

Solving the Nonlinear Dyson Equation

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1 Problem

We solve the following Dyson-like equation:

$$G_i = g_i + g_i \Delta G_i, \quad \text{for } i \in \{1, 2\}, \quad (1)$$

where the *hybridization function* Δ is defined as:

$$\Delta(t, t') = J \frac{G_1(t, t') + G_2(t, t')}{2}. \quad (2)$$

The *free Green functions* correspond to the non-interacting Hamiltonians $h_1(t) = U(t)/2$ and $h_2(t) = -U(t)/2$, where $U(t)$ is a given function. The retarded free Green functions satisfy:

$$\frac{dg_i^R(t, t')}{dt} + ih_i(t)g_i^R(t, t') = -i\delta(t - t'). \quad (3)$$

In the real-time Keldysh formalism, we solve the following equations:

$$G^R = g^R + g^R \Delta^R G^R, \quad (4)$$

$$G^A = G^{R\dagger}, \quad (5)$$

$$G^K = (\mathbb{1} + G^R \Delta^R)g^K(\mathbb{1} + \Delta^A G^A) + G^R \Delta^K G^A, \quad (6)$$

where

$$\Delta^R(t, t') = \frac{G_1^R(t, t') + G_2^R(t, t')}{2}, \quad (7)$$

$$\Delta^K(t, t') = \frac{G_1^K(t, t') + G_2^K(t, t')}{2}. \quad (8)$$

2 Algorithm

2.1 Discretization

The kernels are discretized on a uniform time grid spanning from $t = 0$ to t_f :

$$\mathbf{A}[p, q] \equiv A(t_p, t_q), \quad \text{where } t_p = p\delta_t. \quad (9)$$

The number of time steps is given by $N \equiv t_f/\delta_t$. In the following, we consider the normalized Frobenius norm:

$$\|\cdot\| : A \mapsto \frac{1}{N} \sqrt{\sum_{p,q} (\mathbf{A}[p,q])^2}. \quad (10)$$

This norm can be efficiently evaluated using matrix operations on the compressed representation, leveraging the relation:

$$\|\mathbf{A}\| = \sqrt{\text{tr}(\mathbf{A}^\dagger \mathbf{A})/N}. \quad (11)$$

Integral operator are discretized by the Nystrom method using a trapezoidal quadrature.

2.2 Construction of g_i and J

The operator J is diagonal, making its construction trivial. To compress the free Green functions efficient implementation of the following maps are required

$$\mathbf{u} \mapsto \sum_q g_i(t_p, t_q) u_q, \quad (12)$$

$$\mathbf{u} \mapsto \sum_q g_i^\dagger(t_p, t_q) u_q, \quad (13)$$

$$(p, q) \mapsto g_i(t_p, t_q). \quad (14)$$

From Equation (3), we deduce:

$$g_i^R(t, t') = \Theta(t - t') g_i^R(t, 0) g_i^R(t', 0)^{-1}, \quad (15)$$

where Θ is the Heaviside function. Hence, the maps can be realized by solving $g_i^R(t, 0)$ with a classical ODE solver and leveraging the low-rank structure of g_i^R .

2.2.1 Dealing with relaxation in g^R

Even in presence of relaxation, one expects $\|g^R(t > 0, 0)\| > 0$. Yet, simple relaxation models lead to $\log(\|g^R(t > 0, 0)\|) \propto -t$. Hence, when doing the computation in finite precision arithmetic eq. (15) quickly become useless. A very direct approach to bypass this issue would be to discretize the differential operator directly, and then inverse it.

2.3 Parameters

We set :

$$U(t) = \alpha \sin(2t) \exp(-t/\tau)(1 - \exp(-t/4\tau)) \quad (16)$$

$$J = 1 \quad (17)$$

2.4 Iteration Method

We iteratively compute:

$$G_{i,j+1} = g_i + g_i \Delta_j G_{i,j+1}, \quad (18)$$

$$\Delta_j = \frac{G_{1,j} + G_{2,j}}{2}. \quad (19)$$

2.5 Convergence Monitoring

We define the norm of the discretized kernel $A(t_p, t_q)$ with $t_{i,p}$ Convergence is monitored using the following error measures:

$$\mathcal{E}_{j,\text{abs}} \equiv \sqrt{\|G_{1,j+1}^R - G_{1,j}^R\|^2 + \|G_{2,j+1}^R - G_{2,j}^R\|^2}, \quad (20)$$

$$\mathcal{E}_{j,\text{rel}} \equiv \frac{\mathcal{E}_{j,\text{abs}}}{\sqrt{\|G_{1,j+1}^R\|^2 + \|G_{2,j+1}^R\|^2}}, \quad (21)$$

2.6 Stopping Criterion

The iteration stops when:

- The number of iterations exceeds the preset maximum.
- $\mathcal{E}_{j,\text{rel}}$ plateaus.
- The target accuracy is reached

3 Results

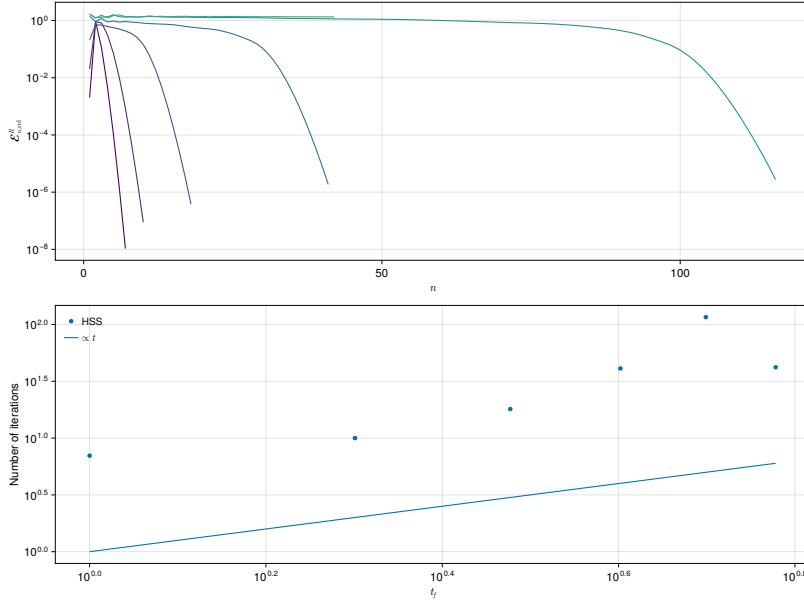


Fig. 1: Convergence toward self-consistent solution for different propagation times t_f . The compression accuracy is maintained at its nominal value throughout the computation. *a:* Real and imaginary part of g_1^R *b:* Real and imaginary part of g_2^R *c:* Evolution of relative difference between successive iterations. *d:* Number of iterations required to reach desired accuracy. *Parameters:* $\alpha = 20, \tau = 5$ and $\delta_t = 0.1$. Compression: $rtol_{\text{nominal}} = 10^{-8}$ and $atol_{\text{nominal}} = 10^{-9}$

References