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4. Quantum spin systems I

* You know the difference between the Ising, the XY, the XXZ and the Heisenberg model
* You can explain the Lanczos algorithm
* You know the Trotter-Suzuki decomposition

4.1 Exact diagonalization

We want to take the step from single to many-particle problems on the example of quantum spin models. These are the simplest examples of we deal with distinguishable particles, where the many-body Hilbert space is simply given by

$$\mathcal{H}^{(N)} = \mathcal{H}^{\otimes N} = \bigotimes_{i=1}^{N} \mathcal{H},$$

where $\mathcal{H}$ is the Hilbert space of a single particle (spin in the current example).

Let us start with spin-$\frac{1}{2}$. A single particle has the Hilbert space $\mathcal{H} = \mathbb{C}^2$. That results in the N-spin Hilbert space $\mathcal{H}^{(N)} = (\mathbb{C}^2)^N = \mathbb{C}^{2^N}$. This has dimension 2^N! It is this exponential scaling which makes our lives so hard. Imagine a spin chain of size $N = 30$ $\Rightarrow$ The Hilbert space size is $2^{30} \approx 10^9$. A single complex vector needs already $\approx 16\,\text{GB}$ of memory!

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In order to push to the limits of what one can do in an exact way, we now learn a few tricks on how to do exact diagonalization. However, to approach the thermodynamic limit, we will need more sophisticated methods that we will learn later in the semester.

Before we start with the real business, let us introduce the standard spin models.

4.1.1 Spin models

4.1.1.1 The transverse field Ising model

We all know the Ising model

$$H = \sum_{\langle ij \rangle} s_i s_j = \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \qquad (s_i = \pm 1)$$

which we wrote in terms of commuting operators σ_i^z. The symbol $\langle i,j \rangle$ is standard for "sum over nearest neighbors". $\langle\langle i,j \rangle\rangle$ would denote next-nearest-neighbors. To turn this into a quantum model we add a transverse field

$$H = \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z + \sum_i \Gamma_i \sigma_i^x$$

As $\sigma_i^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ flips the σ_i^z eigenstates, Γ_i introduces a non-trivial quantum dynamics.

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4.1.1.2 The quantum Heisenberg model

The quantum Heisenberg model is nothing but the generalization of

$$H = \sum_{\langle ij \rangle} J_{ij} \vec{S}_i \vec{S}_j = \sum_{\langle ij \rangle} J_{ij} \left[S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \right].$$

The only change is, that we are using the spin-$\frac{1}{2}$ operators! A convenient way to write the Heisenberg model is

$$H = \sum_{\langle ij \rangle} J_{ij} \left[\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_i^z S_j^z \right].$$

Clearly, the total magnetization $M = \sum_i S_i^z$ is preserved. However the first two terms might change the local magnetization. Using the basis

$$\{ |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle \},$$

the two spin term over one bond of a $S = \frac{1}{2}$ problem looks like

$$\begin{pmatrix} J_{ij}/4 & & & \\ & -J_{ij}/4 & J_{ij}/2 & \\ & J_{ij}/2 & -J_{ij}/4 & \\ & & & J_{ij}/4 \end{pmatrix}.$$

The block-diagonal form reflects the spin-conservation.

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4.1.1.3 The XXZ model

Typically, magnetic materials don't possess the full SO(3) rotational symmetry, which means the Hamiltonian might reduce to

$$H = J \sum_{\langle ij \rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z,$$

which is called the XXZ model. For $\Delta \to 0$, this reduces to the quantum XY-model. For $|\Delta| \to \infty$ we obtain the classical Ising model.

4.1.2 Exact diagonalization

The good news: typically Hamiltonians contain only two-body terms. That means not all $2^N \times 2^N$ elements of an N spin $S = 1/2$ problem are nonzero. But even the storage of a sparse matrix with $\mathcal{O}(2^N)$ matrix elements is prohibitive for large N. The solution is to use iterative solvers.

Imagine you take a random vector

$$v_{\text{random}} = \sum_i c_i |i\rangle \quad \text{with} \quad H|i\rangle = \lambda_i |i\rangle.$$

If we now apply the Hamiltonian

$$H v_{\text{random}} = \sum_i c_i \lambda_i |i\rangle.$$

If we repeat this we obtain

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$H^3 v_{random}$, $H^4 v_{random}$, etc $\Rightarrow$

$H^M v_{random}$ is a good candidate for an extremal eigenvector.

