigh, Ritz

Original system: \( H_{t,U} \)
Reference system: \( H_{t',U'} \)

\[ E_{t,U}[\Psi_{t',U'}] \xrightarrow{\Psi_{t',U'}} \Psi_{t',U'} \]

\[
E_{t,U}[|\Psi\rangle] = \langle \Psi | H_{t,U} | \Psi \rangle
\]

\[
\frac{\partial E_{t,U}[|\Psi_{t',U'}\rangle = 0]}{\partial t'} \neq 0
\]

→ Hartree-Fock approximation
Rayleigh, Ritz

\[ E_{t,U} [\Psi_{t',U'}] = \langle \Psi | H_{t,U} | \Psi \rangle \]

\[ \frac{\partial E_{t,U} [\Psi_{t',U'}=0]}{\partial t'} = 0 \]

→ Hartree-Fock approximation

type of approximation ⇔ choice of reference system
Non-perturbative conserving approximations

Rayleigh, Ritz

\[ E_{t,U}[\Psi_{t',U'}] = \langle \Psi | H_{t,U} | \Psi \rangle \]

\[ \frac{\partial E_{t,U}[\Psi_{t',U'}]}{\partial t'} \bigg|_{t'=0} \neq 0 \]

\[ \rightarrow \text{Hartree-Fock approximation} \]

SFT

\[ \Omega_{t,U}[\Sigma_{t',U'}] = ? \]

\[ \frac{\partial \Omega_{t,U}[\Sigma_{t',U'}]}{\partial t'} \bigg|_{t'=0} \neq 0 \]

\[ \rightarrow \text{new approximations} \]

Type of approximation \(\leftrightarrow\) choice of reference system
non-perturbative, thermodynamically consistent, systematic approximations

$\Lambda_U[\Sigma]$ unknown but **universal**!

**original system:**

$$\Omega_{t,u}[\Sigma] = \text{Tr} \ln \frac{1}{G_{0,t}^{-1} - \Sigma} + \Lambda_U[\Sigma]$$

**reference system:**

$$\Omega_{t',u}[\Sigma] = \text{Tr} \ln \frac{1}{G_{0,t'}^{-1} - \Sigma} + \Lambda_U[\Sigma]$$

**combination:**

$$\Omega_{t,u}[\Sigma] = \Omega_{t',u}[\Sigma] + \text{Tr} \ln \frac{1}{G_{0,t}^{-1} - \Sigma} - \text{Tr} \ln \frac{1}{G_{0,t'}^{-1} - \Sigma}$$

→ non-perturbative, thermodynamically consistent, systematic approximations

→ $\Phi$-derivable, conserving, respecting Luttinger sum rule?
original system, $H_{t,U}$:

lattice model ($D = 2$) in the thermodynamic limit

n.n. hopping: $t$
local interaction: $U$
electron density: $n = N/L$
original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit
- n.n. hopping: $t$
- local interaction: $U$
- electron density: $n = N/L$

reference system, $H'_{t',U}$:

- system of decoupled clusters
- diagonalization
- trial self-energy: $\Sigma = \Sigma(t')$
- self-energy functional: $\Omega_t[\Sigma(t')]$
- stationary point: $\frac{\partial}{\partial t'} \Omega_t[\Sigma(t')] = 0$
original system, $H_{t,U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H'_{t',U}$:

system of decoupled clusters
**original system,** $H_{t,U}$:

lattice model ($D = 2$) in the thermodynamic limit

**reference system,** $H_{t',U}$:

system of decoupled clusters

cluster size: $L_c$

- $L_c \leq 2$: analytic
- $L_c \leq 6$: exact diagonalization
- $L_c \leq 12$: Lanczos method
- $L_c \leq 100$: stochastic techniques
example: \( D = 1 \) Hubbard model

\( T = 0 \), half-filling, \( U = 8 \), nearest-neighbor hopping \( t = 1 \)

variational parameter: nearest-neighbor hopping \( t' \) within the chain

\[ \Omega(t') \equiv \Omega[\Sigma(t')] \text{ stationary at } t'_{\text{min}} \neq t \]

\[ t'_{\text{min}} \approx t \]
original system, $H_{t,U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

system of decoupled clusters
original system, $H_{t,u}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',u}$:

system of decoupled clusters

variational parameters:
intra-cluster hopping
partial compensation of finite-size effects
cluster approximations

original system, \( H_{t,U} \):

lattice model \((D = 2)\) in the thermodynamic limit

reference system, \( H_{t',U} \):

system of decoupled clusters

variational parameters:

hopping between cluster boundaries

boundary conditions
boundary conditions

\[ \Omega \]

exact: Lieb, Wu (1968)

\[ D = 1 \text{ Hubbard model} \]
\[ T = 0, \text{ half-filling, } U = 8 \]
\[ t = 1 \]

open or periodic b.c. ?
open boundary conditions!
original system, $H_{t, U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t', U}$:

system of decoupled clusters
original system, $H_{t, U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H'_{t', U}$:

system of decoupled clusters

variational parameters:
on-site energies
thermodynamic consistency
cluster approximations

original system, $H_{t, U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t', U}$:

