भारतीय विज्ञान शिक्षा एवं अनुसंधान संस्थान पुणे
INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH PUNE

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EXACT DIAGONALISATION AND KRYLOV SPACE METHODS IN MBL

SAGNIK GHOSH

INDIAN INSTITUTE OF SCIENCE EDUCATION & RESEARCH, PUNE

1. Introduction

One of the ways to characterise the dynamical phases of a system (described by a Hamiltonian or Floquet operator) is to look at its level spacing statics, which follows a Poisson distribution for integrable (Berry-Tabor Conjecture) and localised systems and is adequtely reproduced by that of Random Matrices for ergodic/thermal systems (Bohigas-Giannoni-Schmidt Conjecture). The central problem in quantum theory is to obtain the spectral pairs of the Hamiltonian/Floquet operator governing the dynamics of given system and it is in particular useful if the same can be done exactly. This notes deals with numerical exact diagonalisation techniques and the related Krylov Space Methods particularly in the context of their application to Many-Body Systems and MBL. It largely follows the structure and material of lectures by David Luitz (MPI-PKS, Dresden) at the 7th Les Houches Summer School on Numerical Physics.

Typical Model: (Hamiltonian)

The XXZ Model:

$$H = \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \Delta S_i^z S_{i+1}^z + h_i S_i^z \tag{1}$$

where, $h_i \in [-W, W]$ (Znidaric 2008, Pal 2010)

Typical Model: (Floquet)

$$\begin{aligned} H(t) &= \sum_i \Delta S_i^z S_{i+1}^z + h_i S_i^z \quad \text{for} \quad t \mod T < T_1 \\ &= \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \text{for} \quad t \mod T > T_1 \end{aligned} \tag{2}$$

(Ponte 2015).

2. Eigen-pair Properties

The focus here is to numerically studying eigen-pairs of $H, U(t)$. The eigenstate problem can be formally stated as,

Definition 1 (Eigenpairs)**.**

$$\begin{aligned} H\,|n\rangle &= E_n\,|n\rangle \quad (E_n, |n\rangle) \text{ being eigenpairs of } H \\ U\,|n\rangle &= \omega_n\,|n\rangle \quad (\omega_n, |n\rangle) \text{ being eigenpairs of } U \end{aligned} \tag{3}$$

Theorem 1. *Since $H^\dagger = H$ by definition, $E_n \in \mathbb{R} \quad \forall n$. Since U is Unitary,*

$$U^\dagger U = U U^\dagger = \mathbb{I}$$

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$\omega_n \in \mathbb{C}$ and $|\omega_n| = 1\ \forall n$. That is eigen-values of H are real and eigenvalues of U lives on the complex unit circle (and hence can be expressed as frequencies)

3. Krylov Subspace Methods

Used to obtain Eigenstates and eigenvalues of large sparse matrices. It is possible to devise exact diagonalisation algorithms that uses only Matrix Products eg. the power algorithm. Here we are gonna refine this to the so called Projection Method (Rayleigh-Ritz procedure) which finally leads to combinations of Krylov subspaces using either the Arnoldi or the lanczos scheme.

Algortihms like power method and Krylov spaces gives you access to the edge of the spectrum, whereas for MBL we are interested mostly at the centre of the spectrum. For that we need Spectral Transforms which is needed to relate the edge modes with the bulk ones.

The idea behind the Power Method is that if one applies the Hamiltonian successively on any trial wave function then it turns out that it filters the wave function which overlapped with the wave function corresponding to the largest eigen-value. The space that we obtain due to the power iteration is called the Krylov space.

Definition 2 (Krylov Space)**.** *Let $|\psi_n\rangle = H^n |\psi_0\rangle$ as is generated in the n-th iteration of the Power Method for an arbitrary $|\psi_0\rangle$. Then a Krylov Space of dimension m is defined as the vector space spanned by $\{|\psi_n\rangle \Big| n \in [0, m-1]\}$. That is,*

$$K_m(H, |\psi_0\rangle) = span(|\psi_0\rangle, H^1 |\psi_0\rangle, H^2 |\psi_0\rangle, \cdots, H^{m-1} |\psi_0\rangle) \tag{4}$$

for large m, the Krylov subspace contains a subspace that is spanned by the eigen-vectors at the edge of the spectrum.

