ASC summer school on
Numerical methods for correlated many-body systems
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The Numerical Renormalization Group (NRG)

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References: K.G. Wilson (Rev. Mod. Phys, 1975)
Bulla et al. (Rev. Mod. Phys, 2008)

Full-density-matrix NRG (fdm NRG)
AW and von Delft (PRL 2007)

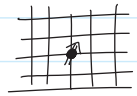
Link to tensor network states (Matrix Product State (MPS) description
AW, PRB 2011, PRB 2012

General implementation of abelian and non-abelian symmetries
AW, Ann. Phys (2012)

Quantum impurity models

NRG was invented for the very specific purpose to deal with (effective) quantum impurity systems

- screening of magnetic impurities in metalls
- quantum dots connected to electronic leads
- quantum bits connected to (dissipative) environment
- consider some arbitrary but fixed lattice site in isotropic medium
  ⇒ self-consistent effective impurity problem
  ⇒ dynamical mean field theory (DMFT)
  Metzner & Vollhardt (1989)



- etc.

Ingredients

- small quantum system with arbitrary interaction that can be (easily) simulated numerically, e.g. Hubbard site
- macroscopic non-interacting bath (typically fermionic) easy to solve analytically
- local coupling of impurity to bath

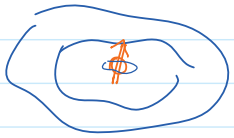
⇒ non-trivial dynamical effects due to strongly-correlated behavior

- dynamically generated low-energy scales which can be
- typically exponentially sensitive, e.g. Kondo temperature T_K
- where the dynamics for temperatures $T \lesssim T_K$ typically is inaccessible to perturbative treatment

⇒ need for unbiased exact methods: analytical (Bethe Ansatz) or numerical based on renormalization group arguments

Prototypical setup:

Single Impurity Anderson Model [SIAM; P.W. Anderson (1961)]



non-interacting metal ($\hat{=}$ Fermi sea, bath)

$$\hat{H}_{bath} \equiv \sum_{k,\sigma} \varepsilon_{k(\sigma)}\, \hat{c}^{\dagger}_{k\sigma}\, \hat{c}_{k\sigma} \qquad (1a)$$

"Magnetic impurity" e.g. iron impurities in noble metals (Au, Ag, ...)
de Haas (1934), J. Kondo (1964), Costi et al. (2009)

$$\hat{H}_{imp} \equiv \varepsilon_d\, \hat{n}_{d\sigma} + U\, \hat{n}_{d\uparrow}\, \hat{n}_{d\downarrow} \qquad (1b)$$

4 states: 0, 1, ↑, ↓

U: short-ranged on-site Coulomb interaction

$\hat{n}_{d\sigma} \equiv \hat{n}_{d\uparrow} + \hat{n}_{d\downarrow}$, $\hat{n}_{d\sigma} \equiv d^{\dagger}_{\sigma} d_{\sigma}$, $\sigma \in \{\uparrow, \downarrow\}$

"d-level", e.g. iron impurity with partially filled d-orbital

Coupling:

$$\hat{V} \equiv \sum_{k\sigma} V_{k(\sigma)}\, \hat{d}^{\dagger}_{\sigma}\, \hat{c}_{k\sigma} + h.c. \qquad (1c)$$

($\hat{c}_{k\sigma}$: spin preserving hopping)

$$= \sum_{\sigma} \hat{d}^{\dagger}_{\sigma} \underbrace{\sum_{k} V_{k\sigma}\, \hat{c}_{k\sigma}}_{\equiv \sqrt{\sum_k V_k^2}\; \hat{f}_{0\sigma}} + h.c. \qquad (2a)$$

$\equiv t_0$

$\hat{f}_{0\sigma}$ defines normalized fermionic mode of the bath such that $\{\hat{f}_{0\sigma}, \hat{f}^{\dagger}_{0\sigma'}\} = \delta_{\sigma\sigma'}$

$$\hat{V} \equiv t_0 \sum_{\sigma} \hat{d}^{\dagger}_{\sigma}\, \hat{f}_{0\sigma} + h.c. \qquad (2b)$$

Interpretation: while the $\hat{c}_{k\sigma}$ are delocalized eigenstates of the bath, their superposition in $\hat{f}_{0\sigma}$ describe an effective localized level that represents the only bath site in the close vicinity of the impurity that the impurity hybridizes with. (2c)

$$\Rightarrow \hat{H}_{SIAM} = \underbrace{\underbrace{\varepsilon_d\, \hat{n}_{d\sigma} + U n_{\uparrow} n_{\downarrow}}_{\equiv H_{imp}} + \underbrace{t_0 \sum_{\sigma} \hat{d}^{\dagger}_{\sigma}\, \hat{f}_{0\sigma} + h.c.}_{\equiv \hat{H}_{cpl} \equiv \hat{V}} + \underbrace{\sum_{k\sigma} \varepsilon_{k\sigma}\, \hat{c}^{\dagger}_{k\sigma}\, \hat{c}_{k\sigma}}_{\equiv H_{bath}}}_{\equiv \hat{H}_0 \equiv \hat{H}_0(\{\hat{f}_{0\sigma}, \hat{f}_{0\sigma}, \ldots\})} \qquad (3)$$