- system of decoupled clusters

  variational parameters:
  ficticious symmetry-breaking fields
  spontaneous symmetry breaking
original system, $H_{t,\mathcal{U}}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',\mathcal{U}}$:

- system of decoupled clusters
- variational parameters:
  - ficticious symmetry-breaking fields
  - different order parameters
antiferromagnetism

$D = 2$ Hubbard model, half-filling
antiferromagnetism

$D = 2$ Hubbard model, half-filling

QMC, VMC: extrapolated to $L \to \infty$, $T \to 0$

QMC: Hirsch (1985)
VMC: Yokoyama, Shiba (1987)
Non-perturbative conserving approximations

antiferromagnetism

\[ D = 2 \text{ Hubbard model, half-filling} \]

\[ \Gamma \quad X \quad M \quad \Gamma \]

QMC / MaxEnt: \( \beta = 10, 8 \times 8 \text{ cluster} \]
classification of approximations

original system, $H_{t,U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

system of decoupled clusters

$L_c = 4$
original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

- system of decoupled clusters

  $L_c = 1$

  Hubbard-I-type approximation
classification of approximations

original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

- system of decoupled clusters with additional bath sites
- $L_c = 1$, $L_b = 2$
- improved description of temporal correlations
classification of approximations

original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

- system of decoupled clusters with additional bath sites
  - $L_c = 1$, $L_b = 5$
- improved mean-field theory
classification of approximations

**original system,** $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

**reference system,** $H_{t',U}$:

- system of decoupled clusters with additional bath sites
  - $L_c = 1$, $L_b = \infty$
- optimum mean-field theory, DMFT
  - *Metzner, Vollhardt* (1989)
  - *Georges, Kotliar, Jarrell* (1992)
classification of approximations

original system, $H_{t, U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t', U}$:

- system of decoupled clusters with additional bath sites
  - $L_c = 4$, $L_b = \infty$
- cellular DMFT
  - Kotliar et al (2001)
  - Lichtenstein and Katsnelson (2000)
classification of approximations

original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

- system of decoupled clusters with additional bath sites
  - $L_c = 4$, $L_b = 5$
- variational cluster approach (VCA)
classification of approximations

original system, $H_{t,U}$:

- lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t',U}$:

- system of decoupled clusters with additional bath sites
  - $L_c = 4$, $L_b = 2$
- variational cluster approach (VCA)
classification of approximations

original system, $H_{t, U}$:

lattice model ($D = 2$) in the thermodynamic limit

reference system, $H_{t', U}$:

system of decoupled clusters with additional bath sites
$L_c = 4$
variational cluster approach (VCA)
classification of approximations

- Dynamical mean-field theory (DMFT): Metzner, Vollhardt (1989), Georges, Kotliar, Jarrell (1992)
- Cellular DMFT
- Dynamical impurity approach (DIA): Kotliar, Savrasov, Palsson (2001)
- Variational cluster approach: Potthoff (2003), Potthoff, Aichhorn, Dahnken (2004)
self-energy functional:

\[
\Omega_{t, U[\Sigma]} = \Omega_{t', U[\Sigma]} + \text{Tr} \ln \frac{1}{G_{0,t}^{-1} - \Sigma} - \text{Tr} \ln \frac{1}{G_{0,t'}^{-1} - \Sigma}
\]

\(\mu\) derivative:

\[
- \frac{\partial \Omega_{t, U[\Sigma]}}{\partial \mu} = - \frac{\partial \Omega_{t', U[\Sigma]}}{\partial \mu} - \frac{\partial}{\partial \mu} \text{Tr} \ln \frac{1}{G_{0,t}^{-1} - \Sigma} + \frac{\partial}{\partial \mu} \text{Tr} \ln \frac{1}{G_{0,t'}^{-1} - \Sigma}
\]

particle number and FS volume:

\[
N = N' - V_{FS}' + V_{FS}
\]

proliferation of the sum rule:

\[
N = V_{FS} \iff N' = V_{FS}'
\]
dynamical impurity approximation

Hubbard model, semielliptical free DOS \((W = 4)\)

\[
\begin{align*}
\varepsilon_c & \quad V \\
\varepsilon_0 &
\end{align*}
\]

two-site DIA:

- total particle number: 
  \((2\text{-site reference system})\)
  \(N' = 2\)
- Kondo regime: 
  \(\varepsilon_0 \ll \varepsilon_c, \mu \ll \varepsilon_0 + U\)
- DMFT: 
  \(\varepsilon_0 = \text{const} = 0\)
mass enhancement: \( \frac{m^*}{m} = z^{-1} = 1 - \Sigma'(\omega = 0) \)