A more systematic approach is to use the Krylov space spanned by

$$\{v, Hv, H^2 v, \ldots, H^M v\} = \mathcal{K}^M$$

This space is only M-dimensional. However to have an orthonormal system we need to orthogonalize

$$r_{n+1} = Hv_n - \underbrace{\sum_{j=1}^{n} v_j \left[v_n^* H v_j\right]}_{\text{Gram-Schmidt}} \qquad \text{Arnoldi}$$

But for this approach we still need to store M-2^N sized vectors! For hermitian problems $H = H^+$ we can use only three of them!

$$r_{n+1} = Hv_n - v_n \underbrace{\left[v_n^* H v_n\right]}_{\alpha_n} - v_{n-1} \underbrace{\left[v_{n-1}^* H v_n\right]}_{\beta_n}$$

$$v_{n+1} = \frac{r_{n+1}}{\|r_{n+1}\|}$$

Lanczos

[Show that the overlap with vectors further back than v_{n-1} are identically zero for $H = H^+$]

In this way, we generated an effective Hamiltonian

$$H \propto \begin{pmatrix} \alpha_1 & \beta_2 & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \beta_4 & & \\ & & \beta_4 & \alpha_4 & \beta_5 & \\ & & & \beta_5 & \alpha_5 & \ddots \\ & & & & \ddots & \ddots \end{pmatrix} = T_{nm}.$$

It is now easy to diagonalize T_{nm}. Like this we get the lowest lying eigenvalues. To find the eigenvectors, we need to go back from $\mathcal{K}^M$ to the full Hilbert space. But we never stored more than three of the basis vectors of $\mathcal{K}^M$! Solution: run the iteration twice!

One problem that we need to be aware of: v_M is orthogonal to $v_1, \dots, v_{M-1}$. In principle. But round-off errors spoil this property, and "new" low-lying eigenvalues appear throughout the iteration. These are called ghost and have to be removed.

Don't code your own Lanczos to do so! Use existing libraries such as scipy.sparse.linalg for Python.

4.2 Time evolution

As for the single particle case, we want to also solve time-dependent problems of the type

$$i\hbar \partial_t |\psi(t)\rangle = H(t) |\psi(t)\rangle$$

both for constant Hamiltonians $H(t) = H$ as well as for time-varying ones.

4.2.1 Time independant Hamiltonians

We already know that the exact solution to the above equation would be

$$|\psi(t+\Delta t)\rangle = e^{-iH\Delta t/\hbar} |\psi(t)\rangle.$$

But we also know that expanding the exponential leads to a non-unitary time evolution. For single-particle problems of the type $H = \hat{T} + \hat{V}$ we got to know the split-operator method, where we knew how to apply $e^{\hat{O}}$ for some operator $\hat{O}$ exactly. Here we go along this line as well.

4.2.1.1 Trotter-Suzuki

We split the Hamiltonian into a sum of K terms

$$H = \sum_{k=1}^{K} h_k$$

which we know how to exponentiate easily. The time evolution operator for a small time-step Δt is then decomposed into multiple products of the non-commuting terms in the Hamiltonian. To first order we have

$$e^{-iH\Delta t/\hbar} = \prod_{k=1}^{K} e^{-ih_k \Delta t/\hbar} + \mathcal{O}(\Delta t^2).$$

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The second-order version reads

$$e^{-iH\Delta t/\hbar} = S\left(\frac{\Delta t}{2}\right) + \mathcal{O}(\Delta t^3)$$

with

$$S(\Delta t) = \left(\prod_{k=1}^{K} e^{-ih_k \Delta t/\hbar}\right)\left(\prod_{k=K}^{1} e^{-ih_k \Delta t/\hbar}\right).$$

For $K=2$, this simplifies to

$$e^{-iH\Delta t/\hbar} = e^{-h_1 \Delta t/2\hbar}\, e^{-ih_2 \Delta t/\hbar}\, e^{-ih_1 \Delta t/2\hbar},$$

which we handle like in the split-operator case with half-time steps in the beginning and the end.

Examples

A: The transverse field Ising model

For the case of the transverse field Ising model we split the Hamiltonian as

$$H = \underbrace{\sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z}_{h_1} + \underbrace{\Gamma\sum_i \sigma_i^x}_{h_2}$$

Each of them can be easily exponentiated. First, the Ising term h_1 is diagonal and is easily written as

$$e^{-ih_1\Delta t/\hbar} = \prod_{\langle ij\rangle} e^{-i\Delta t J_{ij}\sigma_i^z\sigma_j^z/\hbar}.$$

