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Symmetric improved estimators for multipoint vertex functions

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Multipoint vertex functions, and the four-point vertex in particular, are crucial ingredients in many-body theory. Recent years have seen significant algorithmic progress toward numerically computing their dependence on multiple frequency arguments. However, such computations remain challenging and are prone to suffer from numerical artifacts, especially in the real-frequency domain. Here, we derive estimators for multipoint vertices that are numerically more robust than those previously available. We show that the two central steps for extracting vertices from correlators, namely, the subtraction of disconnected contributions and the amputation of external legs, can be achieved accurately through repeated application of equations of motion, in a manner that is symmetric with respect to all frequency arguments and involves only fully renormalized objects. The symmetric estimators express the core part of the vertex and all asymptotic contributions through separate expressions that can be computed independently, without subtracting the large-frequency limits of various terms with different asymptotic behaviors. Our strategy is general and applies equally to the Matsubara formalism, the real-frequency zero-temperature formalism, and the Keldysh formalism. We demonstrate the advantages of the symmetric improved estimators by computing the Keldysh four-point vertex of the single-impurity Anderson model using the numerical renormalization group.

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