Computational Quantum Physics
Exercise 8

PHYS-463
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Problem 8.1 Time-dependent variational principle (TDVP)

In previous lectures we have seen how variational ansätze can be used to study static physical properties of quantum many-body systems. Variational methods can also be used to describe the time evolution of a quantum state, using the Time Dependent Variational Principle (TDVP).
In this exercise we will use TDVP to describe the time evolution of the Transverse Field Ising Model (TFIM) with open boundary conditions, given by:

$$\hat{H} = J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{N} \sigma_i^x. \tag{1}$$

a) Start with the minimal example case considering $N = 2$ spins and the variational ansatz:

$$|\psi(\theta(t))\rangle = \mathrm{e}^{\mathrm{i}\theta(t)(\sigma_1^x + \sigma_2^x)} |\phi(0)\rangle \text{ with } |\phi(0)\rangle = |{\downarrow}\rangle \otimes |{\downarrow}\rangle, \tag{2}$$

and $\theta(t)$ a complex parameter. Use the expression of the S matrix given in the lecture notes and derive the expression for the vector C to solve the equations of motion and compare the variational dynamics to the exact one.

(*Hint:* to compare the variational dynamics with the exact one you can measure some observables on the time evolved state, such as magnetization or energy.)

b) Now we generalize the problem to N spins and consider a mean-field ansatz of the form

$$|\psi\left(\theta_1(t), \ldots, \theta_N(t)\right)\rangle = \prod_{i=1}^{N} \mathrm{e}^{\mathrm{i}\theta_i(t)\sigma_x^i} |\psi(0)\rangle, \tag{3}$$

where $|\psi(0)\rangle = \bigotimes_{i=1}^{N} |{\downarrow}\rangle$. Implement the code that computes S, C and update the parameters θ_i for the given ansatz and system.

c) Fix $\Gamma = 1$ and for $N = 10$ compare the results given by the TDVP with those obtained in Exercise 3.2 for $J \in \{0, 0.1, 0.25, 0.4\}$. What do you observe?

Problem 8.2 Imaginary time evolution

As we have seen in the lecture, we can use the Wick rotation $\mathrm{i}t \to \tau$ to perform imaginary time evolution of a given initial quantum state. The resulting state of this evolution is the ground state of the given quantum mechanical system, as was also shown in the lecture. In this exercise we want to implement this method and analyse its convergence rate. To do this, we consider the TFIM with periodic boundary conditions:

$$\hat{H} = J \sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \Gamma \sum_{i=1}^{N} \sigma_i^x, \tag{4}$$

where $\sigma_{N+1} = \sigma_1$.

For a small imaginary time step δ_τ, we approximate the state evolution to the first order:

$$|\psi(\delta_\tau)\rangle = \mathrm{e}^{-\delta_\tau \hat{H}} |\psi(0)\rangle \approx (1 - \delta_\tau \hat{H}) |\psi(0)\rangle \,. \tag{5}$$

a) Implement the TFIM Hamiltonian using sparse matrices introduced in former exercises.

b) Using exact diagonalization (ED), find the ground state energy E_0 and the first excited state energy E_1 of the TFIM with $N = 10$ spins, $J = 1$, and $\Gamma \in \{0.5, 1, 1.5, 2\}$ respectively.

c) Starting from a random initial state, repeatedly apply Eq. (5) until $\tau = 20$ (using the same values for N, J, and Γ as above), and measure 1000 energies E during the evolution.
Hint: Make sure to normalize your state after each iteration to prevent numerical instability.

d) For each Γ, plot the energy difference $E - E_0$ as a function of τ. How does the energy converge to the ground state?

e) Estimate the exponential convergence rate of this method when E is close to E_0, and plot it as a function of the energy gap $E_1 - E_0$. What can you observe? Can you explain the result?
Hint: The interval of τ where E is steadily converging can be different for each Γ.