Continuum's description of the bath

$$\hat{H}_{bath} \xrightarrow{*)} \sum_{\sigma} \int d\varepsilon \cdot \varepsilon \cdot \hat{c}^{\dagger}_{\varepsilon\sigma}\, \hat{c}_{\varepsilon\sigma} \qquad (4a)$$

$$\hat{H}_{cpl} \xrightarrow{*)} \sum_{\sigma} \int d\varepsilon\, \sqrt{g(\varepsilon)}\, V(\varepsilon)\, \hat{d}^{\dagger}_{\sigma}\, \hat{c}_{\varepsilon\sigma} + h.c. \equiv t_0 \sum_{\sigma} \hat{d}^{\dagger}_{\sigma}\, \hat{f}_{0\sigma} + h.c. \qquad (4b)$$

where

$$t_0^2 \equiv \sum_k V_k^2 \longrightarrow \int d\varepsilon \underbrace{g(\varepsilon)\, V^2(\varepsilon)}_{\equiv \frac{1}{\pi}\Gamma(\varepsilon)} = \frac{1}{\pi}\int d\varepsilon\, \Gamma(\varepsilon) \qquad (4c)$$

with the hybridization function

$$\Gamma(\omega) \equiv -\,\mathrm{Im}\,\Delta(\omega) = \pi\, g(\omega)\, V^2(\omega) \qquad (5)$$

given the retarded bath Green's function

$$\Delta(\omega) \equiv \sum_k \frac{V_k^2}{\omega^+ - \varepsilon_k} \longrightarrow \int d\varepsilon\, g(\varepsilon)\, V^2(\varepsilon)\, \frac{1}{\omega^+ - \varepsilon_k} \qquad (6a)$$

NRG: $\frac{1}{t_0^2} \cdot \Delta(t) = G_0(t) \equiv \langle \hat{f}_{0\sigma} | (\hat{f}_{0\sigma})(t) \equiv -i\vartheta(t) \langle \{\hat{f}_{0\sigma}(t), \hat{f}^{\dagger}_{0\sigma}(0)\} \rangle_T$ (6b)

$\hookrightarrow$ $\frac{1}{t_0^2}\Delta(\omega)$ is the fermionic correlation function of the local bath level $\hat{f}_{0\sigma}$ in the absence of the impurity! Its local density of states (= spectral function) exactly represents the hybridization function $\Gamma(\omega) \geq 0$, up to normalization. (6c)

*) $\{\hat{c}_{k\sigma}, \hat{c}^{\dagger}_{k'\sigma'}\} = \delta_{kk'}\delta_{\sigma\sigma'} \rightleftharpoons \{\hat{c}_{\varepsilon\sigma}, \hat{c}^{\dagger}_{\varepsilon'\sigma'}\} = \delta_{\sigma\sigma'}\delta(\varepsilon - \varepsilon')$ (7)

$[1/\sqrt{\varepsilon}] \leftarrow [1/\varepsilon]$ dimension full!

$\delta(\varepsilon - \varepsilon') = \delta_{kk'} \frac{1}{\left|\frac{\partial \varepsilon}{\partial k}\right|} \equiv g(\varepsilon)$

$\rightarrow$ substitute: $\hat{c}_{k\sigma} \leftrightarrow \frac{\hat{c}_{\varepsilon\sigma}}{\sqrt{g(\varepsilon)}}$, $\sum_k \leftrightarrow \int g(\varepsilon) d\varepsilon$

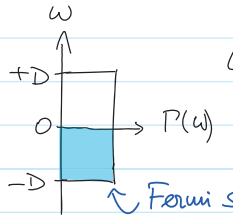
$\varepsilon \rightarrow \varepsilon(k)$ with level spacing $\delta_k = \varepsilon(k+1) - \varepsilon(k)$ such that $g(\varepsilon(k)) \cdot \delta_k \simeq 1$

(g: 1-particle density of states)

Focus on impurity dynamics

from the point of view of the impurity:
all that is relevant is the product $\rho(\varepsilon)*V^2(\varepsilon)$
i.e. the form of $\rho(\varepsilon)$ or $V(\varepsilon)$ individual is irrelevant (8)
↳ this introduces freedom to model the bath!

For simplicity:
Assume "box-distribution" for the hybridization function



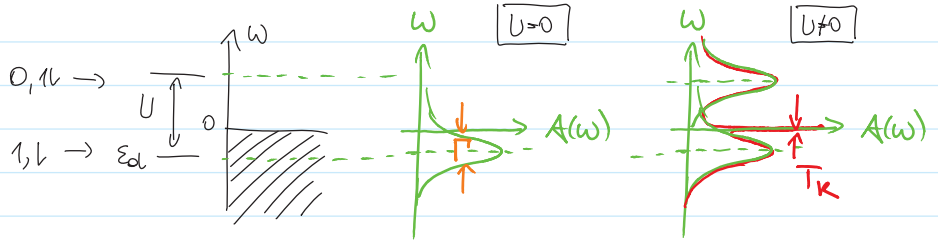
$$\Gamma(\omega) = \theta(|D-\omega|)\cdot\Gamma \qquad (9)$$

↳ two parameters only
- half-bandwidth $D := 1$ (typically sets unit of energy)
- hybridization strength Γ ($[\Gamma]$ = energy)

this allows one to focus on universal physical behavior
e.g. having $T_K \ll D$, for $|\varepsilon_d|, \Gamma, U < D$,
D becomes irrelevant for the physics at the impurity

Local density of states at impurity (≡ spectral function)

$$A_\sigma(\omega) \equiv -\frac{1}{\pi}\,\mathrm{Im}\,G_\sigma(\omega) \quad \text{where } G_\sigma(t) = -i\theta(t)\,\langle\{\hat d_\sigma(t), \hat d_\sigma^\dagger(0)\}\rangle_T \qquad (10)$$



$\Rightarrow$ Lorentzian $A(\omega) = \frac{\Gamma}{\pi}\frac{1}{(\omega-\varepsilon_d)^2+\Gamma^2}$
$\Rightarrow A(t) \sim e^{-\Gamma t}$

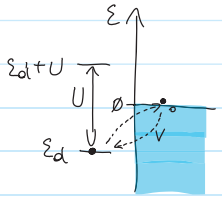
"Kondo resonance" of width T_K at $\omega = 0$

