CT-1/2-HYB-QMC: a new solver for time-dependent Anderson impurity

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Motivation

Continuous-time quantum Monte Carlo methods (CT-QMC) are widely used to solve impurity models in equilibrium [1]. However, they suffer from an inherent dynamical sign problem while treating the nonequilibrium real-time dynamics [2, 3, 4]. Here we propose a method that alleviates the dynamical sign problem in case of the single-orbital Anderson impurity model (AIM).

Model and method

The Hamiltonian of the time-dependent single-orbital AIM in a setup with two leads reads

$$H(t) = H_{\mathrm{loc}}(t) + \sum_{\sigma} \left[H_{\mathrm{bath},\sigma}(t) + H_{\mathrm{hyb},\sigma}(t) \right]$$

$$H_{\mathrm{loc}}(t) = \sum_{\sigma} \mathcal{E}_{d\sigma}(t) d^{\dagger}_{\sigma} d_{\sigma} + U(t)\, d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow}$$

$$H_{\mathrm{bath},\sigma}(t) = \sum_{\alpha=-1,1} \sum_{p}^{N/2} \left(\varepsilon_{p\sigma}(t) + \alpha \frac{\mathcal{V}(t)}{2} \right) c^{\dagger}_{\alpha p\sigma} c_{\alpha p\sigma}$$

$$H_{\mathrm{hyb},\sigma}(t) = \sum_{\alpha=-1,1} \sum_{p}^{N/2} \left(V_{p\sigma}(t)\, c^{\dagger}_{\alpha p\sigma} d_{\sigma} + \mathrm{h.c.} \right).$$

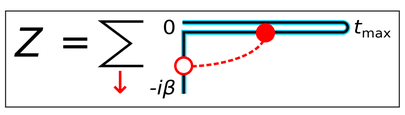
The generating functional for all the time-dependent observables of the interest is the dynamical partition function $\mathcal{Z}(\beta, t_{\max})$

$$\mathcal{Z}(\beta, t_{\max}) = \mathrm{Tr}\left(e^{-\beta H(0)} \mathcal{T}_{-} e^{-i\int_{t_{\max}}^{0} dt H(t)} \mathcal{T}_{+} e^{-i\int_{0}^{t_{\max}} dt H(t)} \right)$$

$$\equiv \mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{C} ds H(s)} \right) = \mathrm{Tr}\left(\mathcal{T}_{\mathcal{C}}\, e^{-i\int_{C} ds (H - H_{\mathrm{hyb}\downarrow})(s)} e^{-i\int_{C} ds H_{\mathrm{hyb}\downarrow}(s)} \right).$$

In contrast to the standard CT-HYB-QMC algorithm we expand $\mathcal{Z}$ perturbatively in in the powers of $H_{\mathrm{hyb}\downarrow}(s)$ only

$$\mathcal{Z}(\beta, t_{\max}) = \sum_{k=0}^{\infty} (-1)^k \int_{0_+}^{-i\beta} ds_1 \cdots \int_{s_{k-1}}^{-i\beta} ds_k \int_{0_+}^{-i\beta} ds'_1 \cdots \int_{s'_{k-1}}^{-i\beta} ds'_k$$
$$w_{\mathrm{loc+bath}\uparrow}(\{s_m\}, \{s'_n\})\, w_{\mathrm{bath}\downarrow}(\{s_m\}, \{s'_n\}).$$



Terms of the expansion are then stochastically sampled within a Monte Carlo simulation. Each term's contribution may be split into the dressed local weight $w_{\mathrm{loc+bath}\uparrow}$ and the spin-down bath weight $w_{\mathrm{bath}\downarrow}$, which is evaluated easily due to Wick's theorem

$$w_{\mathrm{bath}\downarrow} = Z_{\mathrm{bath}\downarrow}\, i^k \det \left[\sum_{\alpha p} V^{*}_{p\downarrow}(s_m) g_{\alpha p\downarrow}(s_m, s'_n) V_{p\downarrow}(s'_n) \right]_{m,n=1,\ldots,k},$$

where $g_{\alpha p\downarrow}(s, s')$ is a non-interacting bath Green function.

