Wilson Chain for a general impurity problem

Žiga Osolin[1], Rok Žitko[1,2]
[1]Jožef Stefan Institute, Ljubljana, Slovenia
[2] Faculty for Mathematics and Physics, Ljubljana, Slovenia

"Jožef Stefan" Institute

Introduction

Wilson chain is a required format of the Hamiltonian to treat with the numerical normalization group (NRG). Construction for a general structure of the impurity problem is not a trivial problem. We need it to treat multiple orbitals with inter-orbital mixing – the problem also appear in the cluster dynamical mean field (DMFT) treatment of the lattice problem.

We would like to transform the Hamiltonian to a chain form with **the following requirements**:

1. The impurity part is the first chain element.
2. Chain has exponential energy separation; the first N chain elements describe the system down to energy exp(-ΛN/2).
3. The transformation should impose as few approximations as possible.

Generalized impurity Hamiltonian

$$H = H_{imp} + \sum_{ki} \epsilon_{ki} c^\dagger_{ki} c_{ki} + \sum_{kij} \left(V_{kij} d^\dagger_i c_{kj} + V^*_{kji} c^\dagger_{kj} d_i \right)$$

Mapping to energy space

The following relation must hold to yield the same action:

$$\frac{\partial f_l(x)}{\partial x} h_{il}(f_l(x)) h^*_{jl}(f_l(x)) = \sum_k V_{ilk} V^*_{jlk} \delta(x - \epsilon_{kl}),$$

where f is the inverse of g. Summing the relation over l

$$\sum_l \frac{\partial f_l(x)}{\partial x} h_{il}(f_l(x)) h^*_{jl}(f_l(x)) = \frac{1}{\pi} \Gamma_{ij}(x). \qquad (1)$$

connects the impurity's hybridization function with the new Hamiltonian with yet unknown functions f (g) and h.

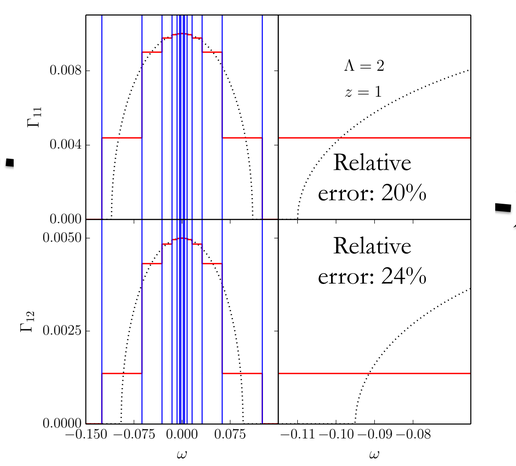
Continuous energy Hamiltonian

$$H = H_{imp} + \sum_i \int_{-1}^{1} \mathrm{d}\epsilon g_i(\epsilon) a^\dagger_{\epsilon i} a_{\epsilon i} + \sum_{ij} \int_{-1}^{1} \mathrm{d}\epsilon \left(h_{ij}(\epsilon) d^\dagger_i a_{\epsilon j} + H.c. \right).$$

Logarithmic discretization (with z-averaging):

$$x_n = \Lambda^{1-n-z}$$
$$I^-_n = [-x_n, -x_{n-1}]$$
$$I^+_n = [x_{n+1}, x_n]$$

Needed for **energy separation**!



Star representation Hamiltonian

$$H = H_{imp} + \sum_{ni} \left(\xi^+_{ni} a^\dagger_{ni} a_{ni} + \xi^-_{ni} b^\dagger_{ni} b_{ni} \right) +$$
$$\frac{1}{\sqrt{\pi}} \left[\sum_{ij} d^\dagger_i \sum_n \left(\gamma^+_{nij} a_{nj} + \gamma^-_{nij} b_{nj} \right) + H.c. \right]$$