$\Rightarrow \Gamma \stackrel{!}{=} \frac{1}{\tau}$ with τ the lifetime of an electron at the impurity (11)

Kondo model (Kondo, 1964)

An effective low-energy model of the SIAM

Consider $\langle n_d\rangle \simeq 1$, energetically favored by Coulomb interaction
↳ "local-moment" regime:



e.g. at particle-hole symmetric point $\varepsilon_d = -\frac{U}{2}$

$$\Rightarrow \hat H_{imp} = -\frac{U}{2}\hat n_d + U\hat n_\uparrow \hat n_\downarrow = \frac{U}{2}\left(\hat n_d - 1\right)^2 + \text{const} \qquad (12a)$$

($\hat n_d^2 = \hat n_d + 2\hat n_\uparrow \hat n_\downarrow$)

$$\Rightarrow \text{energy cost: } 0 \;\underset{\varepsilon_d}{\longleftrightarrow}\; 1,\downarrow \;\underset{\varepsilon_d+U}{\longleftrightarrow}\; 2 \qquad (12b)$$

Charge fluctuations are considered processes of large energy cost
↳ include as 2nd order processes, starting with 1 particle at impurity
(Schrieffer-Wolff transformation (1966))

coupling between low-energy (1, ↓) and high-energy states (0, 2)
determined by the hybridization $\hat V$ in (4b)

$$\hat H_0^{\text{eff}} \simeq \hat V^\dagger \underbrace{\frac{1}{E_0 - \hat H}}_{\simeq \frac{1}{(-\frac{U}{2})}} \hat V \simeq -\frac{2t_0^2}{U}\sum_{\sigma\sigma'}\Big[\underbrace{(\hat d_\sigma^\dagger \hat f_{0\sigma})(\hat f_{0\sigma'}^\dagger \hat d_{\sigma'})}_{=-2\vec S_d\cdot\vec S_0 - \frac{1}{2}\hat n_d(\hat n_0 - 2)} + (\hat f_{0\sigma}^\dagger \hat d_{\sigma'})(\hat d_\sigma^\dagger \hat f_{0\sigma'})\Big]$$

(4b)

*) ↗

$$= +\underbrace{\frac{8t_0^2}{U}}_{=2J_0}\vec S_d\cdot\vec S_0 + \frac{2t_0^2}{U}\underbrace{\left(\hat n_{d\uparrow}\hat n_{0\uparrow} - \hat n_d - \hat n_0\right)}_{=0 \text{ since } \hat n_{d\uparrow} = n_d = 1}$$

factor 2 for convenience (see below)

$$\boxed{\hat H_0^{\text{eff}} \simeq H_0^{\text{Kondo}} = 2J_0\,\vec S_d\cdot\vec S_0} \quad (J_0 \geq 0, \text{ antiferromagnetic}) \qquad (13a)$$

eventually this will lead to full screening of the impurity spin by the bath
↳ Kondo "screening cloud", "Kondo singlet"

*) $\hat S_d^\alpha \equiv \sum_{\sigma\sigma'}\hat d_\sigma^\dagger\left(\frac{1}{2}\tau^\alpha_{\sigma\sigma'}\right)\hat d_{\sigma'}$ with τ^α the Pauli matrices ($\alpha = x, y, z$)

$$\hat S_0^\alpha \equiv \sum_{\substack{\sigma\sigma'\\ k\in a}}\frac{V_{ak}V_{ak'}}{\left(\sum_{k''\in a}V_{ak''}^2\right)}\underbrace{\hat c_{k\sigma}^\dagger\left(\frac{1}{2}\tau^\alpha_{\sigma\sigma'}\right)\hat c_{k'\sigma'}}_{\equiv\,\hat S^\alpha_{ak'}} \qquad (13b)$$

Poor Man's Scaling (Hewson (1993), Anderson (1970))

$$\hat{H}_0^{\text{Kondo}} = \underbrace{\frac{8t_0^2}{UN}}_{=2J} \sum_{kk'} \vec{S}_{0\sigma}\cdot\vec{S}_{kk'} \longrightarrow \sum_{kk'}\left(J_\perp\left(\hat{S}_{0\sigma}^{+}\hat{S}_{kk'}^{-}+\hat{S}_{0\sigma}^{-}\hat{S}_{kk'}^{+}\right)+2J_z\hat{S}_{0\sigma}^{z}\hat{S}_{kk'}^{z}\right) \quad (14a)$$

↑ for simplicity: $V_k = V$ ← generalize to anisotropic coupling

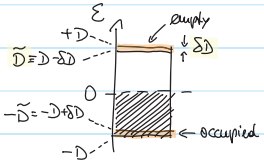
$\rho(\varepsilon) = \rho_0$ (box distribution) $\Rightarrow N \equiv \rho_0 \cdot 2D \hat{=}$ total # levels in bath

$$\hookrightarrow \rho_0 J = \rho_0 \frac{8t_0^2}{UN} = \rho_0 \cdot \frac{8}{U}\cdot\frac{2D}{N}\cdot\frac{\Gamma}{\pi} = \frac{8\Gamma}{\pi U} \quad \text{... dimensionless} \quad (14b)$$

(14c): $\frac{2D}{N} = \frac{1}{\rho_0}$

↳ eg. see (24) below!