- Mott transition for \( n \rightarrow 1 \) and strong \( U \)
- 2S-DMFT: non-conserving two-site approximation
Mott transition

\[ U \ll W \quad U \gg W \]

atom → solid

energy

metal → insulator

\[ IPE \quad PES \]
Mott transition: phase diagram

Hubbard model
half-filling
semielliptical DOS, $W = 4$
two-site DIA ($L_b = 2$)

$\rightarrow$ qualitative agreement with DMFT (QMC, NRG)

*Georges et al (1996), Joo, Oudovenko (2000), Bulla et al (2001)*
convergence with increasing $L_b$

Hubbard model
half-filling
semielliptical DOS
$W = 4$
DIA

Pozgajcic (2004)

→ quantitative agreement with DMFT (QMC, NRG)

Georges et al (1996), Joo, Oudovenko (2000), Bulla et al (2001)

→ extremely fast convergence with increasing $L_b$
Hubbard model, $D = 1, U = 4 = W, T = 0$: exact (Bethe ansatz) vs. DMFT vs. 2S-DIA
Luttinger sum rule for a $k$-independent self-energy:

$\Rightarrow V_{FS} = V_{FS}^{(0)}$

$V_{FS} = 2 \sum_{k} \Theta(\mu - \varepsilon(k) - \Sigma(0))$

$V_{FS}^{(0)} = 2 \sum_{k} \Theta(\mu_0 - \varepsilon(k))$

$\Rightarrow \mu = \mu_0 + \Sigma(0)$

$\rho(\omega) = \sum_{k} \delta(\omega + \mu - \varepsilon(k) - \Sigma(\omega))$

$\rho_0(\omega) = \sum_{k} \delta(\omega + \mu_0 - \varepsilon(k))$

$\Rightarrow \rho(0) = \rho_0(0)$
non-conserving approximations: Hubbard-I, 2S-DMFT
conserving approximation: two-site DIA
single-impurity Anderson model

sum rule fulfilled within 2S-DIA \(\Rightarrow\) sum rule fulfilled exactly for reference system

\[ N = V_{FS} \iff N' = V'_{FS} \]

direct check:
1) \(L_b = 2\): analytically
2) \(L_b = 4\): full diagonalization
3) \(L_b \leq 10\): Lanczos

\(\Rightarrow\) sum rule never violated

Green’s function: \(G_{\alpha\beta}(\omega)\)
diagonalized Green’s function: \(G_k(\omega)\)
Luttinger sum rule:

\[
\sum_{k,m} \alpha_m^{(k)} \Theta(\mu - \omega_m^{(k)}) = \sum_{k,m} \Theta(\mu - \omega_m^{(k)}) - \sum_{k,n} \Theta(\mu - \zeta_n^{(k)})
\]
$N = V_{FS} \Leftrightarrow N' = V'_{FS}$
dynamical cluster approximation (DCA)

Hubbard model, $D = 2$, n.n. hopping $t$, $U = W = 8t$, $T = W/60$, $L_c = 16$, QMC

$n = 0.95$  $n = 0.9$  $n = 0.8$

$A(k, \omega = 0)$  

$\Rightarrow$ sum rule violated close to Mott insulator
sum rule violated for Hubbard clusters?

\[ N = V_{FS} \iff N' = V'_{FS} \]

**direct check:**
1) \( L_c = 2 \): analytically
2) \( L_c = 4 \): full diagonalization
3) \( L_c \leq 10 \): Lanczos

→ sum rule violated for the Mott insulator

\[
\sum_{k,m} \alpha_m^{(k)} \Theta(\mu - \omega_m^{(k)}) = \sum_{k,m} \Theta(\mu - \omega_m^{(k)}) - \sum_{k,n} \Theta(\mu - \zeta_n^{(k)})
\]
finite Hubbard clusters

→ sum rule violated close to Mott insulator
Fermi-liquid theory: $N = V_{FS}$

proof: perturbation theory to all orders $n \ (n \to \infty) \ for \ T \to 0$

(weak-coupling) conserving approximations: truncation of $\Phi[G]$
- macroscopic conservation laws respected
- thermodynamically consistent
- Luttinger’s sum rule respected

non-perturbative construction of $\Phi[G]$ possible ($T > 0$)

self-energy-functional theory: non-perturbative conserving approximations
- dynamical impurity approximation (DIA)
- variational cluster approximation (VCA)
- DMFT, C-DMFT/DCA

sum rule: $N = V_{FS} \iff N' = V'_{FS}$

sum rule respected by DMFT, DIA $\iff$ sum rule holds for the (finite) single-impurity Anderson model (Friedel sum rule)

sum rule violated by DCA, VCA $\iff$ sum rule violated for Hubbard clusters

where is the defect in the proof? proposal: $\lim_{T \to 0} \lim_{n \to \infty} \neq \lim_{n \to \infty} \lim_{T \to 0}$