Computer Physics Communications 184 (2013) 1280–1286

Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

Efficient implementation of the continuous-time hybridization expansion quantum impurity solver☆

Hartmut Hafermann [a], Philipp Werner [b], Emanuel Gull [c,d,*]

[a] *École Polytechnique, CNRS, 91128 Palaiseau Cedex, France*
[b] *Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*
[c] *University of Michigan, Ann Arbor, MI 48109, USA*
[d] *Max Planck Institut für die Physik komplexer Systeme, 01187 Dresden, Germany*

ARTICLE INFO

Article history:
Received 8 October 2012
Received in revised form
25 November 2012
Accepted 5 December 2012
Available online 19 December 2012

Keywords:
CT-QMC
CT-HYB
DMFT
Dynamical mean-field theory

ABSTRACT

Strongly correlated quantum impurity problems appear in a wide variety of contexts ranging from nanoscience and surface physics to material science and the theory of strongly correlated lattice models, where they appear as auxiliary systems within dynamical mean-field theory. Accurate and unbiased solutions must usually be obtained numerically, and continuous-time quantum Monte Carlo algorithms, a family of algorithms based on the stochastic sampling of partition function expansions, perform well for such systems. With the present paper we provide an efficient and generic implementation of the hybridization expansion quantum impurity solver, based on the segment representation. We provide a complete implementation featuring most of the recently developed extensions and optimizations. Our implementation allows one to treat retarded interactions and provides generalized measurement routines based on improved estimators for the self-energy and for vertex functions. The solver is embedded in the ALPS-DMFT application package.

Program summary

Program title: ct-hyb

Catalogue identifier: AEOL_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEOL_v1_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Use of the hybridization expansion impurity solvers requires citation of this paper. Use of any ALPS program requires citation of the ALPS [1] paper.

No. of lines in distributed program, including test data, etc.: 650044

No. of bytes in distributed program, including test data, etc.: 20553265

Distribution format: tar.gz

Programming language: C++/Python.

Computer: Desktop PC, high-performance computers.

Operating system: Unix, Linux, OSX, Windows.

Has the code been vectorized or parallelized?: Yes, MPI parallelized.

RAM: 1 GB

Classification: 7.3.

External routines: ALPS [1, 2, 3], BLAS [4, 5], LAPACK [6], HDF5 [7]

Nature of problem:
Quantum impurity models were originally introduced to describe a magnetic transition metal ion in a non-magnetic host metal. They are widely used today. In nanoscience they serve as representations of

☆ This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

* Corresponding author at: University of Michigan, Ann Arbor, MI 48109, USA. Tel.: +1 212 854 6712.
E-mail addresses: hartmut.hafermann@cpht.polytechnique.fr (H. Hafermann), philipp.werner@unifr.ch (P. Werner), gull@phys.columbia.edu, egull@umich.edu (E. Gull).

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2012.12.013

quantum dots and molecular conductors. In condensed matter physics, they are playing an increasingly important role in the description of strongly correlated electron materials, where the complicated many-body problem is mapped onto an auxiliary quantum impurity model in the context of dynamical mean-field theory, and its cluster and diagrammatic extensions. They still constitutes a non-trivial many-body problem, which takes into account the (possibly retarded) interaction between electrons occupying the impurity site. Electrons are allowed to dynamically hop on and off the impurity site, which is described by a time-dependent hybridization function.

Solution method:
The quantum impurity model is solved using a continuous-time quantum Monte Carlo algorithm which is based on a perturbation expansion of the partition function in the impurity–bath hybridization. Monte Carlo configurations are represented as segments on the imaginary time interval and individual terms correspond to Feynman diagrams which are stochastically sampled to all orders using a Metropolis algorithm. For a detailed review on the method, we refer the reader to [8].

Running time:
1–8 h.

References:

