Contents

Chapter 1

Variational approximation of the partition function of 2D classical lattice models

1.1 Abstract

The variational method is introduced in its historical context – that of interacting 1D quantum lattice systems. An overview of White's density matrix renormalization group [2] is given. Then, the formal connection to 2D classical lattices is made.

1.2 Strongly interacting 1D quantum lattice models

The Hilbert space is enormous

Consider the problem of numerically finding the ground state $|\Psi_0\rangle$ of the N-site 1-dimensional transverse-field Ising-model, given by

$$H = -J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^{N} \sigma_i^x \tag{1.1}$$

The underlying Hilbert space of the system is a tensor product of the local Hilbert spaces $\mathcal{H}_{\text{site}}$, which are spanned by the states $\{|\uparrow\rangle, |\downarrow\rangle\}$. Thus, a general state of the system is a unit vector in a 2^N-dimensional space.

$$|\Psi\rangle = \sum_{i_1, i_2, \ldots \in \{|\uparrow\rangle, |\downarrow\rangle\}} c_{i_1, i_2, \ldots, i_N} |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \ldots \otimes |\sigma_N\rangle \tag{1.2}$$

So, for a system with 1000 particles, the dimensionality of the Hilbert space comes in at about $10^3 01$, some 220 orders of magnitude larger than the number of atoms in the observable universe. As it turns out, nature is very well described by Hamiltonians that are local – that do not contain interactions between an arbitrary number of bodies. And for these Hamiltonians, only an exponentially small subset of states can be explored in the lifetime of the universe [1]. That is, only exponentially few states are physical.

Expand a bit. Refer back to problem of finding ground state.

1.3 Density matrix renormalization group

The density matrix renormalization group (DMRG), introduced in 1992 by White [2], aims to find the best approximation of a many-

body quantum state, given that only a fixed amount of basis vectors is kept. This amounts to finding the best truncation

$$\mathcal{H}_N \to \mathcal{H}_{\text{eff}} \tag{1.3}$$

From the full N-particle Hilbert space to an effective lower dimensional one. This corresponds to renormalizing the Hamiltonian H. Before the DMRG paper, several methods for achieving this truncation were proposed, most notably Wilson's real-space renormalization group [4].

Real-space renormalization group

Consider the problem of finding the ground state of a many-body Hamiltonian H. A natural way of renormalizing H in real-space is by partitioning the lattice in blocks, and writing H as

$$H = H_A \otimes \ldots \otimes H_A \tag{1.4}$$

where H_A is the Hamiltonian of a block.

Make figures.

The blocking procedure now entails finding an effective Hamiltonian H'_A of the two-block Hamiltonian $H_{AA} = H_A \otimes H_A$. In numerical renormalization introduced by Wilson, H'_A is formed by keeping the m lowest lying eigenstates $|\epsilon_i\rangle$ of H_{AA}.

$$H'_A = \sum_{i=1}^{m} \epsilon_i \, |\epsilon_i\rangle \, \langle\epsilon_i| \tag{1.5}$$

This is equivalent to writing

$$H'_A = O H_{AA} O^\dagger \tag{1.6}$$

With O an $m \times 2^L$ matrix, with rows being the m lowest-lying eigenvectors of H_{AA}, and L the number of lattice sites of a block.

At the fixed point of this iteration procedure, H_A represents the hamiltonian of a half-infinite chain. In choosing this truncation, it is assumed that the low-lying eigenstates of the system in the thermodynamic limit are composed of low-lying eigenstates of smaller blocks. It turns out that this method gives poor results for many lattice systems. Following an example put forth by White and Noack [3], we establish here an intuition why.

Single particle in a box

Consider the Hamiltonian

$$H = 2\sum_i |i\rangle\langle i| - \sum_{\langle i,j\rangle} |i\rangle\langle j| \tag{1.7}$$

Where the second summation is over nearest neighbors $\langle i, j\rangle$. H represents the discretized version of the particle-in-a-box Hamiltonian, so we expect its ground state to be approximately a standing wave with wavelength double the box size. However, the blocking procedure just described tries to build the ground state iteratively from ground states of smaller blocks. No matter the amount of states kept, the final result will always incur large errors.

For this simple model, White and Noack solved the problem by diagonalizing the Hamiltonian of a block with different boundary conditions, and combining the lowest eigenstates of each. Additionally, they noted that diagonalizing $p > 2$ blocks, and projecting out $p - 2$ blocks to arrive at H_{AA}, also gives accurate results, and that this is a generalization of applying multiple boundary conditions. It is a slightly changed version of this last method that is know known as DMRG.

Density matrix method

Bibliography

[1] David Poulin et al. "Quantum simulation of time-dependent Hamiltonians and the convenient illusion of Hilbert space". In: *Physical review letters* 106.17 (2011), p. 170501.

[2] Steven R White. "Density matrix formulation for quantum renormalization groups". In: *Physical Review Letters* 69.19 (1992), p. 2863.

[3] Steven R White and RM Noack. "Real-space quantum renormalization groups". In: *Physical review letters* 68.24 (1992), p. 3487.

[4] Kenneth G Wilson. "The renormalization group: Critical phenomena and the Kondo problem". In: *Reviews of Modern Physics* 47.4 (1975), p. 773.