Assume bandwidth of bath $D \gg J$



→ trace out largest energy shell of the bath by accounting for it's effective contribution via 2nd order perturbation theory (15)

Coupling between states with $|\varepsilon|<\tilde{D}$ and $|\varepsilon'|>\tilde{D}$ mediated by $\hat{c}^{+}_{k\tilde{\varepsilon}}\hat{c}_{k\varepsilon}$ in $\hat{S}^{\alpha}_{kk'}$ which can scatter an electron $k\varepsilon$ at low energy $|\varepsilon|<\tilde{D}$ into a state $k\tilde{\varepsilon}$ in the outer shell at large energy $|\tilde{\varepsilon}|\geq\tilde{D}$ (16a)

Two 2nd order processes:

- remove, then reinsert particle at $\tilde{\varepsilon} < -\tilde{D}$
- add, then remove particle at $\tilde{\varepsilon} > +\tilde{D}$ (16b)

By tracing out states at large energies, only the empty (full) state contributes at energies $\tilde{\varepsilon} > +\tilde{D}$ ($\tilde{\varepsilon}<-\tilde{D}$), respectively. (16c)

Got spin-half impurity → $(\hat{S}_{0\sigma}^{\pm})^2 = 0$, $(\hat{S}_{0\sigma}^{z})^2 = \mathbb{1}$, etc.

↳ this constrains the relevant 2nd order processes in (14a) to

$$\hat{S}_{0\sigma}^{-}\hat{S}_{0\sigma}^{+},\ \hat{S}_{0\sigma}^{+}\cdot\hat{S}_{0\sigma}^{-},\ \hat{S}_{0\sigma}^{\pm}\hat{S}_{0\sigma}^{z},\ \hat{S}_{0\sigma}^{z}\hat{S}_{0\sigma}^{\pm} \quad (16d)$$

(the $\hat{S}_{0\sigma}^{z}\cdot\hat{S}_{0\sigma}^{z}$ cancels by symmetry)

$$\text{e.g. } \delta\hat{H}_{\uparrow}^{(1)} \simeq \sum_{kk'}\sum_{|\tilde{\varepsilon}|>\tilde{D}}\left[\frac{J_\perp^2}{\emptyset-|\tilde{\varepsilon}|}\left(\hat{S}_{0\downarrow}^{-}\cdot\sum_{k}\hat{c}^{+}_{k\uparrow}\hat{c}_{k\downarrow}\right)\left(\hat{S}_{0\downarrow}^{+}\sum_{k'}\hat{c}^{+}_{k'\downarrow}\hat{c}_{k'\uparrow}\right)\right] \quad (17a)$$

(A): $|\tilde{\varepsilon}|>\tilde{D}$; (B): $|\tilde{\varepsilon}'|>\tilde{D}$

$\to \langle \hat{c}_{k\downarrow}\hat{c}^{+}_{k'\downarrow}\rangle \simeq \delta_{kk'}$

interested in low-energy properties $|\varepsilon|\ll\tilde{D}$

- need to destroy the particle that was created
- only contributes for positive $\tilde{\varepsilon}$

$$\simeq \frac{J_\perp^2}{-D}\,\hat{S}_{0\downarrow}^{-}\hat{S}_{0\downarrow}^{+}\cdot\sum_{kk'}\hat{c}^{+}_{k'\uparrow}\hat{c}_{k\uparrow}\cdot\rho(D)\cdot\delta D \quad (17b)$$

reversed order of (A) and (B) in (17a) → only contributes for neg. $\tilde{\varepsilon}$

$$\hookrightarrow \delta\hat{H}_{\uparrow}^{(2)} \simeq \frac{J_\perp^2}{-D}\,\hat{S}_{0\downarrow}^{+}\hat{S}_{0\downarrow}^{-}\cdot\sum_{kk'}\underbrace{\hat{c}_{k\uparrow}\hat{c}^{+}_{k'\uparrow}}_{=-\hat{c}^{+}_{k'\uparrow}\hat{c}_{k\uparrow}+\delta_{kk'}}\cdot\rho(D)\cdot\delta D \quad (17c)$$

must vanish by symmetry i.e. after $\sum_G(\dots)$ in (17e)

$$\delta\hat{H}_{\uparrow}^{(1)}+\delta\hat{H}_{\uparrow}^{(2)} = \frac{J_\perp^2}{+D}\underbrace{\left[\hat{S}_{0\downarrow}^{+},\hat{S}_{0\downarrow}^{-}\right]}_{=2\hat{S}_{0\downarrow}^{z}}\sum_{kk'}\hat{c}^{+}_{k\uparrow}\hat{c}_{k'\uparrow}\cdot\rho(D)\cdot\delta D \quad (17d)$$

include reverse spin orientation in (17a)

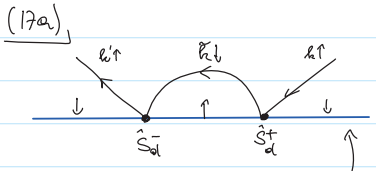
$$\sum_G\left(\delta\hat{H}_G^{(1)}+\delta\hat{H}_G^{(2)}\right) = \frac{J_\perp^2}{D}\,2\hat{S}_{0\sigma}^{z}\cdot\sum_{kk'}2\hat{S}_{kk'}^{z}\cdot\rho(D)\cdot\delta D \quad (17e)$$

with $dD = -\delta D < 0$ (D is decreased) and $\frac{dD}{D} = d\ln D$ (17f)

$$\frac{\partial J_\perp}{\partial\ln D} = -2\rho_0 J_\perp^2 \quad \text{(assuming constant } \rho(\varepsilon)=\rho_0) \quad (18)$$

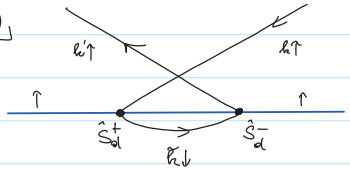
diagrammatic representation (e.g. read above equations right to left)

(17a)



blue line represents impurity

(17c)



(19)

Crossing of fermionic lines (blocks) yield the minus sign in (17c)

