Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

An efficient continuous-time quantum Monte Carlo impurity solver in Kondo Regime CHANGMING YUE, YILIN WANG, Institute of Physics, Chinese Academy of Science, XI DAI, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — An efficient continuous-time quantum Monte Carlo impurity solver with high acceptation ratio at low temperature is developed to study the strongly correlated heavy-fermion materials. In this solver, the imaginary time evolution operator for the high energy multiplets, which decays very rapidly with time, is approximated by a δ function, and as a result the virtual charge fluctuations of $f^n \rightarrow f^{n\pm1}$ are all included without applying Schrieffer-Wolff transformation explicitly . As benchmarks, our algorithm perfectly reproduces the results for both Coqblin-Schriffeer and Kondo lattice models obtained by ct-J method developed by Junya Otsuki et al. Furthermore, it allows us to study low energy physics of heavy-fermion materials directly without fitting the exchange coupling J in the Kondo model. As an example, we test our solver on CeCoIn5, the famous heavy fermion material within the framework of LDA+DMFT to obtain its quasi-particle spectrum.

Changming Yue
Chinese Academy of Sci (CAS)

Date submitted: 27 Oct 2015 Electronic form version 1.4