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CTSEG: A segment picture quantum impurity solver based on TRIQS

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Summary

Electron-electron interactions are a key determinant of the electrical and optical response properties in solid-state materials. Yet, the many-electron problem is outstandingly difficult, and can be tackled analytically only when interactions are weak, or in rare exactly solvable cases. One of the popular numerical schemes for addressing strongly interacting systems is dynamical mean-field theory (DMFT; Georges et al., 1996). In DMFT, the many-body problem formulated on a crystal lattice is self-consistently mapped onto a single atom (or impurity) immersed in an effective environment (or bath). The remaining computational task is then the solution of the impurity problem, which can be carried out through various quantum Monte Carlo algorithms (Gull et al., 2011). Here, we present an implementation of the continous time hybridization expansion algorithm in the segment picture (`CTSEG`) based on `TRIQS`, a comprehensive library for the numerical investigation of interacting quantum systems (Parcollet et al., 2015).

Statement of need

The Monte Carlo algorithms for quantum impurity problems are based on stochastically exploring the terms in the perturbative expansion of the solution around an exactly solvable limit. Continuous time hybridization expansion algorithms – chief of which `CTHYB` – involve expanding around the limit of an isolated atom (Gull et al., 2011). Currently, there exist implementations of `CTHYB` within three different libraries: `ALPS` (Shinaoka et al., 2017), `w2dynamics` (Wallerberger et al., 2019) and `TRIQS` (Seth et al., 2016).

However, a simpler and potentially faster version of the `CTHYB` algorithm, called `CTSEG`, can be used under the restriction of density-density interactions on the impurity (Haule, 2007; Werner et al., 2006; Werner & Millis, 2006). `CTSEG` can be further generalized to allow for time-dependent (Werner & Millis, 2007, 2010) and spin-spin interactions (Otsuki, 2013; Steiner et al., 2015): see Werner & Casula (2016) for a review. To our knowledge, there exists so far one published implementation of `CTSEG` based on ALPS (Hafermann et al., 2013), but it does not allow for spin-spin interactions.

Our `CTSEG` solver is about twice as fast as `TRIQS-CTHYB` for a single orbital problem, and has better scaling with the number of orbitals (40 times faster in our 5 orbital test case, see Fig. 1a). `CTSEG` has already allowed us to obtain the first numerically-exact solution of the quantum Heisenberg spin glass (Kavokine et al., 2024).

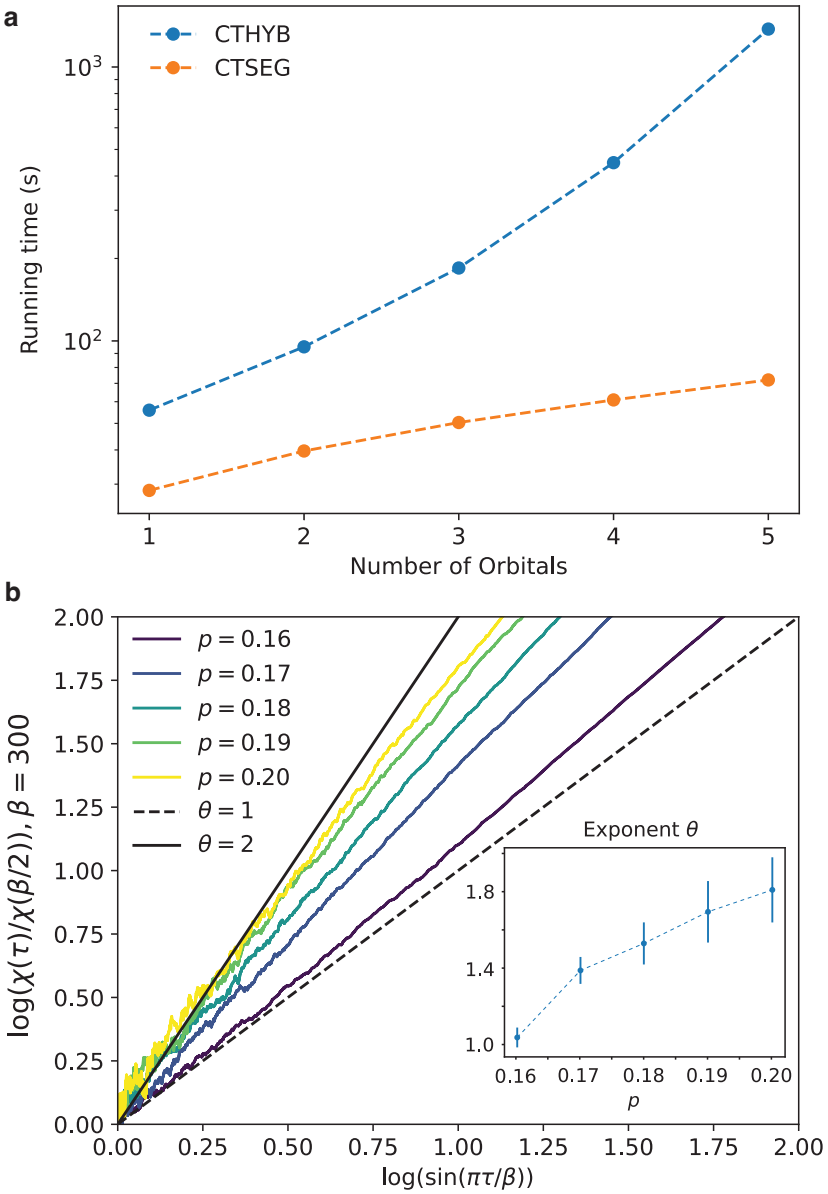

Figure 1: **a**. Running time comparison between the TRIQS implementations of CTSEG and CTHYB. The test system is a multi-orbital impurity at half-filling and inverse temperature $\beta = 20$. The Coulomb repulsion is $U = 2$ for two electrons on the same orbital and $U' = 1$ for two electrons on different orbitals. The hybridization is diagonal and identical for all orbitals: $\Delta(\omega) = 1/(\omega - 0.3)$. **b**. Spin-spin correlation function $\chi(\tau) = \langle \mathbf{S}(\tau) \cdot \mathbf{S}(0) \rangle$ of the $t - J - U$ model studied by Dumitrescu et al., obtained using CTSEG at inverse temperature $\beta = 300$ and different values of doping p. At long times $\chi(\tau) \sim 1/\tau^{\theta}$, with $\theta = 1$ at the QCP. Inset: exponent θ as a function of doping p. The QCP is located at $p \approx 0.16$.

Example of use

As a further illustration of our solver's performance, we apply it to the fully connected $t-J-U$ model, which has been previously studied (Dumitrescu et al., 2022). At half-filling, the model forms a spin glass phase, which melts into a metal at a doping-induced quantum critical point (QCP). Dumitrescu et al. obtained solutions at inverse temperatures up to $\beta = 65$, limited by the fermionic sign problem of their interaction expansion solver. The hybridization expansion carried out by CTSEG is sign-problem-free for the $t-J-U$ model, allowing us to reach $\beta = 300$

and to obtain a more accurate localization of the QCP at doping $p \approx 0.16$ (Fig. 1b).

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