Evaluation of the dressed local weight - *discretized bath*

The novel aspect is the evaluation of the dressed local weight, which incorporates both local and spin-up bath degrees of freedom. This auxiliary system is governed by the Hamiltonian $H_0 = H_{\mathrm{loc}} + H_{\mathrm{bath}\uparrow} + H_{\mathrm{hyb}\uparrow}$ and is effectively non-interacting since H_0 conserves $n_{\downarrow} = \langle d^{\dagger}_{\downarrow} d_{\downarrow} \rangle$. Using the well-known result from determinant QMC [5] we get (for $s_k > s'_k$)

$$w_{\mathrm{loc+bath}\uparrow} = \mathrm{Tr}_{\mathrm{loc,bath}\uparrow}\left(e^{-\beta H_0(0)} d^{\dagger}_{\downarrow}(s_k) d_{\downarrow}(s'_k) \ldots d^{\dagger}_{\downarrow}(s_1) d_{\downarrow}(s'_1) \right)$$
$$= e^{-i\int_{s_k}^{-i\beta} ds\, \mathcal{E}_{d\downarrow}(s)} e^{-i\int_{s'_{k-1}}^{s'_k} ds\, \mathcal{E}_{d\downarrow}(s)} \ldots e^{-i\int_{0_+}^{s_1} ds\, \mathcal{E}_{d\downarrow}(s)}$$
$$\det\left[\mathbb{1} + u_1(-i\beta, s_k) u_0(s_k, s'_k) u_1(s'_k, s_{k-1}) \ldots u_0(s_1, s'_1) u_1(s'_1, 0_+) \right],$$

where $u_{n_{\downarrow}}$ is a single-particle time-evolution matrix

$$u_{n_{\downarrow}}(s, s') = \mathcal{T}_{\mathcal{C}} \exp\left(-i \int_{s'}^{s} d\bar{s} \begin{bmatrix} \mathcal{E}_{d\uparrow}(\bar{s}) + U(\bar{s}) n_{\downarrow} & V^{*}_{1}(\bar{s}) & \cdots & V^{*}_{k}(\bar{s}) \\ V_1(\bar{s}) & \varepsilon_{1\downarrow}(\bar{s}) & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ V_k(\bar{s}) & 0 & 0 & \varepsilon_{k\downarrow}(\bar{s}) \end{bmatrix} \right).$$

The computational cost is $\mathcal{O}(N^3)$, where N is the size of the bath.

Evaluation of the dressed local weight - *discretized time*

Formally one can integrate out the bath levels and work directly with the hybridization function

$$\Delta_{\uparrow}(s, s') = \sum_{\alpha p} V^{*}_{p\uparrow}(s) g_{\alpha p\uparrow}(s, s') V_{p\uparrow}(s')$$

The impurity spin-up Green function for a given MC configuration $n_{\downarrow}(s)$ satisfies Dyson equation

$$G_{\uparrow}(s, s') = G_{0\uparrow}(s, s') + \left(G_{0\uparrow} \circ \Delta_{\uparrow} \circ G_{\uparrow} \right)(s, s'),$$

where

$$G^{-1}_{0\uparrow}(s, s') = \left[i\frac{\partial}{\partial s} - \mathcal{E}_{d\uparrow}(s) - U(s) n_{\downarrow}(s) \right] \delta(s, s').$$

One can discretize contour times $s_i = \sum_{j=0}^{i-1} (\Delta s)_j$ and obtain the local weight as a determinant in the contour-time space in the limit $\Delta s \to 0$

$$w_{\mathrm{loc+bath}\uparrow} = \det\left[i G_{\uparrow}(s_i, s_j) \right]_{i,j} = \left(1 + e^{-i\int_{0_+}^{-i\beta} ds [\mathcal{E}_{d\uparrow}(s) + U(s) n_{\downarrow}(s)]} \right) \det\left[\delta_{ij} - \left(G_{0\uparrow} \circ \Delta_{\uparrow} \right)(s_i, s_j) \right]_{i,j}.$$

The computational cost is $\mathcal{O}(N^3_{\mathrm{times}})$ but does not depend on N. In principle, one can also introduce retarded interaction $U_{\uparrow\downarrow}(s, s')$ at no additional cost.

