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Improved measurement scheme of the self energy in the worm-sampled hybridization-expansion quantum Monte Carlo MANCHEON HAN, CHOONG-KI LEE, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University — Hybridization-expansion continuous-time quantum Monte Carlo (CT-HYB) is a popular approach in real material researches because it allows to deal with non-density-density-type interaction. In the conventional CT-HYB, we measure Green's function and find the self energy from the Dyson equation. Because one needs to compute the inverse of the statistical data in this approach, obtained self energy is very sensitive to statistical noise. For that reason, the measurement is not reliable except for low frequencies. Such an error can be suppressed by measuring a special type of higher-order correlation function and is implemented for density-density-type interaction [1]. With the help of the recently reported worm-sampling measurement [2], we developed an improved self energy measurement scheme which can be applied to any type of interactions. As an illustration, we calculated the self energy for the 3-orbital Hubbard-Kanamori-type Hamiltonian with our newly developed method. This work was supported by NRF of Korea (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039). [1] H. Hafermann et al., Phys. Rev. B, 85, 205106 (2012) [2] P. Gunacker et al., Phys. Rev. B, 92, 155102 (2015)

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