Entanglement spectra in the NRG

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Outline

- Brief introduction to the Numerical Renormalization Group (NRG)
  - iterative diagonalization of quantum impurity models
  - energy flow diagram and finite size scaling
  - entanglement entropy and area law
- Natural emergence of reduced density matrices
- Entanglement flow diagram
  - low-energy fixed point spectra
  - Important “feed-back” from small to large energy scales
- Summary and outlook
Kondo Hamiltonian

\[ \mathcal{H} = B \cdot \hat{s} + 2J \hat{s} \cdot \hat{S} + \int_{-D}^{D} d\epsilon \, \epsilon \, \hat{c}^\dagger_{\epsilon \mu} \hat{c}_{\epsilon \mu} \]

\[ \hat{S} \equiv \frac{1}{2} \int_{-D}^{D} d\epsilon d\epsilon' \rho \, \hat{c}^\dagger_{\epsilon \mu} \sigma_{\mu \mu'} \hat{c}_{\epsilon' \mu'} \]

\[ T_K = \sqrt{2\rho J} e^{-\frac{1}{2\rho J}} \]

logarithmic discretization + tridiagonalization → Wilson chain:

\[ \hat{H} = \hat{H}_{\text{dot}} + (2\rho J D) \hat{s} \cdot \hat{\tau} + \frac{1}{2} \left( 1 + \frac{1}{\Lambda} \right) \sum_{n=0}^{\infty} \xi_n \Lambda^{n/2} \left( \hat{f}^\dagger_{n\mu} \hat{f}_{n+1,\mu} + \text{H.c.} \right), \quad \hat{\tau} \equiv \hat{f}^\dagger_{0\mu} \sigma_{\mu \mu'} \hat{f}_{0\mu'} \]

Review Bulla et al. (RMP 2008)
Kondo (1964)
Entanglement spectra in the numerical renormalization group

NRG energy eigenstates

Anders and Schiller (2005)

Black-box algorithms for dynamical correlation functions (Lehmann representation)
Single impurity Anderson model

\[ \hat{H} = \sum_{\sigma} \varepsilon_{d\sigma} \hat{n}_\sigma + U \hat{n}_\uparrow \hat{n}_\uparrow + \sqrt{\frac{2\Gamma}{\pi}} \sum_{k,\sigma} \left( \hat{c}^\dagger_{k\sigma} \hat{d}_\sigma + H.c. \right) + \sum_{k,\sigma} \varepsilon_{k\sigma} \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} \]

**Entanglement spectra in the numerical renormalization group**
Correlation functions (Lehmann representation)

- Correlation functions
  \[ G_d(t) = \langle e^{i\hat{H}t} \hat{d} e^{-i\hat{H}t} \cdot \hat{d}^\dagger \rangle_T \]

  \[ A_d(\omega) \equiv \int \frac{dt}{2\pi} e^{i\omega t} G_d(t) = \sum_n \sum_{ss' \notin KK, e} \rho_{ss'}^{[n]} \cdot |n\langle se|\hat{d}|s'e\rangle_n|^2 \cdot \delta(\omega - E_{ss'}) \]

  \[ \int A(\omega)d\omega = \langle \{d, d^\dagger\} \rangle_T = 1 \]

  fulfilled up to double precision noise! \((10^{-16})\)

- \( \text{tr}(\hat{C}^\dagger \cdot \rho_T \cdot \hat{B}(s)) \)

- Collecting spectral data in a single sweep having \((s,s') \notin \{KK\}\)

- \( R_n \equiv \sum_{n' \geq n} w_{n'} \rho_{n,n'}^{FD_M}(T) \)

- See also DM-NRG (Hofstetter, 2000)
NRG and area law

- NRG and DMRG are based on the same algebraic structure: matrix product states (MPS)
- MPS successful in 1D because of area law: entanglement entropy $S$

$$S = \text{tr} (\rho_A \log \rho_A) = \text{tr} (\rho_B \log \rho_B)$$
$$\propto \text{area between } A \text{ and } B$$
$$\lesssim \log L \text{ (for ground states in 1D)}$$

Wolf et al. (PRL 2008); Eisert et al. (RMP 2010)
NRG and area laws

Entanglement spectra in the numerical renormalization group

calculated w.r.t. “overall ground state”

Entanglement entropy $S_E$

Wilson shell $n$ (even iterations)

$E_K = 8$

$\Lambda = 2$, $N = 99$, $N_k \leq 380$ (2260)

using $SU(2)_{\text{charge}} \otimes SU(2)_{\text{spin}}$
Entanglement spectra in the numerical renormalization group

Exponentially reduced importance of states at higher energy

\[ \rho(E) \sim e^{-4.6E} \]

\( \varepsilon_{\chi=5\%}=6 \cdot 10^{-12} \)

For each iteration \( n \):

\[ \hat{H}|s\rangle = E_s|s\rangle \iff \rho_s \equiv \langle s|\hat{\rho}|s\rangle \]

\[ \hat{\rho}|r\rangle = \rho_r|r\rangle \iff E_r \equiv \langle r|\hat{H}|r\rangle \]

\( \text{eig}(\rho) \) decays exponentially with excitation energy (non-gapped system!)

\[ \Rightarrow \text{a consequence of energy scale separation} \]
Entanglement spectra in the numerical renormalization group

Entanglement flow diagram (SIAM, B=0)

Entanglement spectra
Li, Haldane (2008)
Strong coupling fixed point spectra (SIAM, B=0)
Entanglement spectra in the numerical renormalization group

Entanglement flow diagram (SIAM, $B>0$)

- $n_0 = 8$
- $n_0 \rightarrow \infty$
Entanglement spectra (SIAM, B>0)
Important “feed-back” from small to large energy scales

DM-NRG (Hofstetter 2000): $B \approx T_K$

- requires reduced density matrices which *properly* encode the low-energy physics
- the resulting DM is *not necessarily* a thermal density matrix at intermediate iteration $n$!
- important for DMFT in the presence of (small) symmetry breaking perturbations
Implications

- Within NRG / DMRG / VMPS / PEPS typically got **both**: \( H_{\text{eff}}(n) \) and \( \rho(n) \)

![Diagram showing entangled system and environment](image)

- Q. How does \( H_{\text{eff}}(n) \) compare with entanglement Hamiltonian of \( \rho(n) \)?

- Taking overall ground state: if \( H_{\text{eff}}(n) \) differs strongly from the entanglement Hamiltonian of \( \rho(n) \), this indicates
  - importance of physics at significantly smaller energy scale
  - not just finite size effect: also affects dynamics at large energies
Summary and Outlook

- Analyzed entanglement spectra within the NRG
  - unique perspective: $H_{\text{eff}}(n)$ built from large energies
  - $\rho_{\text{red}}(n)$ represents the traced out low-energy physics

- Two regimes at higher energies
  - entanglement spectrum $\text{ES}[\rho_{\text{red}}(n)]$ w.r.t. overall ground state
    - does / does not agree with eigenspectrum of $H_{\text{eff}}(n)$

- Clear relevance for dynamical quantities at finite (high) energies

- Linked to “further relevant information” at the low-energy scale

Outlook

- “non-thermal” reduced density matrices
- better quantitative understanding of connection between $H_{\text{eff}}(n)$ and $\rho_{\text{red}}(n)$

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