Logarithmic discretisation - crude

We can choose $f_l(x) = x$, greatly simplifying Eq. (1) to

$$\boldsymbol{h}(x)\boldsymbol{h}^\dagger(x) = \frac{1}{\pi}\boldsymbol{\Gamma}(x), \qquad \boldsymbol{h}(x) = \frac{1}{\sqrt{\pi}}\sqrt{\boldsymbol{\Gamma}}(x).$$

For each interval only **retain only constant** wave function (approximation).

$$\gamma^\pm_{nij} = \left(\int^{\pm,n} \mathrm{dx} \boldsymbol{\Gamma}(x) \right)^{1/2}_{ij} \qquad \xi^\pm_{ni} = \frac{1}{d_n} \int^{\pm,n} x \cdot \mathrm{dx}$$

Logarithmic discretisation - fitting

For each interval, h(x) is constant (so we only couple to k=0 wave) but f(x) is chosen so that difference between the left and right side of the Eq. (1) is minimal using least squares fitting:

- Linearly discretize interval to M points – f is different in each point
- MN(N+1)/2 equations and MN+N(N+1)/2 unknowns
- f is monotonic on each interval (so we can calculate its inverse to get g) – we use unconstrained least squares using re-parameterization

$$\gamma^\pm_{nij} = \sqrt{\pi d_n} h^\pm_{ij} \qquad \xi^\pm_{ni} = \int \mathrm{dx} \cdot f^{-1}_i(x)$$

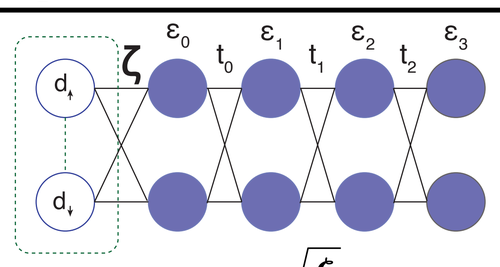
The **same results** as conventional discretization scheme for the diagonal case!
We use correction factor: $A_\Lambda = \frac{1}{2}\frac{\Lambda+1}{\Lambda-1}\ln\Lambda$

Star to chain transformation (Lanzcos)

The first state is the one that directly coupled to the impurity:

$$\boldsymbol{f}_0 = \frac{1}{\boldsymbol{\xi}} \sum_n \left(\gamma^+_n \boldsymbol{a}_n + \gamma^-_n \boldsymbol{b}_n \right), \qquad \boldsymbol{\xi} = \sum_n \left((\gamma^+_n)^2 + (\gamma^-_n)^2 \right).$$

New states are produced with iterative block diagonalisation. Special care must be taken with the order of multiplication and conjugation for complex coefficients. The procedure is numerically unstable: we use GMP arbitrary precision floating points with 3000 mantissa bits. This suffices for stability of 4x4 internal space matrices for chain lengths up to 30.



Wilson chain Hamiltonian

$$H = H_{imp} + \sum_n \left(\boldsymbol{f}^\dagger_n \boldsymbol{\epsilon}_n \boldsymbol{f}_n + \boldsymbol{f}^\dagger_n \boldsymbol{t}_n \boldsymbol{f}_{n+1} + H.c. \right) + \sqrt{\frac{\boldsymbol{\xi}}{\pi}} \left(\boldsymbol{d}^\dagger \boldsymbol{f}_0 + H.c. \right).$$

References

- R. Bulla, T. A. Costi and T. Pruschke: Numerical renormalization group method for quantum impurity systems. RMP 80, 395, 2008.
- V. L. Campo and L. Oliveira: Alternative discretization in the numerical renormalization-group method. PRB 72, 104432, 2005.
- R. Zitko and T. Pruschke: Energy resolution and discretization artifects in the numerical renormalization group. PRB 79, 085106, 2009.
- J. G. Liu, D.Wang and Q. H. Wang: Quantum impurities in channel mixing baths. arXiv 1509.01461, 2015.

Conclusion

We have tested Wilson chain generation for 4 channel problem (2 orbitals with spin flavour). The NRG code must use symmetries to handle so big problems using iterative diagonalisation.
We plan to use the discretization scheme for the cluster DMFT loop with the NRG as an impurity solver.