References

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Measurement of current - *discretized bath*

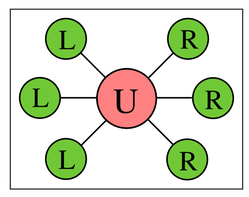
The current to the left ($\alpha = -1 \equiv L$) lead is given by

$$I_{\sigma}(t) = -2\,\mathrm{Im} \sum_{p} V_{p\sigma}(t) \left\langle c^{\dagger}_{Lp\sigma} d_{\sigma} \right\rangle (t).$$

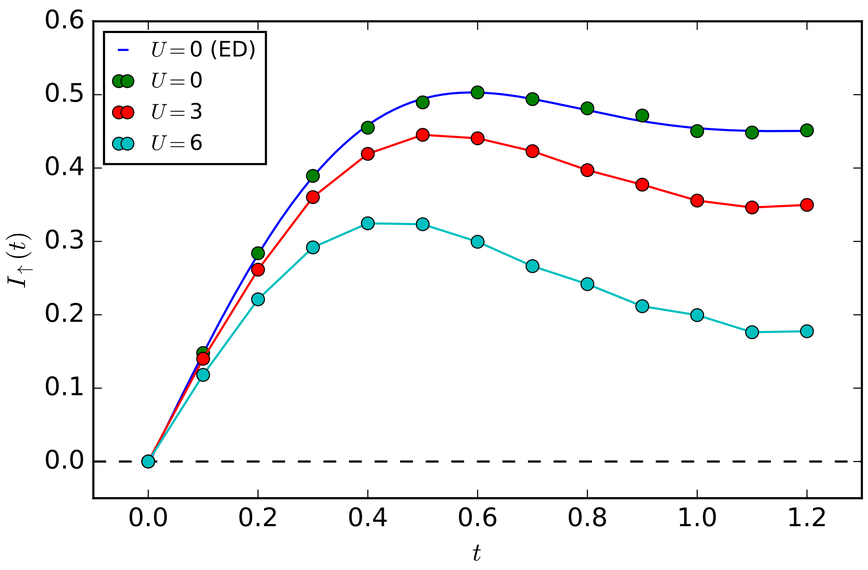
Since the spin-up subsystem is solved explicitly for each MC configuration, one has a direct access to the relevant expectation values

$$\left\langle c^{\dagger}_{\alpha p\uparrow} d_{\uparrow} \right\rangle (t) = \left\langle - \left[\mathbb{1} + u_{0/1}(t, \tilde{s}_i) \ldots u_1(\tilde{s}_1, 0_+) u_1(-i\beta, \tilde{s}_{2k}) \ldots u_{0/1}(\tilde{s}_{i+1}, t) \right]^{-1}_{\alpha p, d} \right\rangle_{\mathrm{QMC}}.$$

