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Computational Quantum Physics (M2) *T. Roscilde, F. Mezzacapo, F. Caleca, S. Bocini*

General rule for the TD sessions: the TD sessions are fully *hands-on* – namely, in every TD session you are supposed to *write computer codes* to learn about the phenomenology and efficiency of important algorithms for problems in quantum physics. You should choose a programming platform (Python, Matlab, Mathematica, C, Fortran, etc.), and you should be able to plot your results in the form of two-dimensional functions $y = f(x)$ (using matplotlib in Python, the plotting utilities of Matlab and Mathematica, Gnuplot, etc.), or occasionally in a more complicated form. We assume that you have some familiarity with at least one programming platform; if this is not the case, you should be able to familiarize yourself rapidly *e.g.* by attending online tutorials.

TD5: Quantum Monte Carlo for the quantum Ising model

In this exercise sheet, we shall use the Trotter-Suzuki mapping of the thermodynamics of the quantum Ising model in d dimensions onto that of the classical Ising model in $d+1$ dimensions; and we will perform a numerical evaluation of the statistical averages of the quantum model via the standard Monte Carlo approach.
We shall focus on the one-dimensional version of the model, with Hamiltonian

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

where the index i runs on a ring of N sites with periodic boundary conditions, $N+1 \equiv 1$. The Trotter-Suzuki mapping relates the partition function of this model to that of a two-dimensional classical Ising model with spatially anisotropic interactions:

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) \approx \cosh(\beta g/M)^{NM} \left[\sum_{\{\vec{\sigma}_k\}} e^{-\beta H_{\mathrm{eff}}(\{\vec{\sigma}_k\})} + O(\beta^2/M)\right] \tag{2}$$

where

$$\frac{H_{\mathrm{eff}}(\{\vec{\sigma}_k\})}{J} = -\frac{1}{M}\sum_i \sum_{k=1}^{M} \sigma_{i,k}\sigma_{i+1,k} - \frac{J_\tau}{J}\sum_i\sum_k (\sigma_{i,k}\sigma_{i,k+1} - 1) \tag{3}$$

and

$$J_\tau = \frac{k_B T}{2} \left|\log\left[\tanh(\beta g/M)\right]\right| \ . \tag{4}$$

Notice that the system has periodic boundary conditions also in the extra (Trotter) dimension ($k = M+1 \equiv 1$), due to the cyclic property of the trace.

1 Setting up the code for the quantum Ising chain

1.1

Define an array `spin(i,k)` of integer (± 1) numbers containing the spin configuration, with $i = 1, N$ and $k = 1, M$.
Define also dimensionless parameters

$$t = \frac{k_B T}{J} \qquad \epsilon = \frac{\beta g}{M} = \frac{g/J}{tM} \ \ (\ll 1) \tag{5}$$

such that $J_\tau/J = (t/2)|\log\tanh(\epsilon)|$. By experience, a good choice is $\epsilon = 10^{-2}$ to keep the Trotter error under control; and $t = 1/N$ to observe the physics of the ground state of the system.
Fixing N fixes t; and, moreover, fixing g/J fixes $M = (g/J)/(t\epsilon)$.
For the choice of N, you can start small (e.g. $N = 10$), and then go up with the size if time permits.

1.2

Choose a random initial configuration. Program a single-spin-flip Metropolis algorithm, by choosing a spin at random, proposing its flip, and accepting it with probability $p = \min(1, \exp(-\beta\Delta H_{\text{eff}})$. A single MC step is defined as $N \times M$ attempts to flip randomly chosen spins. You should perform P_{therm} thermalization steps in which you do nothing; and P_{meas} measurement steps during which you accumulate the averages of estimators (see below) – and, if you have time, you can also calculate the error bars on them! Good choices for the parameters could be $P_{\text{therm}} = 10^3 \div 10^4$ and $P_{\text{meas}} = 10^4 \div 10^5$.
You want to keep track as well of the acceptance rate of the spin flips (ratio of accepted spin flips to proposed ones), and understand how the value of g affects this rate.

1.3

For the measurement part of your simulation, keep track of a few observables

1. The longest-distance correlations $C_{N/2} = \langle \sigma_i^z \sigma_{i+N/2}^z \rangle$, which captures the existence (or not) of long-range ferromagnetism. For this quantity, you can use the estimator

$$C_{N/2} = \frac{1}{NM} \left\langle \sum_{i,k} \sigma_{i,k}\sigma_{i+N/2,k} \right\rangle_{\text{MC}} \tag{6}$$

   where $i+N/2$ should be read as $\min(i+N/2, N-i)$ in a system with periodic boundary conditions, and $\langle ... \rangle_{\text{MC}}$ denotes the Monte Carlo average.

2. The transverse magnetization $m^x = \langle \sigma_i^x \rangle$. To write an estimator for it, one can use the fact that

$$m^x = \frac{1}{N}\frac{d}{dg}(-k_B T \log Z) \tag{7}$$

   which leads to

$$m^x = \frac{1}{\sinh(2\epsilon)}\left(\cosh(2\epsilon) - C_\tau\right) \tag{8}$$

   where

$$C_\tau = \frac{1}{NM}\sum_{ik} \langle \sigma_{i,k}\sigma_{i,k+1} \rangle_{\text{MC}} \ . \tag{9}$$

2 Reconstructing the quantum phase transition

2.1

Choose a value of N, and for a grid of field values g/J (centered around $g/J = 1$), calculate $C_{N/2}$ and m^x. Plot the resulting values as a function of g/J. You should observe that the two quantities have a complementary behavior, and you may guess where the critical field sits.

2.2

If you repeat this study for several values of N – e.g. $N = 8,\ 16,\ 24, \ldots$ – then you can try and reconstruct the quantum critical behavior by testing the finite-size scaling Ansatz

$$C_{N/2} = N^{-2\beta/\nu} F\left(|g - g_c| N^{1/\nu}\right) \tag{10}$$

where $\beta = 1/8$ and $\nu = 1$ for a transition of the 2d Ising type. Namely, if you plot $C_{N/2} N^{2\beta/\nu}$ vs. $|g - g_c| N^{1/\nu}$, you should see that the data for different system sizes collapse onto the same universal curve $F(x)$, provided that you have properly guessed the critical field g_c.

3 Looking at spectral properties

The correlations in imaginary time contain precious information about the gap over the ground state. You can look at the correlation function $C_\tau(p) = \langle \sigma_{i,k} \sigma_{i,k+p} \rangle$, which, in the quantum paramagnetic phase, is supposed to decay as

$$C_\tau(p) \sim \exp(-p\beta\Delta/M) \qquad (p \gg 1) \tag{11}$$

where Δ is the spectral gap between the ground state and the first excited state. You can

3.1

test this behavior on your data, by working at a fixed g/J (e.g. $g/J = 2$); and trying to extract the gap from an exponential fit to the data; or via the second-moment estimator $\Delta/J \approx \xi_\tau^{-1}$ where

$$\xi_\tau = \frac{1}{2\pi t} \sqrt{\frac{S(0)}{S(2\pi/M)} - 1} \tag{12}$$

ξ_τ is the correlation length in imaginary time, and

$$S(l) = \sum_p C(p) \cos(lp) \ . \tag{13}$$

And then

3.2

repeat the calculation for a few values of g/J, to observe that a) the gap grows linearly with g, for large g; and b) the gap is closing at the quantum critical point (in the thermodynamic limit).