Self-energy trick

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Abstract

Notes on the self-energy trick and its implementation using `NRG Ljubljana` library.

Contents

1 Self-energy trick

The most straightforward way of computing the self-energy Σ is the Dyson equation

$$G(z)^{-1} = G_0(z)^{-1} - \Sigma(z)^{-1}. \tag{1}$$

However, since G_0 is exact and G is calculated numerically, taking the difference of these two quantities introduces numerical errors. These can be avoided by using various combinations of correlation functions. This technique is known in the literature as self-energy trick and was first introduced by Bulla et. al. [1] Recently, Kugler [2] proposed an improvement of this technique by introducing further correlation functions. We use this technique in our implementation of the DMFT loop.

Kugler's self-energy trick relies on the following four fermionic correlation function, which can in principle be matrix valued:

$$G_{\alpha\alpha',z} = \langle\langle d_\alpha; d^\dagger_{\alpha'}\rangle\rangle_z, \quad I_{\alpha\alpha' z} = \langle\langle q_\alpha, q^\dagger_\alpha\rangle\rangle_z, \tag{2a}$$

$$F^{\mathrm{L}}_{\alpha\alpha',z} = \langle\langle q_\alpha; d^\dagger_{\alpha'}\rangle\rangle_z; \quad F^{\mathrm{R}}_{\alpha\alpha',z} = \langle\langle d_\alpha; q^\dagger_\alpha\rangle\rangle_z \tag{2b}$$

which are numerically computed in the NRG part of the code. Here, d_α is the impurity operator labeled by an index α which enumerates spin and possibly other quantum numbers. The auxiliary operator is defined as

$$q_\alpha \equiv [d_\alpha, H_{\mathrm{int}}], \quad q^\dagger_\alpha = [H_{\mathrm{int}}, d^\dagger_\alpha], \tag{3}$$

where H_{int} is the interacting part of the Hamiltonian. When the correlation functions in Eq. (2) are diagonal (and are thus labeled by only one index α), it then follows $F^{\mathrm{L}}_{\alpha z} = F^{\mathrm{R}}_{\alpha z}$. In the general case, they are still related by symmetry.

Matrix-valued correlation functions are obtained from the quadratic Hamiltonian

$$H_0 = \sum_{\alpha\alpha'} d^\dagger_{\alpha'} \epsilon_{d,\alpha'\alpha} d_\alpha + \sum_{k,\alpha\alpha'} c^\dagger_{k\alpha'} \epsilon_{k,\alpha'\alpha} c_{k\alpha'} + \sum_{k,\alpha\alpha'} \left(d^\dagger_{\alpha'} V_{k,\alpha'\alpha} c_{k\alpha} + \mathrm{H.c.} \right) \tag{4}$$

if the off-diagonal elements ($\alpha \neq \alpha'$) are non-zero; here, ϵ_d, ϵ_k and V_k are matrices. The bare propagator G_z^0 can be written in terms of the hybridization function

$$\Delta_z = \sum_k V_k (z\mathbf{1} - \epsilon_k)^{-1} V_k^\dagger \tag{5}$$

as

$$\left(G_z^0\right)^{-1} = z\mathbf{1} - \epsilon_d - \Delta_z. \tag{6}$$

The two main formulas to calculate the self-energy Σ_z are then

$$\Sigma_z^{\mathrm{FG}} = F_z^{\mathrm{L}} G_z^{-1} = G_z^{-1} F_z^{\mathrm{R}}, \tag{7a}$$

$$\Sigma_z^{\mathrm{IFG}} = \Sigma^{\mathrm{H}} + I_z - F_z^{\mathrm{L}} G_z^{-1} F_z^{\mathrm{R}}, \tag{7b}$$

where the superscripts indicate the correlation functions used to calculate Σ_z; Eq. (7a) corresponds to the old(er) trick by Bulla [1] and Eq. (7b) to the new Kugler formula [2]. The Hartree self-energy is defined as

$$\Sigma^{\mathrm{H}}_{\alpha\alpha'} = \langle\{[d_\alpha, H_{\mathrm{int}}], d^\dagger_{\alpha'}\}\rangle = \langle\{q_\alpha, d^\dagger_{\alpha'}\}\rangle. \tag{8}$$