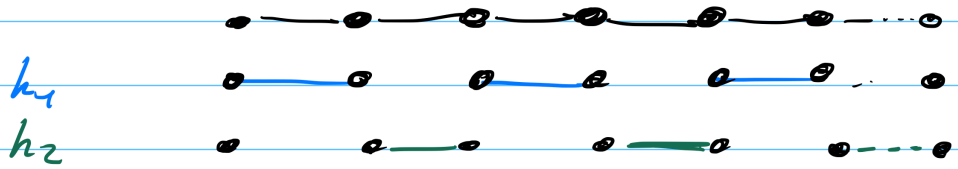
The local term h_2, on the other hand is not diagonal but can be exponentiated for each site individually.

$$e^{i\alpha t P_0 \sigma^x} = \begin{pmatrix} \cos(\alpha t P/k) & i\sin(\alpha t P/k) \\ -i\sin(\alpha t P/k) & \cos(\alpha t P/k) \end{pmatrix}.$$

It is important to note, that both terms h_1 and h_2 can be calculated on the fly given a specific state in the σ^z-basis. So we never have to store the full Hamiltonian!

B: Heisenberg, XXZ and XY

The good thing about the transverse Ising model was, that terms connecting different sites were diagonal. For the Heisenberg-like models we need to work harder to find simple h_i's. One way to go is to split into disjoint bonds:



$$H = h_1 + h_2 = H_{even} + H_{odd}$$

with

$$H_{even} = J \sum_i \frac{1}{2}\left(S_{2i}^+ S_{2i+1}^- + S_{2i}^- S_{2i+1}^+\right) + \Delta S_{2i}^z S_{2i+1}^z,$$

$$H_{odd} = J \sum_i \frac{1}{2}\left(S_{2i+1}^+ S_{2i+2}^- + S_{2i+1}^- S_{2i+2}^+\right) + \Delta S_{2i+1}^z S_{2i+2}^z.$$

Both H_{even} and H_{odd} contain commuting terms that can be individually exponentiated:

$$e^{i\epsilon\Delta J/4}\begin{pmatrix} e^{-i\epsilon\Delta J/4} & & \\ & \cos(\epsilon\Delta J/2) & i\sin(\epsilon\Delta\frac{J}{2}) \\ & -i\sin(\epsilon\Delta J/2) & \cos(\epsilon\Delta J/2) \\ & & e^{-i\epsilon\Delta J/2} \end{pmatrix}.$$

4.2.1.2 Imaginary time evolution

We can use the time-evolution protocoll discussed above to obtain the ground-state. Imagine we replace

$$it \to \tau.$$

Then, the "imaginary time" evolution reads

$$|\psi(\tau)\rangle = e^{-\tau H}|\psi(0)\rangle.$$

Let us see what happens to a random state, that we again write with respect to the energy eigenstates

$$H|i\rangle = \lambda_i|i\rangle \qquad |\psi_0\rangle = \sum_i c_i|i\rangle$$

$$\Rightarrow$$

$$e^{-\tau H}|\psi_0\rangle = \sum_i c_i e^{-\lambda_i\tau}|i\rangle$$

$$= e^{-\epsilon_0\tau}\Big[c_0|0\rangle + \underbrace{\sum_{k>0} e^{-\Delta\lambda_k\tau} c_k|k\rangle}_{\to 0}\Big].$$

Indeed, provided that $c_0 \neq 0$, we find the ground-state.

4.2.2. Time dependent Hamiltonians

In principle, we can use the Trotter-Suzuki approach also to problems where $H(t)$ explicitly depends on time. The only issue is that

$$|\psi(t+\Delta t)\rangle \neq e^{-iH(t)\Delta t}|\psi(t)\rangle$$

or $[H(t'), H(t)] \neq 0$, i.e., the Hamiltonians at different times do not commute. We need to use

$$U(t,t') = \hat{T}_s\, e^{-i\int_t^{t'} H(s)\,ds},$$

where $\hat{T}_s$ is the time ordering operator.

4.2.2.1 The Magnus expansion

There are various ways of dealing with the time-ordering operator. It is often convenient to use the Magnus expansion

$$U(\Delta t) = e^{-i\Delta t \bar{H}_t} \quad \text{with}$$

$$\bar{H}_t = \bar{H}_t^{(1)} + \bar{H}_t^{(2)} + \ldots \quad \text{where we write}$$

$$\bar{H}_t^{(1)} = \frac{1}{\Delta t}\int_t^{t+\Delta t} H(s)\,ds,$$

$$\bar{H}_2^{(2)} = -\frac{i}{\Delta t}\int_t^{t+\Delta t} ds \int_t^{s} dt\, [H(s), H(t)].$$

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We can now use $\bar{H}_t$ instead of H and use all techniques discussed above.