Theory of Quantum Systems for Beginners

During this two-day lab class, you will learn basic analytic and computational methods we use in the Theory of Mesoscopic Quantum Systems group. On both days, you will receive lectures in the morning, followed by programming sessions in the afternoon. The course requires a solid knowledge of linear algebra and basic quantum mechanics, and programming will be done using the Julia language.

The basics will be studied hands-on on particular assignments under the subject: "The Ising model: spontaneous symmetry breaking, local order parameters, order and disorder in quantum magnets". Depending on the progress in the first topic, follow-up assignments may be chosen from one of the following: "The Bose-Hubbard model: superfluids and Mott-insulators" (intermediate), "Matrix Product States: A variational approach to the quantum many-body problem" (intermediate) or "Topological quantum matter: exotic bound modes and non-local order parameters" (advanced).

Exact Diagonalization

This technique is a brute-force approach to numerical simulations of condensed matter systems, because it constructs the Hamiltonian operator in a suitable vector space, followed by a straightforward diagonalization in order to access the spectrum.

Mathematically, exact diagonalization corresponds to finding solutions of the stationary Schrödinger equation in Dirac notation

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

in which $\hat{H}$ corresponds to the Hamiltonian operator and $|\psi_n\rangle \in \mathcal{H}$ is the corresponding eigenstate of $\hat{H}$ with eigenvalue E_n. Note that the Hamiltonian can be represented as a matrix in an arbitrary basis $\{\phi_n\}$, with matrix elements $H^{\phi}_{mn} = \langle\phi_m|\hat{H}|\phi_n\rangle$. The Hamiltonian in this notation is simply

$$\hat{H} = H^{\phi}_{mn}\,|\phi_m\rangle\,\langle\phi_n|\,.$$

Please note that I use the sum convention. The matrix elements depend of course on the choice of the basis, and $H^{\psi}_{mn} = E_n\delta_{mn}$ is diagonal. In a typical situation, the Hamiltonian is written in a canonical basis (e.g. in a real-space basis where $|\phi_n\rangle$ is localized at position n), such that the matrix elements H^{ϕ}_{mn} are known, but the eigenvalues E_n are not.

> Convince yourself that the eigendecomposition of H^{ϕ}_{mn} leads to the spectral decomposition of $\hat{H}$.

Now, if we want to measure eigenstate observables in the canonical basis, they can be expressed in terms of the unitary transformation U which diagonalizes H^{ϕ}.

Find a formula for the expectation value of a general Hermitian operator $\langle\psi_i|\hat{O}|\psi_j\rangle$. Double-check your result by computing $\langle\psi_i|\hat{H}|\psi_j\rangle$.

The transverse-field Ising model (TFIM)

The TFIM is the quantum analog of the classical (Ernst) Ising model, motivated from the study of ferromagnetism in statistical mechanics. The initial idea is the following: elementary magnets can only assume two values. They don't have dipolar magnetic interactions in the solid body (everything is rather screened) and their interaction range is limited to their very neighbors, resulting in a short-ranged exchange interaction. Futhermore, there is an external field which induces quantum fluctuations relative to the axis of the exchange interaction. The effect of these fluctuations in 1D is equivalent to thermal fluctuations in a 2D classical system, which can be seen in the path integral formulation. Furthermore, the 1D quantum Ising model is THE example of quantum phase transitions, because it can be solved analytically in full glory via the transfer-matrix method. Both analytic approaches will be presented if you want to pursue project 1.

The Hamiltonian reads

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}^z_{\boldsymbol{r}_i} \hat{S}^z_{\boldsymbol{r}_j} + h \sum_i \hat{S}^x_{\boldsymbol{r}_i}$$

in which $\boldsymbol{r}_i$ denotes some position in a Bravais lattice, and $\hat{S}^k_{\boldsymbol{r}_i}$ is the local spin-1/2 operator along the k direction. J denotes the binding energy between adjacent spins ($\langle i,j \rangle$ denotes a constrained sum over nearest neighbors only), and h is the magnetic field amplitude associated with the Zeeman coupling. The spin operators satisfy the same algebraic commutation relations as orbital angular momentum, i.e.

$$[\hat{S}^i, \hat{S}^j] = i\hbar\varepsilon_{ijk}\hat{S}^k$$

and they can be represented in terms of the Pauli matrices

$$\hat{S}^i \simeq \frac{\hbar}{2}\sigma^i,$$

$$\sigma^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},\ \sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Keep in mind that the Pauli matrices are a good basis for any 2×2 matrix, it might be imortant for some of the assignments.

