

The bath Green's function from the augmented propagator

Notes to `XX_Interactive.Quantity`, lines 249–276

1 What the script does

The last block of the script computes, for the Ni 3*d* shell of NiO, the bath Green's function (the Weiss field of dynamical mean-field theory)

$$\mathcal{G}(\omega)^{-1} = G(\omega)^{-1} + \Sigma(\omega), \quad (1)$$

where G is the local Green's function of the Ni 3*d* orbitals in the lattice with a local self energy Σ on every Ni site, and Σ is that self energy. In words: the interacting lattice Green's function with the local self energy taken out again. $\mathcal{G}$ is the non-interacting Green's function of the Anderson impurity model whose interacting Green's function equals G when the impurity has the self energy Σ , which is why DMFT needs it.

The relevant lines are (slightly reformatted)

```
U=8
Sigma = ResponseFunction.New({{Matrix.Zero(5), 0},
    {Matrix.New({{0,0,0,0,0},{0,0,0,0,0},{0,0,U^2/4,0,0},
        {0,0,0,0,0},{0,0,0,0,U^2/4}})},
    mu = 0, type = "ListOfPoles"})

G, Aug = CalculateG(TB,{Sigma, 0},{{"HybridizationFunction",true},
    {"Emin",-12},{"Emax",7},{"NE",380},{"Nk",{40,40,40}}})

Hybridisation = ResponseFunction.Downfold(Aug[1], Matrix.New({
    {0,0,0,0,0,1,0,0,0,0},{0,0,0,0,0,0,1,0,0,0},
    {0,0,0,0,0,0,0,1,0,0},{0,0,0,0,0,0,0,0,1,0},
    {0,0,0,0,0,0,0,0,0,1}}))

Hloc = ResponseFunction.New({{OnsiteFromAug(Aug[1])}, {}},
    mu = 0, type = "Tri")

Gbath = ResponseFunction.FromEffectiveHamiltonian( Hybridisation + Hloc)
```

together with the small function `OnsiteFromAug` (lines 252–261). Nowhere does the script invert G or subtract Σ . This note explains why the result is nevertheless (1), and why it is done this way.

2 Notation and the quantity we want

Let h be the one-particle matrix of the tight-binding Hamiltonian of the whole crystal (here Ni 3*d* and O 2*p* Wannier orbitals from FPLO), and let $\hat{\Sigma}(\omega)$ be the self energy $\Sigma(\omega)$ placed on every Ni site and zero on the O sites. The lattice Green's function is

$$\mathbb{G}(\omega) = (\omega - h - \hat{\Sigma}(\omega))^{-1}. \quad (2)$$

Let $|c\rangle = (|c_1\rangle, \dots, |c_n\rangle)$ be the $n = 5$ Ni 3*d* orbitals of one site, say the one at $R = 0$. We use the block notation $\langle c|X|c\rangle$ for the $n \times n$ matrix with elements $\langle c_m|X|c_{m'}\rangle$, so that

$$G(\omega) = \langle c|\mathbb{G}(\omega)|c\rangle, \quad \varepsilon_0 = \langle c|h|c\rangle \quad (3)$$

are the local Green's function and the onsite energy matrix of the Ni 3d shell.

The hybridisation function $\Delta(\omega)$ is defined by writing

$$G(\omega)^{-1} = \omega - \varepsilon_0 - \Sigma(\omega) - \Delta(\omega). \quad (4)$$

It describes everything the rest of the crystal does to the site: an electron hops away and comes back. With (4) the goal (1) becomes

$$\boxed{\mathcal{G}(\omega) = (\omega - \varepsilon_0 - \Delta(\omega))^{-1}} \quad (5)$$

so what we need is ε_0 and Δ . It is convenient to introduce

$$\zeta(\omega) = \omega - \Sigma(\omega), \quad \Delta(\omega) = \zeta(\omega) - \varepsilon_0 - G(\omega)^{-1}. \quad (6)$$

Why not simply subtract?