[1] B. Bauer, L. D. Carr, H. G. Evertz, A. Feiguin, J. Freire, S. Fuchs, L. Gamper, J. Gukelberger, E. Gull, S. Guertler, A. Hehn, R. Igarashi, S. V. Isakov, D. Koop, P. N. Ma, P. Mates, H. Matsuo, O. Parcollet, G. Pawlowski, J. D. Picon, L. Pollet, E. Santos, V. W. Scarola, U. Schollwöck, C. Silva, B. Surer, S. Todo, S. Trebst, M. Troyer, M. L. Wall, P. Werner and S. Wessel, Journal of Statistical Mechanics: Theory and Experiment 2011, P05001 (2011).
[2] F. Alet, P. Dayal, A. Grzesik, A. Honecker, M. Körner, A. Läuchli, S. R. Manmana, I. P. McCulloch, F. Michel, R. M. Noack, G. Schmid, U. Schollwöck, F. Stöckli, S. Todo, S. Trebst, M. Troyer, P. Werner, S. Wessel, J. Phys. Soc. Japan 74S (2005) 30.
[3] A. Albuquerque, F. Alet, P. Corboz, P. Dayal, A. Feiguin, S. Fuchs, L. Gamper, E. Gull, S. Gürtler, A. Honecker, R. Igarashi, M. Körner, A. Kozhevnikov, A. Läuchli, S. Manmana, M. Matsumoto, I. McCulloch, F. Michel, R. Noack, G. Pawlowski, L. Pollet, T. Pruschke, U. Schollwöck, S. Todo, S. Trebst, M. Troyer, P. Werner and S. Wessel, J. Magn. Magn. Mater. 310, 1187 (2007), proceedings of the 17th International Conference on Magnetism The International Conference on Magnetism.
[4] C. L. Lawson, R. J. Hanson, D. R. Kincaid, and F. T. Krogh, ACM Transactions on Mathematical Software 5, 324 (1979).
[5] L. S. Blackford, J. Demmel, I. Du, G. Henry, M. Heroux, L. Kaufman, A. Lumsdaine, A. Petitet, and R. C. Whaley, ACM Trans. Math. Softw. 28, 135 (2002).
[6] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, and D. Sorensen, LAPACK Users' Guide, 3rd ed. (Society for Industrial and Applied Mathematics, Philadelphia, PA, 1999).
[7] The HDF Group, Hierarchical data format version 5, http://www.hdfgroup.org/HDF5 (2000–2010).
[8] E. Gull, A. J. Millis, A. I. Lichtenstein, A. N. Rubtsov, M. Troyer and P. Werner, Rev. Mod. Phys. 83, 349 (2011).

1. Introduction

Quantum impurity models describe a set of correlated sites or orbitals embedded in a bath of non-interacting states. Quantum impurity models appear in a range of contexts, including magnetic impurities embedded in a non-magnetic host material [1], nanoscience, where they are used to describe quantum dots and molecular conductors [2], and surface science [3], for the description of molecules adsorbed on a substrate. Quantum impurity solvers are also an essential ingredient of the dynamical mean-field (DMFT) [4–7] approximation to correlated lattice systems, which has had enormous success in recent years in the simulation of correlated material systems [8–10] and lattice models [11].

With this article we provide a description and a state-of-the-art implementation of the continuous-time [12–14] 'hybridization expansion' quantum Monte Carlo impurity solver for density–density interactions [15]. Our implementation includes in particular the important numerical and conceptual advances developed over the last few years: improved estimators [16], frequency and Legendre measurements [17], measurement of vertex functions [14], treatment of retarded interactions [18,19], and parallelization to a large number of cores [20–23].

General fermionic impurity models have the form $H_{\mathrm{imp}} = H_{\mathrm{loc}} + H_{\mathrm{bath}} + H_{\mathrm{hyb}}$, where

$$H_{\mathrm{loc}} = \sum_{ab} E^{ab} d_a^\dagger d_b + \sum_{abcd} U^{abcd} d_a^\dagger d_b^\dagger d_c d_d, \tag{1}$$

$$H_{\mathrm{bath}} = \sum_{k\alpha} \varepsilon_{k\alpha} c_{k\alpha}^\dagger c_{k\alpha}, \tag{2}$$

$$H_{\mathrm{hyb}} = \sum_{k\alpha b} V_k^{\alpha b} c_{k\alpha}^\dagger d_b + \mathrm{h.c.} \tag{3}$$

The term H_{loc} corresponds to the impurity with level energies and intra-orbital hoppings described by E and the interaction terms parametrized by U (roman indices label the different interacting orbitals including spin). H_{bath} describes the non-interacting bath with quantum numbers k and spin/orbital index α. The hybridization term H_{hyb} represents the exchange of electrons between the impurity and the bath, parametrized by the hybridization matrix $V_k^{\alpha b}$. All the relevant properties of the bath are encoded in the hybridization functions

$$\Delta_{ab}(i\omega_n) = \sum_{k,\alpha} \frac{V_k^{a\alpha *} V_k^{\alpha b}}{i\omega_n - \varepsilon_{k\alpha}}. \tag{4}$$