In the following, we set $\hbar = 1$, and remember that we thereby changed our unit of energy to a reduced Planck quantum. Furthermore, to make our discussion easier for now, we consider a one-dimensional chain such that $\boldsymbol{r}_i = ia$, and set the lattice constant $a = 1$. We don't need to be careful about that because a does not enter in $\hat{H}$, although in an actual experiment, J will of course decrease if the distance between the spins is increased.

Remember that a general many-body state, composed by N instances of a local Hilbert space $|i_n\rangle \in \mathcal{H}_n$, reads

$$|\Psi\rangle = \sum_{\{i_n\}} C_{i_1,i_2,\ldots,i_n} |i_1, i_2, \ldots, i_n\rangle$$

where

$$|i_1, i_2, \ldots, i_n\rangle = |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_n\rangle$$

denotes the Kronecker product. In order to construct the local spin operators of $\hat{H}$, we apply the same strategy:

$$\hat{S}^k_n \simeq \frac{1}{2} \left(\bigotimes_{j<n} \sigma^0 \right) \sigma^k \left(\bigotimes_{j>n} \sigma^0 \right)$$

> Consider $N = 8, 16, 32, 64$ instances and assume that each coefficient of $C_{\{i_n\}}$ is a `float64`. How much memory is needed to store the wavefunction? How much memory do you need for a naïve matrix expression of H? What is the maximum N that you can simulate on your laptop? What if the Hamiltonian is perturbed by just a single term $\hat{S}^y_{\boldsymbol{r}_i}$?
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> Construct the operators $\hat{S}^k_n$ in a `julia` script and demonstrate that $[\hat{S}^k_m, \hat{S}^l_n] = 0 \ \forall m \neq n$. Use the operators to construct the Hamiltonian.

The eigenvalue problem

Given a $n \times n$ Hermitian matrix A, we want to find m extremal eigenvalues and -vectors.

> Develop a method to get the job done.
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> Compare your implementation with the precision and runtime of an appropriate implementation in `KrylovKit.jl`. Bonus: look up the Lanczos algorithm, implement it and compare your version against the KrylovKit.

A blind run into the Ising model

Now that we know a bit about how to numerically solve the eigenvalue problem, let's go back to the Ising model and apply it to our first physics problem.

> Can you guess the energy and ground state for $J = \pm 4$ and $h = 0$? Is there a degeneracy of the ground state? What do you expect happens for $|h| \ll |J|$?
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> Describe two more trivial examples of $\mathbb{Z}_2$, involving integer numbers. Show that $\hat{X}$ is a symmetry of the Ising model, i.e. $[\hat{H}, \hat{X}] = 0$. What does that mean?

The lowest energy state is two-fold degenerate, and the most general ground state is $|\Psi\rangle = \alpha\,|\Psi_\uparrow\rangle + \sqrt{1-\alpha^2}\,|\Psi_\downarrow\rangle$. However, the system is not truly "quantum". What we mean by that is that the degenerate ground state is infinitely sensitive to perturbations, which leads to a so-called spontaneously symmetry-broken state in the thermodynamic limit.

> Consider a perturbation of the form $-h_z \sum_j \hat{S}^z_j$ (with $h_z > 0$). What happens to the degenerate $\mathbb{Z}_2$ symmetric ground state $|\Psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\Psi_\uparrow\rangle \pm |\Psi_\downarrow\rangle\right)$? Make your statement formal by a first order perturbation theory. From your result, argue that the unperturbed model in the thermodynamic limit can be approached in two different (non-commuting) limits.
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> Now that you have an idea of the underlying physics, try to confirm your intuition numerically.