4. Rayleigh-Ritz Procedure

We start from the Krylov space $K_m(H, |\psi_0\rangle)$ and create an ortho-normal basis for the same and construct the matrix $V = \{v_1, \cdots, v_m\}$. The Rayleigh-Ritz Procedure is also a projection method because in the next step we project the Hamiltonian onto the Krylov space using this basis,

Definition 3 (Rayleigh Quotient Matrix)**.**

$$R = V^\dagger H V \tag{5}$$

The idea then is to solve the eigen-problem for R, which is a much more tractable problem than the original one, since $m << d$.

$$R\overline{w}_i = \lambda_i \overline{w}_i \tag{6}$$

Definition 4 (Ritz Pairs)**.** *The eigen-pairs that are solution to the problem as states by the equation (6) are called Ritz Pairs, $(\lambda_i, \overline{w}_i)$*

The Ritz values λ_i are actually approximate eigenvalues of the original Hamiltonian and $\overline{w}_i$ are projection of original eigen-vectors to the Krylov subspace. We can go back to the original computation basis by,

$$V\overline{w}_i = \overline{x}_i \tag{7}$$

Conjecture 1. *If m is large enough then some of the Ritz pairs will converge very close to the original eigen-pairs of the Hamiltonian, and the ones that are faster to converge in terms of m, are the ones which have the largest modulus of eigen-value.*

Corollary 1. *The edges converges first.*

The convergence of various modes can be checked by computing the residual,

$$r_i = ||H\overline{x}_i - \lambda_i \overline{x}_i|| \tag{8}$$

This scheme is the central idea for the Arnoldi and lanczos algorithm. But in its present form the Rayleigh-Ritz Procedure is fairly inefficient, especially as for every higher m, you have to create a new orthogonal basis and repeat the procedure all over again. The Arnoldi and Lanczos schemes tries to address some of these issues.

5. Arnoldi Algorithm

Lanczos is the special case for Arnoldi for Hermitian Matrices. (Lanczos, 1950 and Arnoldi 1951, Y. Saad). Arnoldi in general works for non-Hermitian matrices too so in our notation we will denote the same as A. The first step is to generate the orthonormal basis for $K_m(A, |\psi\rangle)$ using only matrix products.

In the first step we choose a random $\overline{v_1}$ and normalise the same. In the next step we iteratively generate for $j = 1 \cdots m$

$$\overline{w} \leftarrow A\overline{v}_j \tag{9}$$

Then we apply an modified Graham-Schmidt orthogonalisation scheme,

$$\begin{aligned} \forall i \in [1, j] \qquad & h_[i, j] = \langle \overline{w}, \overline{v}_i \rangle \\ & \overline{w} = \overline{w} - \sum h_{i,j} \overline{v}_i \end{aligned} \tag{10}$$

Then we normalise the same and obtain the $j + 1$th eigen-vector of the higher dimensional Krylov Space.

$$h_{j+1,j} = ||\overline{w}|| \qquad \overline{v}_{j+1} = \frac{\overline{w}}{h_{j+1,j}} \tag{11}$$

Corollary 2. *The $R_{i,j}$ So it has a upper Hessenberg structure. (Upper-diagonal+plus the first off diagonal term)*

Theorem 2. *Define $R_{i,j} = h_{i,j}$. Then R is the Rayleigh Quotient Matrix. That is, it is the projection of the Hamiltonian to the Krylov Space.*

So the problem now just boils down to diagonalising R. Now, If A is Hermitian then by property $R^\dagger = R$.

Theorem 3. *If A is Hermitian, then R is a tri-diagonal matrix.*

This tri-diagonal structure in the Hermitian case also reduces the loop (10) to just one element. One also makes use of the fact that $h_{j,j+1} = h^*_{j+1,j}$

6. Problems and Comments

All algorithms comes with Round off errors and in this case this means gradual loss of orthogonality. One cure to this is explicit re-orthogonalisation. The other method is to restart. The idea here is that after some finite steps, you reuse the approximation of the obtained ground state as the starting vector and repeat the Lanczos scheme. This usually gives much better convergences. There also exists methodology such as Implicit Restarting, Deflation (removes parts of the Krylov space which has already converged, essentially once the state has converged you can subtract the projection of the subspace spanned by them).

If you have symmetries then it is always better to block-diagonalise the Hamiltonian first anyways as that significantly reduces the matrix sizes.

