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Eigenmodes in nearly integrable quantum chains

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Abstract

Apparent incompatibility of classical irreversible thermodynamics with

Keywords: *integrals of motion, ETH, integrability breaking, XXZ model*

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Introduction

The results concerning spin transport in the long range XXZ have already been published in Mierzejewski et al. [1]. Writing something about computational basis

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Krylov subspace methods for quantum many-body systems

One of the two purposes of this thesis is to develop and test a set of numerical tools based on the Krylov subspace methods, which is a family of iterative methods concerned with projecting high dimensional problems into smaller dimension subspaces and solving them therein. Therefore, this chapter serves as a pedagogical introduction to the core ideas of these methods, including some of the usually omitted mathematical details. For the initial part of this exposition we follow the excellent textbook of numerical linear algebra by Trefethen and Bau [4], whereas for further applications to quantum many-body physics we rely on the excellent treatments of the topic found in Sandvik [2] and PhD thesis by Crivelli [3].

Reproduce Figure 32.1 about the difference between direct and iterative algorithms

We start this chapter by quickly sketching the problems with "direct" algorithms such as Exact Diagonalization, and quickly follow with the fundamental iterative algorithm for sparse nonhermitian matrices, the Arnoldi iteration. Its outputs admits several possible interpretations, however we shall focus on the problem of locating extremal eigenvalues. Afterwards, we restrict our attention to the class of hermitian matrices, to which of course all typical tigh-binding Hamiltonians belong to, and describe the Lanczos algorithm, which allows for efficient calculation of the ground state eigenvalue and eigenvector, and thus the ground state properties of a system. Yet in this work we are mainly interested in infinite temperature calculations, for which in principle sampling of the whole spectrum is required. To this end, in subsequent sections we develop a scheme for time evolution of arbitrary state, called the Krylov propagator [5], and combine it with the idea of Dynamical Quantum Typicality (DQT), which states that a single pure state can have the same properties as an ensemble density matrix [6, 7, 8]. We finish this chapter with a proposal of employing this method to the identification of local integrals of motion in a given tight-binding system. (cite my bachelors)

2.1 Problems with Exact Diagonalization

The most straightforward numerical method for studying discrete quantum many-body systems is without a doubt Exact Diagonalization (ED) [9]. It belongs to the family of the so-called direct algorithms and allows one to obtain numerically exact set of eigenvalues and eigenvectors and subsequently compute any desired properties of the system, be it thermal expectation values, time evolution, Green's functions etc. Unfortunately, the starting point of any ED calculation is the expression of the Hamiltonian as a dense matrix, in the Hilbert space basis of choice. Taking into account the fact that the dimension many-body Hilbert space grows exponentially with the size of the system, the memory cost quickly becomes prohibitive, even when exploiting conservation laws and related symmetries. For example, in the case of a spin chain of length L, with on-site basis dimension being 2, the full dimension of the Hilbert space would be $\mathcal{D} = 2^L$. Taking a modest length of 25 sites, that gives $2^{25} = 33554432 \approx 3.36 \cdot 10^7$ basis states and a memory footprint of Hamiltonian matrix of around 9PB (using double-precision floating point numbers), which is 9000 times more than the typical consumer hard drive capacity of 1TB. Even assuming some kind of distributed memory platform allowing for handling such large matrices, the computational complexity of ED, requiring $O(\mathcal{D}^3)$ operations, is the next major hurdle. Therefore, it is exceedingly difficult to probe the thermodynamic limit physics and ED calculations suffer from finite size effects.

Closer investigation of the Hamiltonian matrix, expressed in computational basis[1] quickly reveals the inefficiency of dense storage. Looking at Figure (Here figure with Hamiltonian, basis ordered by magnetization), we see that most of the matrix elements are zero. In fact only about $\mu \propto \mathcal{D}$ out of $\mathcal{D}^2$ matrix elements are non-zero. Hence, a numerical scheme leveraging this sparsity is highly desirable. This is exactly what the Krylov subspace algorithms do, by the virtue of requiring only a "black box" computation of matrix-vector product, which can be fairly easily implemented in a way requiring only $O(\mu\mathcal{D})$ operations.

2.2 Calculation of extremal eigenvalues

Our goal in this section is to develop the Lanczos algorithm for ground state search of hermitian matrices, and along the way understand how and why it works.

2.2.1 Arnoldi iteration

The Lanczos algorithm is special case of a more general algorithm, called Arnoldi iteration, designed to transform a general, nonhermitian matrix $A \in \mathbb{C}^{m\times m}$ via a orthogonal [2] similarity transformation to a Hessenberg form $A = QHQ^\dagger$.

Definition 2.1 *A square, $m \times m$ matrix H is said to be in upper **Hessenberg** form if $\forall i, j \in \{1, \ldots, n\} : i > j + 1 \implies (A)_{i,j} = 0$. It is said to be in **lower Hessenberg form**, if its transpose is in upper Hessenberg form.*

[1] For spin systems, it is the eigenbasis of S^z operator.

[2] Orthogonal in this context means that $Q^\dagger Q = I_{m\times m}$

A Hessenberg matrix differs from a triangular one by one additional super- or subdiagonal. Such form is desirable, because many numerical algorithms in linear algebra experience considerable speedup from leveraging triangular structure of a matrix, and sometimes those benefits carry over to this almost-triangular case. A particularly important strength of the Arnoldi iteration is that it can be interrupted before completion (cf. fig 32.1), thus producing only an approximation of the Hessenberg form in situation where m is so large, that full computations are infeasible (eg. in quantum many-body physics).

Assume now that we are able to only compute the first $n < m$ columns of the equation $AQ = QH$. Let Q_n be the restriction of Q to n columns and let them be denoted by $q_1, q_2, \dots q_n$.

2.2.2 Restriction to hermitian case: Lanczos iteration

2.3 Time evolution via the Krylov propagator

2.4 Physical interlude: Quantum Typicality

2.5 Correlation functions and the search for integrals of motion

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Spin transport in long range XXZ model

The results concerning spin transport in the long range XXZ have already been published in Mierzejewski et al. [1].

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Relaxation eigenmodes in long range XXZ model

The results concerning spin transport in the long range XXZ have already been published in Mierzejewski et al. [1].

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Summary

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Hilbert subspaces with fixed momentum