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Correlation functions from a unified variational principle: Trial Lie groups

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ABSTRACT

Time-dependent expectation values and correlation functions for many-body quantum systems are evaluated by means of a unified variational principle. It optimizes a generating functional depending on sources associated with the observables of interest. It is built by imposing through Lagrange multipliers constraints that account for the initial state (at equilibrium or off equilibrium) and for the backward Heisenberg evolution of the observables. The trial objects are respectively akin to a density operator and to an operator involving the observables of interest and the sources. We work out here the case where trial spaces constitute Lie groups. This choice reduces the original degrees of freedom to those of the underlying Lie algebra, consisting of simple observables; the resulting objects are labeled by the indices of a basis of this algebra. Explicit results are obtained by expanding in powers of the sources. Zeroth and first orders provide thermodynamic quantities and expectation values in the form of mean-field approximations, with dynamical equations having a classical Lie–Poisson structure. At second order, the variational expression for two-time correlation functions separates – as does its exact counterpart – the approximate dynamics of the observables from the approximate correlations in the initial state. Two building blocks are involved: (i) a commutation matrix which stems from the structure constants of the Lie algebra; and (ii) the second-derivative matrix of a free-energy function. The diagonalization of both matrices, required for practical calculations, is worked out, in

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a way analogous to the standard RPA. The ensuing structure of the variational formulae is the same as for a system of non-interacting bosons (or of harmonic oscillators) plus, at non-zero temperature, classical Gaussian variables. This property is explained by mapping the original Lie algebra onto a simpler Lie algebra. The results, valid for any trial Lie group, fulfill consistency properties and encompass several special cases: linear responses, static and time-dependent fluctuations, zero- and high-temperature limits, static and dynamic stability of small deviations.

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