A Numerical Method to Study Highly Correlated Nanostructures: The Logarithmic Discretization Embedded Cluster Approximation

E. ANDA, G. CHIAPPE, C. BUSSER, M. DAVIDOVICH, G. MARTINS, F. H-MEISNER, E. DAGOTTO, Oakland University — A numerical algorithm to study transport properties of highly correlated local structures is proposed. The method, dubbed the Logarithmic Discretization Embedded Cluster Approximation (LDECA), consists of diagonalizing a finite cluster containing the many-body terms of the Hamiltonian and embedding it into the rest of the system, combined with Wilson’s ideas of a logarithmic discretization of the representation of the Hamiltonian. LDECA’s rapid convergence eliminates finite-size effects commonly present in the embedding cluster approximation (ECA) method. The physics associated with both one embedded dot and a string of two dots side-coupled to leads is discussed. In the former case, our results accurately agree with Bethe ansatz (BA) data, while in the latter, the results are framed in the conceptual background of a two-stage Kondo problem. A diagrammatic expansion provides the theoretical foundation for the method. It is argued that LDECA allows for the study of complex problems that are beyond the reach of currently available numerical methods.

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