Similar for the remaining two processes in (16d)

$$\delta \hat{H}^{(3)}_{+} \simeq \frac{J_\parallel J_z}{-D} \underbrace{\hat{S}^z_d \hat{S}^z_d}_{\to -\frac{1}{2}} \cdot \sum_{kk'} \underbrace{\hat{c}^\dagger_{k\downarrow} \hat{c}_{k'\downarrow}}_{=\hat{S}^-_{kk'}} \cdot g(D)\,\delta D \qquad \text{(20a)}$$

↑ only $\tilde{\varepsilon} > \tilde{D}$ contributes

$$\hat{c}^\dagger_{k\downarrow} \hat{c}_{k'\downarrow} \cdot \left(\hat{c}^\dagger_{k\uparrow} \hat{c}_{k'\uparrow} - \hat{c}^\dagger_{k\downarrow} \hat{c}_{k'\downarrow} \right)$$

$$+ \frac{J_\parallel J_z}{-D} \underbrace{\hat{S}^z_d \hat{S}^+_d}_{\to +\frac{1}{2}} \cdot \sum_{kk'} \underbrace{\hat{c}^\dagger_{k\uparrow} \hat{c}_{k'\downarrow}}_{=\hat{S}^-_{kk'}} \cdot g(D)\,\delta D \qquad \text{(20b)}$$

↑ only $\tilde{\varepsilon} > \tilde{D}$ contributes

$$\left(\hat{c}^\dagger_{k\uparrow} \hat{c}_{k'\uparrow} - \hat{c}^\dagger_{k\downarrow} \hat{c}_{k'\downarrow} \right) \cdot \hat{c}^\dagger_{k\downarrow} \hat{c}_{k\uparrow} \qquad (-1)$$

$$= +2 \cdot \frac{J_\parallel J_z}{D} \hat{S}^+_d \sum_{kk'} \hat{S}^-_{kk'} \qquad \text{(20c)}$$

(17f) → (18):

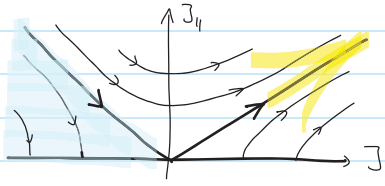
$$\frac{\partial J_\parallel}{\partial \ln D} = -2 g_0 J_z J_\parallel \qquad \text{(21a)}$$

$$\frac{\partial J_z}{\partial \ln D} = -2 g_0 J_\parallel^2 \qquad \text{(21b)}$$

Scaling trajectories / renormalization group (RG) flow

(21) defines renormalization group flow

- $\frac{(21b)}{(21a)} \Rightarrow \frac{\partial J_z}{\partial J_\parallel} = \frac{J_\parallel}{J_z} \Rightarrow J_z^2 = J_\parallel^2 + \text{const} \;\hat{=}$ parabolic/hyperbolic curves (22a)
  ↑ assuming g = const (e.g. box distribution)
- (21b) → J_z is strictly increasing when tracing out and thus reducing large D (22b)



ferromagnetic Kondo

regular/antiferromagnetic Kondo model flows towards
- strong coupling
- isotropic Kondo

(22c)

Ex, Isotropic Kondo

(21) $\xrightarrow{J_\parallel = J_z = J}$ $\frac{dJ}{d\ln D} = -2gJ^2$ (23a)

$$\int \frac{dJ}{J^2} = -2g \int d\ln D \Rightarrow \frac{1}{2gJ} = \ln D + \text{const} \Rightarrow D(J)\, e^{-\frac{1}{2gJ}} = \text{const} \qquad \text{(23b)}$$

assume constant density of states (box distribution), for simplicity

e.g. J grows to infinity *before* D is integrated out/down to zero

$$D_0(J_0)\, e^{-\frac{1}{2gJ_0}} = D^*(\infty)\, \underbrace{e^{-\frac{1}{\infty}}}_{=1} \equiv D^* =: T_K \qquad \text{(23c)}$$

↑ initial bare parameters in Kondo Hamiltonian

$$\boxed{T_K = D_0\, e^{-\frac{1}{2gJ_0}}}$$ (no phase transition; cross over scale) (24)

⇒ at the Kondo scale $T_K = D^*$ the perturbative treatment assuming small J breaks down

⇒ for energies (e.g. temperatures) smaller than T_K non-perturbative methods are required

In summary:

Impurity models with local spin moment generically feature Kondo type physics

- yields dynamically generated low-energy scale
- exponentially sensitive
- non-perturbative (e.g. cannot expand T_K in terms of small J)

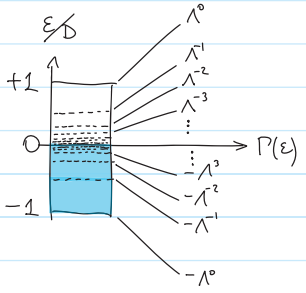
how to deal with this in practice?

Numerical renormalization group (NRG, Wilson, 1975)

For numerical treatment
need to discretize / coarse grain the bath continuum

Wilson: not by real space finite-size modelling
but by direct discretization in energy
("NRG" is much about "en-er-gy") (25a)

Logarithmic discretization: energy intervals $\begin{cases} I_n^+ \equiv [\frac{1}{\Lambda^{n+1}}, \frac{1}{\Lambda^n}] \\ I_n^- \equiv [-\frac{1}{\Lambda^n}, -\frac{1}{\Lambda^{n+1}}] \end{cases}$ (25b)



- $\Lambda > 1$ is a dimensionless discretization parameter (typically $\Lambda \gtrsim 2$; $n \in \mathbb{N}$) (25c)

$\Rightarrow$ can zoom in to arbitrarily small energies $\Rightarrow$ this can resolve dynamically generated, likely exponentially small energy scales