2 Operator definitions in NRG Ljubljana

In the package NRG Ljubljana, there is a set of predefined operators as well as an option to define new arbitrary operators through Mathematica. Since the package exploits the symmetries of the model and the operators to speed up diagonalization, the defined operators must match the symmetry type given as an input parameter at the beginning of a calculation. The required operators for a given symmetry type are

1. `QS`: $U(1)_{\mathrm{charge}} \otimes SU(2)_{\mathrm{spin}}$, charge and spin conservation.
2. `QSZ`: $U(1)_{\mathrm{charge}} \otimes U(1)_{\mathrm{spin}}$, again $U(1)$ symmetry in the charge space and a broken symmetry in the spin space (usually due to an external magnetic field in z-direction).
3. `U1`: $U(1)_{\mathrm{charge}}$, only charge conservation, no symmetry in spin space.
4. `SPSU2`: $SU(2)_{\mathrm{spin}}$, no charge conservation (superconductivity)
5. `SPSU1`: $U(1)_{\mathrm{spin}}$ (S_z component), no charge conservation (superconductivity)

We define one auxiliary operator in the `model.m` file

```
opcd[#1, #2] = (-1)^#2 d[1 -#1, 1 - #2];
```

this operator has the correct symmetry properties in the superconducting case. For the correlation functions F^{L}, F^{R} and I we need

```
selfopd =  ( Chop @ Expand @ komutator[Hselfd /. params, d[#1, #2]] )&;
```

while for the constant Hartree term we define

```
SigmaHd = Expand @ antikomutator[ selfopd[#1, #2], d[#3, #4] ] /. params &;
```

In the `QS` and `SPSU2` case we need to take the average of both spin species, i.e.,

$$\Sigma^{\mathrm{H}} = \frac{1}{2}\left(\Sigma^{\mathrm{H}}_{\uparrow} + \Sigma^{\mathrm{H}}_{\downarrow}\right). \tag{9}$$

The elements of this matrix in the `SPSU2` case are thus calculated as

```
SigmaHdAvg11 := Expand @ (SigmaHd[CR, UP, AN, UP]+SigmaHd[CR, DO, AN, DO])/2;
SigmaHdAvg12 := Expand @ (SigmaHd[AN, DO, AN, UP]+SigmaHd[AN, UP, AN, DO])/2;
SigmaHdAvg21 := Expand @ (SigmaHd[CR, UP, CR, DO]+SigmaHd[CR, DO, CR, UP])/2;
SigmaHdAvg22 := Expand @ (SigmaHd[AN, DO, CR, DO]+SigmaHd[AN, UP, CR, UP])/2;
```

3 Results for various symmetry classes

We focus on the single impurity Anderson model with the bath electrons in a normal or superconducting state. The results are gathered in the folders with their respective symmetry type indicated by the file name, e.g., `spsu2-U0` corresponds to the superconducting case without interaction. Each of the folders contains two scripts `1_run` and `2_proc`: the first one runs the NRG calculation and stores the output for each z-value, and the second one averages over z to calculate the spectral functions and the self-energy. Some of the folders contain plots comparing Kugler's trick with the old way of calculating Σ.

References

[1] R. Bulla, A. C. Hewson and T. Pruschke, *Numerical renormalization group calculations for the self-energy of the impurity Anderson model*, Journal of Physics: Condensed Matter **10**(37) (1998) 8365, doi:10.1088/0953-8984/10/37/021.

[2] F. B. Kugler, *Improved estimator for numerical renormalization group calculations of the self-energy*, Phys. Rev. B **105** (2022) 245132, doi:10.1103/PhysRevB.105.245132.