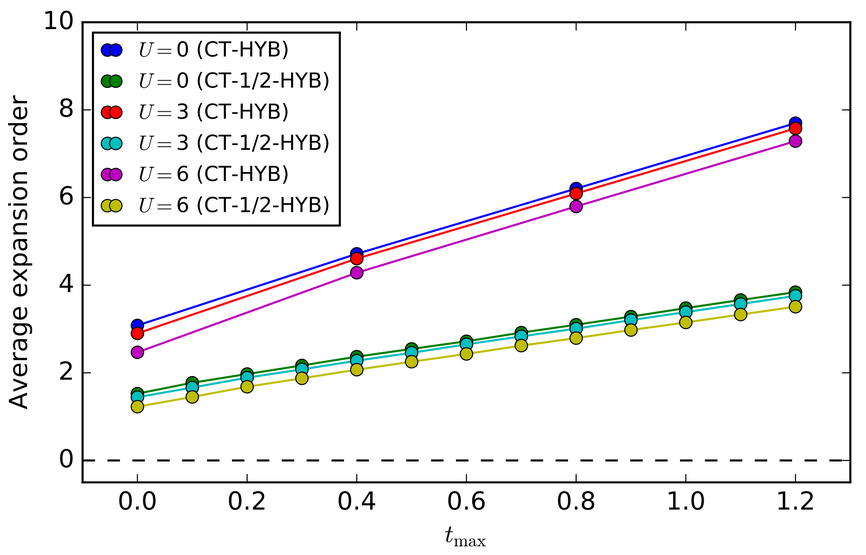
Here we consider the voltage quench from $\mathcal{V}(0) = 0$ to $\mathcal{V}(t > 0) = 4$ for $U(t) = 3$ and 6. Each lead is composed of $N/2 = 15$ bath states $\varepsilon_{\alpha p\sigma}$ equidistantly spaced around 0 in the interval of half-width $D = 3$. We use the integrated impurity-bath coupling $\Gamma = \frac{\pi N |V_p|^2}{4D}$ as energy unit. The inverse temperature $\beta = 2$.

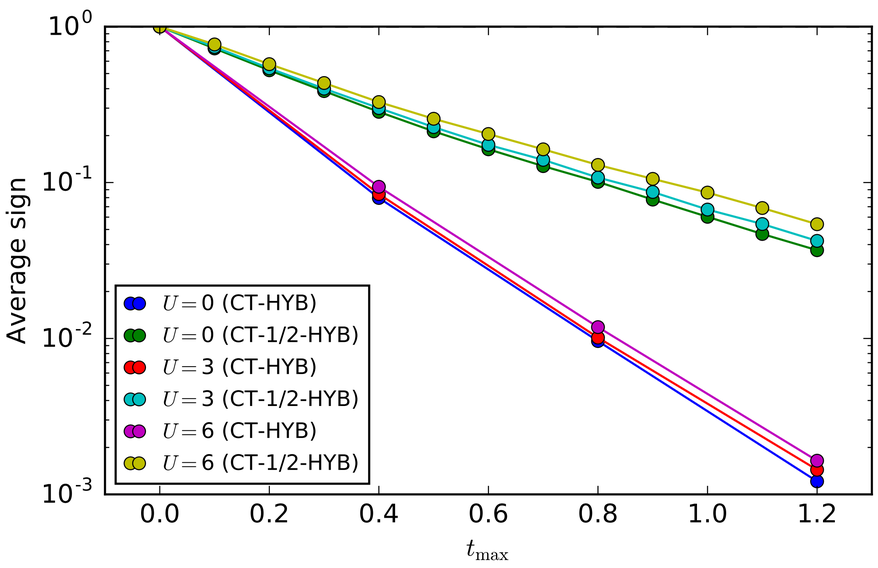


Current from CT-1/2-HYB



Average expansion order





Conclusions

- CT-1/2-HYB-QMC allows one to solve the finite-size single-orbital Anderson impurity model exactly on twice as long time scales as within the standard CT-HYB-QMC.
- The average expansion order is reduced by a factor of 2, which decreases the computational burden of the bath weight evaluations with respect to CT-HYB by 4.
- The computational complexity of the *discretized bath* algorithm is $\mathcal{O}(N^3)$ as opposed to $\mathcal{O}(e^N)$ for exact-diagonalization methods.
- The computational complexity of the *discretized time* algorithm is $\mathcal{O}(N^3_{\mathrm{times}})$ and the extrapolation $\Delta s \to 0$ shall be performed.
- CT-1/2-HYB can be extended to multiorbital problems with density-density interactions. However, the increase in the time span that can be simulated is only $\frac{n}{n-1}$, where n is the number of electronic flavors ($n = 2$ for the single-orbital AIM).

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