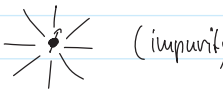
E.g. SIAM in Eqs.(1):

$$\hat{H}_{\text{opt}} = \sum_\sigma \int d\varepsilon \sqrt{\tfrac{\Gamma(\varepsilon)}{\pi}}\, \hat{d}_\sigma^\dagger \hat{c}_{\varepsilon\sigma} \stackrel{!}{=} \sum_{n\sigma} \hat{d}_\sigma^\dagger \underbrace{\int_{I_n} d\varepsilon \sqrt{\tfrac{\Gamma(\varepsilon)}{\pi}}\, \hat{c}_{\varepsilon\sigma}}_{\equiv V_n \hat{c}_{n\sigma}} \tag{26a}$$

$$\hookrightarrow V_n^2 = \frac{1}{\pi}\int_{I_n} \Gamma(\varepsilon)\, d\varepsilon \tag{26b}$$

$$\hat{H}_{\text{bath}} = \sum_\sigma \int d\varepsilon\, \varepsilon\, \hat{c}_{\varepsilon\sigma}^\dagger \hat{c}_{\varepsilon\sigma} \simeq \sum_{n\sigma} \varepsilon_n \hat{c}_{n\sigma}^\dagger \hat{c}_{n\sigma} \tag{27a}$$

$$\hookrightarrow \varepsilon_n \simeq \langle \hat{H}_{\text{bath}} \rangle_n \equiv \langle | \hat{c}_{n\sigma} \cdot \hat{H}_{\text{bath}} \cdot \hat{c}_{n\sigma}^\dagger | \rangle = \frac{1}{\int_{I_n} \Gamma(\varepsilon) d\varepsilon} \int_{I_n} d\varepsilon \cdot \varepsilon \cdot \Gamma(\varepsilon) \tag{27b}$$

"Star geometry":  (impurity couples to "diagonal" levels)

$$\hat{H}_{\text{SIAM}} \simeq \hat{H}_{\text{imp}} + \sum_\sigma \hat{d}_\sigma^\dagger \underbrace{\sum_n V_n \hat{c}_{n\sigma}}_{\equiv t_0 \hat{f}_{0\sigma}} + \sum_{n\sigma} \varepsilon_n \hat{c}_{n\sigma}^\dagger \hat{c}_{n\sigma} \tag{28a}$$

"chain geometry"
exact mapping onto effective 1D chain ("Wilson chain")

given: (1) diagonal bath Hamiltonian: matrix $H \equiv \begin{pmatrix} \ddots & & 0 \\ & \varepsilon_n & \\ 0 & & \end{pmatrix}$ in basis $\{\hat{c}_{n\sigma}\}$
(2) single normalized vector $|f_0\rangle \equiv \frac{1}{\sqrt{\sum_n V_n^2}} \begin{pmatrix} V_0 \\ V_1 \\ V_2 \\ \vdots \end{pmatrix}$ (28b)

↳ Lanczos tridiagonalization:
given arbitrary hermitian matrix H together with arbitrary starting vector $|f_0\rangle$

$$H|f_0\rangle = \varepsilon_0 |f_0\rangle + t_1 |f_1\rangle \tag{29a}$$

($|f_1\rangle$: this defines new normalized orthogonal component to $|f_0\rangle$)
(ε_0: captures component parallel to original $|f_0\rangle$)
here: matrix-vector multiplication in 1-particle space

For general n: 3-term recurrence relation

$$H|f_n\rangle = t_n^* |f_{n-1}\rangle + \varepsilon_n |f_n\rangle + t_{n+1} |f_{n+1}\rangle \tag{29b}$$

($|f_{n+1}\rangle$: this defines)

↳ e.g. by multiplication with $\langle f_{n-1}| \cdot$ from the left
$\langle f_{n-1}| \cdot H |f_n\rangle = \langle f_n | \cdot \underbrace{H^\dagger}_{=H} |f_{n-1}\rangle^* = t_n^*$ ... this was the definition for t_n!

no contributions for $n' < n-1$ since by multiplying $\langle f_{n'}| \cdot$
$\langle f_{n'}| \cdot H |f_n\rangle = \langle f_n | \cdot \underbrace{H^\dagger |f_{n'}\rangle}^* = 0$ if $n' < n-1$
(by construction, can be expressed in terms of the vectors $|f_0\rangle, \ldots, |f_{n'+1}\rangle$)

here: given diagonal matrix $H = \begin{pmatrix} \ddots & & 0 \\ & \varepsilon_n & \\ 0 & & \end{pmatrix}$ together with $|f_0\rangle$
↳ generate tridiagonal matrix $T \equiv \begin{pmatrix} \varepsilon_0 & t_1 & 0 \\ t_1^* & \varepsilon_1 & t_2 \\ & t_2^* & \ddots \\ 0 & & \end{pmatrix}$ together with basis $|f_n\rangle$ (29c)

Generic impurity Hamiltonian in Wilson chain setup

$$\hat{H} = \underbrace{\hat{H}_{imp}(\hat{d}_\sigma; U, \varepsilon_d, \dots) + \hat{H}_{cpl}(\hat{d}_\sigma, \hat{f}_{0\sigma}; \Gamma_0, \dots)}_{= \hat{H}_0(\hat{d}_\sigma, \hat{f}_{0\sigma}; U, \varepsilon_d, \Gamma, \dots)} + \hat{H}_{bath}(\hat{f}_{n\sigma}; t_n, \varepsilon_n) \quad (30a)$$

$$= \hat{H}_0(\hat{d}_\sigma, \hat{f}_{0\sigma}; U, \varepsilon_d, \Gamma, \dots) \quad (30b)$$

where $\hat{H}_{bath} = \sum_\sigma \sum_{n=0}^{\infty} \left(\varepsilon_n \hat{f}^\dagger_{n\sigma} \hat{f}_{n\sigma} + \left(t_{n+1} \hat{f}^\dagger_{n\sigma} \hat{f}_{n+1,\sigma} + \text{h.c.} \right) \right)$ (30c)

with the set $\{\hat{f}_{n\sigma}, \varepsilon_n, t_n\}$ fully determined

- by the hybridization function $\Gamma(\omega)$
- together with NRG discretization parameters $(\Lambda, z, \dots)$

shift in logarithmic discretization ↗

$\Lambda^{-n} \longrightarrow \Lambda^{-(n+z)}$ with $z \in [0, 1[$ (30d)

