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Improved determination of the self-energy and vertex function in Strong-Coupling Continuous-time Quantum Monte Carlo HARTMUT HAFERMANN, Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau Cedex, France, KELLY R. PATTON, Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, PHILIPP WERNER, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland — The continuous-time quantum Monte Carlo method based on the strong coupling expansion is an efficient and flexible tool for the solution of multiorbital Anderson impurity models. However it is known that it is difficult to accurately compute the intermediate and high-frequency behavior of measured quantities. This leads to large errors, in particular for the self-energy when computed from Dyson's equation. A similar problem occurs for the vertex function when computed directly from the two-particle Green function. We propose an improved way of measuring these quantities, based on higher-order impurity correlation functions. The method yields very accurate estimates for the self-energy and vertex function over the full frequency range. In the segment representation, the improved estimators can be accumulated at essentially no additional computational cost.

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