7. Probing the Center of the Spectrum: Spectral Transforms

The Arnoldi/Lanczos scheme gives us access to the edge of the spectrum. The Lanczos type convergence is inversely proportional to the gaps and for MBL systems typically the center of the spectrum is densely populated. But for studying dynamical phases we are more keen about the center of the spectrum.

Typically in a finite size system we have a maximum and a minimal energy. The role of the spectral transformations are essentially to map the central of the spectra to the edge modes. The simplest form is called spectral fold.

$$A = (H - \sigma \mathbb{I})^2 \tag{12}$$

Where σ is set close to a the levels we are interested in. This brings the interesting modes to the edges but the edge modes are still dense. So it has convergence issues.

The second choice for spectral transform is,

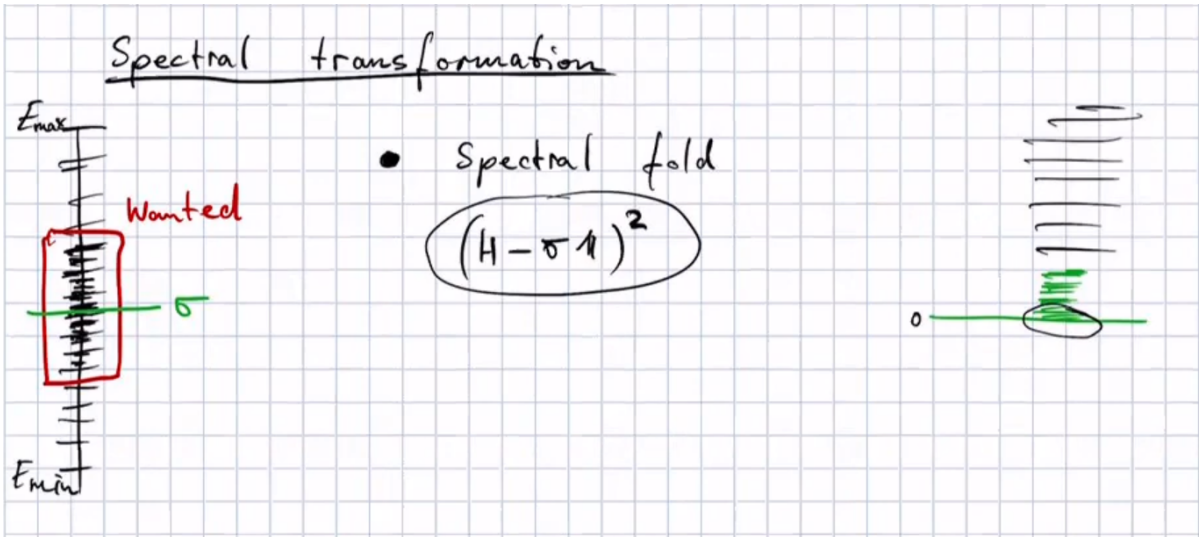

FIGURE 1. Caption: Mapping of modes using Spectral Fold (From lecture of David Luitz)

$$A = (H - \sigma\mathbb{I})^{-1} \tag{13}$$

and this goes by the name of *Shift Inverse*. It is in particular designed at mapping the states with less bang gaps to the ones with larger gaps after the transform, which makes Lanczos convergence faster. However, numerically the transform poses an issue as it involves a matrix inversion. The work around the same is as following.

First we construct the LU decomposition of $(H - \sigma\mathbb{I})$ using Gauss algorithm.

$$(H - \sigma\mathbb{I}) = LU \tag{14}$$

Then instead of solving for,

$$(H - \sigma\mathbb{I})^{-1} |\psi\rangle = |\tilde{\psi}\rangle \tag{15}$$

we solve for $|\tilde{\psi}\rangle$ in,

$$\begin{aligned} (H - \sigma\mathbb{I}) |\tilde{\psi}\rangle &= |\psi\rangle \\ \text{or} \quad LU |\tilde{\psi}\rangle &= |\psi\rangle \end{aligned} \tag{16}$$

which is a much faster algorithm than *dsyevd*. The module for LU decomposition is callled *zgetrf* and solving the equation is called *zgetrs*. You can also implement Massively Parallel Implementations of LU decomposition such as (**STRUMPACK, MUMPS**), using which you can do really large system sizes such as $d \simeq 2 \times 10^6 - 10^7$. (technical article: Pietracaprina Sci. Post. Phys. 5,045 (2018))