NB! no real space resolution! "Site" $\triangleq$ energy shell ("Wilson shell")

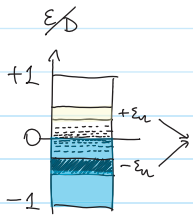
Energy scale separation

Crucially: log. discretization $\Leftrightarrow$ exponentially decaying hoping amplitudes

$$t_n \sim \Lambda^{-n/2} \quad (31)$$

↑

Why $t_n \sim \Lambda^{-n/2}$ and not Λ^{-n}?



1 energy level in the star geometry at energies $+\varepsilon_n \sim \Lambda^{-n}$ combined with the energy level at $-\varepsilon_n$

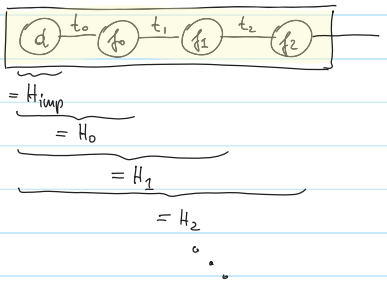
↳ contribute 2 sites in Wilson chain

↳ lowest energy scale e.g. Λ^{-N} in the star geometry reached after $2N$ sites in the chain geometry

↳ $t_{2N} \sim \Lambda^{-2N/2} \Lambda^{N}$ ✓

⇒ this justifies iterative complete diagonalization of the Wilson chain!

Iterative Diagonalization



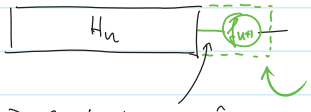
... proceed until dimension of many body Hilbert space reaches some max. number of states D, say at iteration n_0

$$\hat{H}_{n_0} |s\rangle_{n_0} = E_{sn_0} |s\rangle_{n_0} \quad (32)$$

↑

exact diagonalization

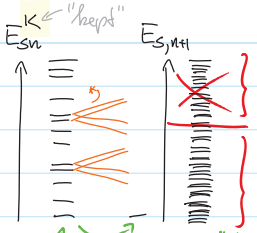
NRG iteration: enlarge Wilson chain by including next site/shell n+1



newly added site with d local states
e.g. d=4 for spinful fermionic site (33a)

D kept states in $\hat{H}_n$ (33b)

↳ (typically hundreds to thousands)



(34a)

$|s\rangle^K_{n+1} \Rightarrow$ next iteration n+2

$\Rightarrow$ refined level structure (34b)

d fold degenerate levels if $t_{n+1} = 0$

↳ by adding a smaller energy scale, due to energy scale separation the additional site splits levels within a closeby range in energy

↳ negligible influence of high-energy spectrum to low-energy spectrum (34c)

↳ this justifies truncation of high-energy states

Complete basis sets

Introduce environmental states for the sake of bookkeeping

$$|se\rangle_n = |s_n\rangle \otimes |e\rangle_n \qquad (35)$$

$|e\rangle_n$: complete basis for sites $n' > n$, e.g. Fock space

(approx.) many-body eigenstates for $\hat{H}_n$ i.e. spanning sites $n' \le n$

By considering some arbitrary but fixed max. Wilson chain length N

$$\Rightarrow \hat{H}_N |se\rangle_n^X \simeq E_{sn} |se\rangle_n^X \qquad (36a)$$

- approx eigenbasis for entire Wilson chain
- d^{N-n}-fold degenerate wrt. states $|e\rangle_n$

$$\Rightarrow |se\rangle_n^D \text{ forms complete (eigen) basis of Wilson chain}$$

$$\sum_{sen} |se\rangle_n^D {}_n^D\langle se| = \mathbb{1}^{(d^N)} \quad \text{(Anders \& Schiller, 2005)} \qquad (36b)$$

Complete eigenbasis that is efficiently tractable in practice

- real-time evolution (quantum quench) [Anders & Schiller, 2005]
- clean systematic framework for
  - dynamical correlation functions
  - statistical observables
  - at arbitrary temperatures

$\Rightarrow$ full-density matrix NRG ("fdm-NRG") [AW 2007, 2012]

- generalizes Hofstetter's DM-NRG (PRL 2000)
- can compute textbook Lehmann expressions exactly in a quantum-many-body context!
  exp. larger Hilbert space? here partly an illusion since tractable!