Equation (6) looks like a recipe: evaluate ζ and G^{-1} on an energy grid and subtract. For a Mott insulator this fails. The self energy used here,

$$\Sigma(\omega) = \frac{U^2/4}{\omega} \quad \text{on the } e_g \text{ orbitals,} \quad (7)$$

is the atomic-limit self energy of a half filled level: it splits the e_g band into a lower and an upper Hubbard band. Its pole sits at the chemical potential, $\omega = 0$. Close to it ζ diverges, $G \approx \zeta^{-1}$ goes to zero and G^{-1} diverges as well. Δ stays finite, so (6) is the difference of two large numbers. All significant digits are lost exactly in the energy range that matters most, around the gap. The route taken by the script never forms ζ or G^{-1} at all.

3 The self energy as auxiliary orbitals

A self energy given as a list of poles,

$$\Sigma(\omega) = \Sigma_0 + \sum_p \frac{W_p}{\omega - e_p}, \quad W_p = W_p^\dagger \succeq 0, \quad (8)$$

can be written as $\Sigma(\omega) = \Sigma_0 + V(\omega - A)^{-1}V^\dagger$ with A the diagonal matrix of the pole energies e_p and $V_p V_p^\dagger = W_p$. On every Ni site we attach auxiliary orbitals with energies A , coupled to the 3d orbitals by V . The extended one-particle Hamiltonian

$$P = \begin{pmatrix} h + \hat{\Sigma}_0 & \hat{V} \\ \hat{V}^\dagger & \hat{A} \end{pmatrix} \quad (9)$$

is Hermitian and does not depend on ω . Partitioning (Löwdin downfolding) of its resolvent $Q(\omega) = (\omega - P)^{-1}$ onto the physical orbitals gives back the lattice Green's function,

$$Q(\omega)_{\text{phys,phys}} = (\omega - h - \hat{\Sigma}(\omega))^{-1} = \mathbb{G}(\omega). \quad (10)$$

This is what `CalculateG(TB,{Sigma,0},...)` does: the 0 says that the second atom of the unit cell, O, has no self energy. Note that this requires every residue W_p to be a Hermitian, positive semi-definite matrix; otherwise P is not Hermitian.

4 The augmented propagator

The trick is to look not only at the orbitals $|c\rangle$ but also at the states $h|c\rangle$, the result of one hop away from the Ni $3d$ orbitals. In second quantisation these are the operators $[c_m, H_0] = \sum_j h_{mj} c_j$, the commutator of the annihilation operator with the one-particle Hamiltonian. With the option `{"HybridizationFunction", true}`, `CalculateG` returns as its second result, for every atom of the unit cell, the $2n \times 2n$ matrix-valued response function

$$\mathcal{A}(\omega) = \begin{pmatrix} \langle c | \mathbb{G} | c \rangle & \langle c | \mathbb{G} h | c \rangle \\ \langle c | h \mathbb{G} | c \rangle & \langle c | h \mathbb{G} h | c \rangle \end{pmatrix} \equiv \begin{pmatrix} G & \bar{K} \\ K & M \end{pmatrix}. \quad (11)$$

`Aug[1]` is this matrix for Ni (10×10), `Aug[2]` the one for O (6×6).

Three identities

The lattice Green's function satisfies $(\hat{\zeta} - h)\mathbb{G} = \mathbb{G}(\hat{\zeta} - h) = \mathbb{K}$ with $\hat{\zeta} = \omega - \hat{\Sigma}(\omega)$. The self energy is local: it maps the orbitals of the site $R = 0$ onto themselves, so

$$\langle c | \hat{\zeta} = \zeta \langle c |, \quad \hat{\zeta} | c \rangle = | c \rangle \zeta. \quad (12)$$

Sandwiching the two forms of the resolvent equation between $\langle c |$, $\langle c | h$ and $| c \rangle$ gives

$$\langle c | (\hat{\zeta} - h) \mathbb{G} | c \rangle = \langle c | c \rangle \implies \zeta G - K = \mathbb{K}, \quad (13)$$

$$\langle c | \mathbb{G} (\hat{\zeta} - h) | c \rangle = \langle c | c \rangle \implies G \zeta - \bar{K} = \mathbb{K}, \quad (14)$$

$$\langle c | h \mathbb{G} (\hat{\zeta} - h) | c \rangle = \langle c | h | c \rangle \implies K \zeta - M = \varepsilon_0. \quad (15)$$

