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Cluster expansion for ground states of local Hamiltonians

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Abstract

A central problem in many-body quantum physics is the determination of the ground state of a thermodynamically large physical system. We construct a cluster expansion for ground states of local Hamiltonians, which naturally incorporates physical requirements inherited by locality as conditions on its cluster amplitudes. Applying a diagrammatic technique we derive the relation of these amplitudes to thermodynamic quantities and local observables. Moreover we derive a set of functional equations that determine the cluster amplitudes for a general Hamiltonian, verify the consistency with perturbation theory and discuss non-perturbative approaches. Lastly we verify the persistence of locality features of the cluster expansion under unitary evolution with a local Hamiltonian and provide applications to out-of-equilibrium problems: a simplified proof of equilibration to the GGE and a cumulant expansion for the statistics of work, for an interacting-to-free quantum quench.

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1. Introduction

One of the main goals of quantum many body physics is to determine the ground state of physically interesting models. Whenever the ground state wavefunction is known, all other ground state properties and observables of interest can be derived. In practice in order to extract physically important information about the ground state, it is valuable to know it in a form that reflects its general physical properties and allows a systematic expansion of observables from more to less relevant information. For example, Renormalization Group methods are supposed to capture the universal ground state properties of physical systems in the thermodynamic limit. One of the most fundamental physical principles that characterize physical systems is *locality* and this is clearly reflected on the properties of their ground state. Indeed physical Hamiltonians are expected to involve only local couplings or interactions between near different points and this imposes constrains on the form of their ground state. In particular, ground states of local Hamiltonians possess an extensive number of particles, energy and other thermodynamic quantities; relative fluctuations of such extensive quantities about their average values decay rapidly with the system size; local observables, like multi-point correlations, in general have a well-defined limit for large system sizes. These properties are deeply linked to the extensivity of a suitably defined ‘free energy’ from which all other thermodynamic quantities and local observables can be calculated.

The extensive part of this quantity can be expressed conveniently as a *cluster expansion* which, roughly speaking, is an expansion in terms of ‘joint cumulants’ or connected multi-point correlation functions in the state. Cluster expansions have been used extensively in statistical physics, both in classical and quantum systems, typically for the study of the partition function of thermal states [1–3]. They have also played an important role in the constructive approach to quantum field theory [4,5] and systematic applications have been developed in various fields, from nuclear physics [6] to quantum optics [7]. Although most studies focused mainly on the partition function, it is also possible to define such expansions directly for the quantum states themselves, which is the approach adopted in the present work.

This approach has the advantage of expressing the state in an exact form, yet and more importantly organizing its information content in order of decreasing physical relevance, while clearly demonstrating its locality properties at any order. It also provides the possibility to study the thermodynamic properties of overlaps between different states. Such overlaps are useful in quantum information theory where they are known as *fidelity* between two states, which has been shown to manifest criticality by exhibiting non-analytic behavior when one of the two states approaches a critical point [8–13]. It is also useful in out-of-equilibrium problems where a quantum system undergoes a rapid change in some parameter, a process known as *quantum quench* [14]. Quantum quenches have attracted significant interest partially due to experimental implementation in cold atom systems [15–22] and due to the possibility of studying thermalization and more generally equilibration in closed quantum systems [23–32] (for a review [33]). In this context, overlaps between the initial state and post-quench excited states are relevant in the study of out-of-equilibrium quantum thermodynamics as they capture information about quantum fluctuation relations [34] and in particular the statistics of work done by such quenches [35,36]. As we will see, the cluster expansion provides an exact spectral expansion of the state, allowing the systematic derivation of thermodynamic quantities, like the quench work statistics, as well as their quantum fluctuations. We suppose the existence of fields $\psi^\dagger(\vec{x})$ and $\psi(\vec{x})$ in a d dimensional