Many-body state space representation

Get iterative construction of low-energy basis

$$|s\rangle_{n+1} = \sum_{\substack{\sigma_{n+1} \\ s_n}} A^{[\sigma_{n+1}]}_{s_n, s_{n+1}} |\sigma_{n+1}\rangle \otimes |s\rangle_n \equiv |s_n\rangle \to \boxed{A} \to s_{n+1} \qquad (37a)$$

($|\sigma_{n+1}\rangle$ on A)

$$= |s_{n-1}\rangle \to \boxed{A} \to s_n \quad (|\sigma_n\rangle \text{ on } A)$$

$$\equiv |\varnothing\rangle \to \boxed{A_{-1}} \to \boxed{A_0} \to \boxed{A_1} \to \cdots \to \boxed{A_{n-1}} \to \boxed{A_n} \to \boxed{A_{n+1}} \to \qquad (37b)$$

($|\sigma_{-1}\rangle$ $|\sigma_0\rangle$ $|\sigma_1\rangle$ … $|\sigma_{n-1}\rangle$ $|\sigma_n\rangle$ $|\sigma_{n+1}\rangle$)

$$\equiv \quad \sigma_{-1}\ \sigma_0\ \sigma_1\ \sigma_2\ \cdots\ \sigma_{n-1}\ \sigma_n\ \sigma_{n+1} \qquad (37c)$$

$$\equiv \sum_{\sigma_{-1}, \ldots, \sigma_{n+1}} \prod_{n' \le n} A^{[\sigma_{n'}]}_{n'} |\sigma_{n+1}, \sigma_n, \ldots, \sigma_0, \sigma_{-1}\rangle \qquad (37d)$$

… "matrix product state"

exactly the same as in DMRG (White, 1992)
Rommer (1995), Schollwöck (2005, 2011)

In a sense: Since NRG zooms in exponentially into the low-energy state space

$\Rightarrow$ NRG computes the ground state of the semiinfinite Wilson chain
$\Rightarrow$ at any finite intermediate iteration got many "block states" $|s\rangle_n$

Indeed, may do variational optimization for ground state on Wilson chain of length N (Sakai, 2008)
↳ for all practical purposes, negligable difference with NRG basis for $n' < N - 10$ (e.g. for $\Lambda \ge 2$)

$\Rightarrow$ energy scale separation governed by Λ
$\Rightarrow$ NRG fails when applied to uniform systems e.g. $\Lambda \to 1^+$

Ex. Impurity spectral function

In Lehmann representation

$$G_{ab}(t) = -i\vartheta(t)\,\langle\{\hat{a}_a(t), \hat{a}_b^\dagger(0)\}\rangle_T \equiv -i\vartheta(t)\,\langle\{\hat{B}(t), \hat{C}^\dagger(0)\}\rangle_T$$

$$\hookrightarrow A(\omega) = -\tfrac{1}{\pi}\mathrm{Im}\,G(\omega) = \sum_{a,b} (\delta_a + \delta_b)\, \underbrace{\langle a|\hat{B}|b\rangle}_{\equiv B_{ab}} \underbrace{\langle b|\hat{C}^\dagger|a\rangle}_{= C_{ab}^*}\, \delta(\omega - E_{ab})$$

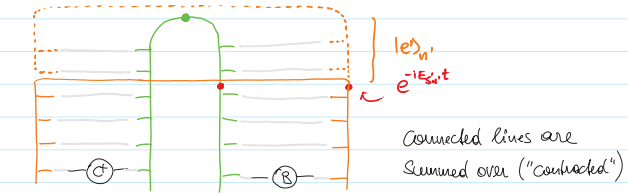
complete eigenbasis $H|a\rangle = E_a|a\rangle$
where in thermal equilibrium $\delta_a(T) = \frac{1}{Z} e^{-\beta E_a}$
with $\beta \equiv \frac{1}{T}$, $Z(T) = \sum_a e^{-\beta E_a}$

Typical structure: $\mathrm{tr}\left(\frac{1}{Z} e^{-\beta\hat{H}} \cdot e^{i\hat{H}t}\, \hat{B}\, e^{-i\hat{H}t} \cdot \hat{C}^\dagger\right)$

complete basis $|s\rangle_n^D$ → $e^{i E_{sn}^D}$; $e^{-i E_{sn}^D}$

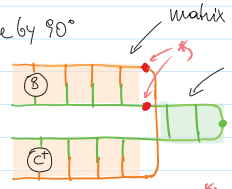
$\hat{\mathbb{1}}'$ ... need to insert another complete basis set $|s'\rangle_{n'}$ to reduce $e^{-i\hat{H}t}$ to simple phase factors

$${}_n\langle s|\, \hat{C}^\dagger\, |s\rangle_n^D\, \frac{e^{-\beta E_{sn}^D}}{Z}\, {}_n^D\langle s|\, e^{i\hat{H}t} \hat{B} e^{-i\hat{H}t}\, |s'\rangle_{n'}$$



Connected lines are summed over ("contracted")

Rotate by 90°



matrix elements in basis $|s'\rangle_{n'}$ } D×D matrices
reduced density matrix }

$$\rho_{s'n} \equiv \mathrm{tr}_{n''>n'}\left(\sum_s \frac{e^{-\beta E_{sn}^D}}{Z_n} |s\rangle_n^D\, {}_n^D\langle s|\right)$$

phase factors $e^{-i(E_{s'n'} - E_{sn})t}$
Fourier trafo $\delta(\omega - (E_{s'n'} - E_{sn}))$

Summary

NRG is tailor made for quantum impurity models including effective impurity models e.g. in the context of DMFT

NRG can deal with exponentially small energy scales at linear additional cost!
NRG intrinsically deals with finite temperature T but this can be T=0!

NRG computes correlation functions directly on the real frequency axis
↳ this is contrast to Quantum Monte Carlo (QMC) which operates on imaginary frequency axis (Matsubara)
↳ no need for numerically ill-conditioned analytic continuation

NRG operates on effective, mapped 1D chain geometry
↳ ideally suited for matrix product states (MPS)
↳ can generate hybrid algorithms with DMRG (same algebraic framework (AW et al, 2009)

Same as for other methods, numerical cost scales exponentially in number of flavors / channels
↳ in case of symmetric flavors can efficiently explore abelian + non-abelian symmetries (AW, 2012)

Note for hands-on session in the afternoon:
X11 window server required for graphical windows
↳ non-mac/linux users may want to install X11 or equivalent.