The Schur complement is the hybridisation function

The Schur complement of the upper-left block of $\mathcal{A}$ is

$$S = M - K G^{-1} \bar{K}. \quad (16)$$

Using (15) for M and (14) for $\bar{K}$,

$$S = (K \zeta - \varepsilon_0) - K G^{-1} (G \zeta - \mathbb{K}) = K G^{-1} - \varepsilon_0, \quad (17)$$

and with (13), $K = \zeta G - \mathbb{K}$,

$$S = (\zeta G - \mathbb{K}) G^{-1} - \varepsilon_0 = \zeta - G^{-1} - \varepsilon_0 = \Delta. \quad (18)$$

Comparing with (6), *the Schur complement of the augmented propagator onto its second block is exactly the hybridisation function*. This holds for matrices: ζ , G and ε_0 need not commute, and Σ may have off-diagonal elements as long as it is local to the site.

By the block-inversion formula the Schur complement equals

$$S = (R \mathcal{A}^{-1} R^\dagger)^{-1}, \quad R = (0_n \mid \mathbb{K}_n), \quad (19)$$

the lower-right block of the inverse, inverted again. This is precisely what `Downfold` computes when called as `ResponseFunction.Downfold(Aug[1], R)` with the 5×10 matrix R of line 271. So

$$\text{Hybridisation} = \Delta(\omega). \quad (20)$$

Why is this better than the subtraction? $\mathcal{A}$ is a list of poles, the eigenvalues of the Hermitian matrix P , with positive semi-definite residues (section 7). `Downfold` works on this pole representation: it writes $\mathcal{A}$ as the resolvent of an effective Hamiltonian and projects, which is

a Hermitian matrix operation, and it returns Δ again as a list of poles. ζ is never formed and nothing is evaluated at an energy, so nothing large is subtracted, also not near the Mott pole of Σ . In the same way as G , Δ is the Green's function of a Hermitian problem: its poles are real and its weights positive, so it can be represented by bath orbitals.

The same construction with the commutator taken with the interaction instead of the one-particle Hamiltonian, $q_m = [a_m, H_U]$, gives the self energy (the improved estimator). Here the commutator with H_0 gives the hybridisation.

5 The onsite energy and a sum rule

At large ω , $\mathbb{G} = \omega^{-1} + h\omega^{-2} + \dots$, so

$$\mathcal{A}(\omega) = \frac{1}{\omega} \begin{pmatrix} \mathbb{K} & \varepsilon_0 \\ \varepsilon_0 & \langle c|h^2|c \rangle \end{pmatrix} + \mathcal{O}(\omega^{-2}). \quad (21)$$

The total weight (the sum of all residues) of the upper-right block $\bar{K}$ is therefore ε_0 . This is what `OnsiteFromAug` does: `ResponseFunction.ToTable(A)` returns $\{\{A0, e1, e2, \dots\}, \{W1, W2, \dots\}\}$, n is half the block size of A , and the loop adds up the elements `W[p][i][n+j]` of the upper-right block of all residues. The result is the bare onsite energy of the lattice; the static part Σ_0 of the self energy is not included, it is part of Σ .

`Downfold` leaves out any constant: $\Delta(\omega) \rightarrow 0$ for $\omega \rightarrow \infty$. The onsite energy must be added by hand. Line 272 makes ε_0 a response function that is only a constant (a "Tri" with first element $A0 = \varepsilon_0$ and no further chain), so

$$\text{Hybridisation} + \text{Hloc} = \varepsilon_0 + \Delta(\omega) \equiv E_{\text{bath}}(\omega), \quad (22)$$

the frequency dependent effective Hamiltonian of the site.

The same expansion gives a useful check. To leading order

$$\Delta(\omega) \rightarrow \frac{\langle c|h^2|c \rangle - \varepsilon_0^2}{\omega} = \frac{1}{\omega} \sum_{j \notin \text{site } 0} h_{mj} h_{jm'}, \quad (23)$$

the sum over all hoppings from the Ni 3d shell to other orbitals and back. The total weight of Δ depends only on the tight-binding model, *not on* Σ . `Downfold` returns this weight as its second result. For the NiO model it is 4.547 for each e_g orbital and 1.711 for each t_{2g} orbital, with and without the self energy, while $\varepsilon_0 = -1.130$ (e_g) and -1.341 (t_{2g}).

6 The bath Green's function

`ResponseFunction.FromEffectiveHamiltonian(E)` returns the response function $(\omega - E(\omega))^{-1}$; it is the inverse of `ResponseFunction.EffectiveHamiltonian`, which for G returns $\omega - G^{-1}$. Applied to E_{bath} (line 273),

$$\text{Gbath} = (\omega - \varepsilon_0 - \Delta(\omega))^{-1} \stackrel{(4)}{=} (G^{-1} + \Sigma)^{-1} = \mathcal{G}(\omega), \quad (24)$$

which is (1). `Gbath.Chop(1E-5)` only removes numerical noise below 10^{-5} .

Written as an effective Hamiltonian, $\mathcal{G}$ is directly an Anderson impurity model: the impurity level is ε_0 , the bath energies are the poles of Δ and the hopping to the bath is given by the square roots of its residues. The impurity model with this bath and the interaction U has the local Green's function G when its self energy is Σ , since $(\mathcal{G}^{-1} - \Sigma)^{-1} = G$. That is the DMFT self-consistency condition.

7 How CalculateG computes $\mathcal{A}$

h is diagonal in the crystal momentum k , with h_k the 8×8 Bloch Hamiltonian, and the local orbitals are $|c_m\rangle = N^{-1/2} \sum_k |k, m\rangle$. For every k the extended matrix P_k (the Bloch Hamiltonian plus the auxiliary orbitals of the self energy) is diagonalised, $P_k = \sum_\nu \lambda_{k\nu} u_{k\nu} u_{k\nu}^\dagger$. With

$$v_{k\nu} = \begin{pmatrix} (u_{k\nu})_{\text{Ni}} \\ (h_k u_{k\nu})_{\text{Ni}} \end{pmatrix}, \quad \mathcal{A}(\omega) = \frac{1}{N} \sum_k \sum_\nu \frac{v_{k\nu} v_{k\nu}^\dagger}{\omega - \lambda_{k\nu}}, \quad (25)$$

where $(\cdot)_{\text{Ni}}$ takes the five Ni $3d$ components and h_k acts on the physical components of the eigenvector only. The residues $vv^\dagger$ are positive semi-definite. The upper-left block is the familiar residue of G ; computing the other three blocks costs one matrix-vector product per eigenvector, the diagonalisation is shared with G .

As for G , the poles $\lambda_{k\nu}$ are put onto the energy grid given by **Emin**, **Emax** and **NE**: each pole is split over its two neighbouring grid points, conserving its weight and its first moment, and one extra pole below and one above the grid collect the weight outside. **Aug[1]** is thus a list of **NE** + 2 poles with 10×10 residues. The Schur complement of this binned function is exact; the only approximation is the binning itself, the same one made for G .

8 Summary

line	Quanty	mathematics
269	<code>CalculateG(...)</code> with <code>HybridizationFunction</code>	G and $\mathcal{A} = \begin{pmatrix} G & \bar{K} \\ K & M \end{pmatrix}$
271	<code>Downfold(Aug[1], R)</code>	$S = M - K G^{-1} \bar{K} = \Delta$
272	<code>OnsiteFromAug(Aug[1])</code>	weight of $\bar{K} = \varepsilon_0$
273	<code>FromEffectiveHamiltonian(...)</code>	$(\omega - \varepsilon_0 - \Delta)^{-1} = (G^{-1} + \Sigma)^{-1}$

The requirements are those of single-site DMFT: the self energy is local to the site (block diagonal in the atom index) and given as a list of poles with Hermitian, positive semi-definite residues. Under these conditions the bath Green's function is obtained without ever subtracting the self energy, which keeps it accurate near the Mott pole of Σ , and the construction is exact for matrix-valued self energies.