Homework 7; due Friday, December 14

PY 502, Computational Physics, Fall 2018

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QUANTUM ANNEALING OF A SPIN GLASS

In a quantum annealing process, some parameter s in a Hamiltonian $H(s)$ is changed slowly as a function of time, i.e., $s = s(t)$ and the Hamiltonian is time dependent; $H(t) = H(s(t))$. In typical protocols used in quantum computing based on quantum annealing, the Hamiltonian is written in the following way with two non-commuting parts H_0 and H_1;

$$H(t) = [1 - s(t)]H_0 + s(t)H_1, \tag{1}$$

where s is changed smoothly from $s = 0$ to $s = 1$ at fixed velocity v between the initial time $t = 0$ and final time $t = T$;

$$s(t) = vt, \quad v = 1/T. \tag{2}$$

The term H_0 is in some sense simple, so that the system (wave function) at $t = 0$ can be prepared to be in the ground state of $H(t = 0) = H_0$. In the basis considered, this state should be highly fluctuating, i.e., it is a superposition of many basis states (often the equal superposition of all basis states). At the other end, $H(t = T) = H_1$, the Hamiltonian corresponds to a purely classical (diagonal in the basis used) potential energy. In quantum computing applications, this potential energy is obtained as a result of a mapping from some complex optimization problem and the goal is to find the ground state of this Hamiltonian H_1. A main focus has been on Ising-type models with highly frustrated random interactions (spin glasses and related satisfiability problems of interest in quantum information science).

The motivation for this kind of setup is that, if the annealing process is sufficiently slow, the adiabatic theorem guarantees that the system will stay in its ground state of $H(s)$ at all times, assuming that the system can be regarded as completely isolated from its environment. Thus, we start by preparing the system in a trivial but highly fluctuating state at $t = 0$, and at $t = T$ we end up with a state—a single basis state—which is the ground state of a complicated Hamiltonian H_1. In principle the ground state can be degenerate, and if so one would obtain one of these when detecting the state at the end of the process.

Spin glass model

In this assignment you will solve the time dependent Schrödinger equation for an annealing process on a quantum spin model (an Ising model in a transversal field) defined by the Hamiltonian (1) with the terms

$$H_0 = -\sum_{i=1}^{N} \sigma_i^x = -\sum_{i=1}^{N}(\sigma_i^+ + \sigma_i^-), \tag{3}$$

$$H_1 = -\frac{2}{N-1}\sum_{i=1}^{N}\sum_{j>i} J_{ij}\sigma_i^z\sigma_j^z, \tag{4}$$

where $\sigma_i^z = \pm 1$ and $\sigma_i^x = \sigma_i^+ + \sigma_i^-$ are z and x Pauli spin matrices for the spins $i = 1, \ldots, N$.

The term (3) is trivial, having a ground state with all spins fully polarized in the x direction, i.e., at $t = 0$ we start the annealing process with the state

$$|\Psi(t = 0)\rangle = \prod_{i=1}^{N} \frac{1}{\sqrt{2}} (|\uparrow\rangle_i + |\downarrow\rangle_i) = 2^{-N/2} \sum_{\sigma^z} |\sigma_1^z, \ldots, \sigma_N^z\rangle, \tag{5}$$

which is the equal superposition of all the 2^N basis state in the basis used the computation. The Ising interactions J_{ij} in (3) couple all the spins in a random way, with the numbers J_{ij} drawn from a distribution of the type illustrated in Fig. 1;

$$P(J) = \begin{cases} a, & \text{for } -1 \leq J < 0, \\ 1 - a, & \text{for } 0 \leq J \leq 1. \end{cases} \tag{6}$$

There are $N(N-1)/2$ distinct pairs of spins and double-counting is avoided by restricting the second sum in Eq. (4) to $j > i$. The N-dependent factor in front of the Ising sum gives en extensive energy when all the couplings have the same signs, but this is not obvious—in fact, in some cases it is not true—when the signs are mixed (but this is nothing we need to worry about here).
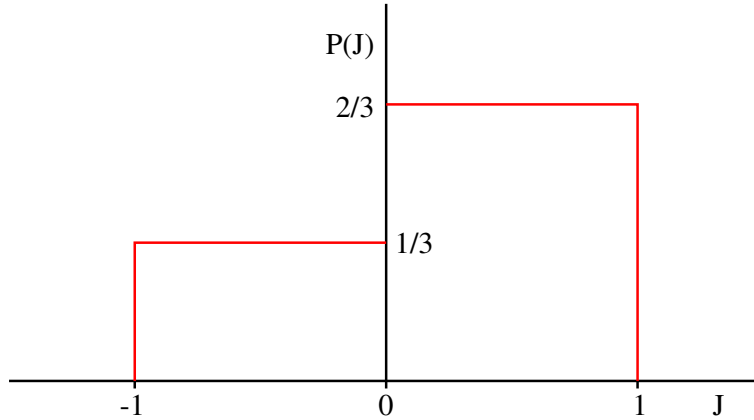

Figure 1: Example of the probability distribution (6), here with the parameter $a = 1/3$.

For $a = 0$, all the couplings are ferromagnetic [note the negative sign in front of the Ising term in the Hamiltonian (4)] and the ground state is a trivial ferromagnet with a doubly-degenerate ground state (all spins "up" or all spins "down"). For $a > 0$, the ground state can be very complicated and, if N is large, it can be very difficult to find the ground state, with the time taken to find it scaling exponentially with N with all known classical algorithms. The question is whether quantum annealing can find the ground state in a time scaling only as a power law in N. Here we will consider only small N, of the order 10, and we will not be able to answer this question. The goal is only to investigate how the quantum annealing process behaves as a is increased from 0.

Runge-Kutta solution of the Schrödinger equation

Recall the Runge-Kutta (RK) method, which we used earlier to solve classical equations of motion. It is a general method for a first-order differential equation of the form

$$\frac{dx(t)}{dt} = f[x(t), t]. \tag{7}$$

On a uniform time grid with $\Delta_t = t_{n+1} - t_n$ and $x(t_n) \equiv x_n$, the fourth-order RK algorithm (with step error of order Δ_t^5) can be written as

$$
\begin{aligned}
k_1 &= \Delta_t f(x_n, t_n), \\
k_2 &= \Delta_t f(x_n + k_1/2, t_{n+1/2}), \\
k_3 &= \Delta_t f(x_n + k_2/2, t_{n+1/2}), \\
k_4 &= \Delta_t f(x_n + k_3, t_{n+1}), \\
x_{n+1} &= x_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),
\end{aligned}
\tag{8}
$$

where the intermediate numbers $k_1 - k_4$ have to be evaluated successively.

This RK algorithm can be directly generalized to a matrix differential equation. We are interested in the Schrödinger equation with a time dependent Hamiltonian;

$$
\frac{\partial \Psi(\{\sigma^z\}, t)}{\partial t} = -iH(t)\Psi(\{\sigma^z\}, t),
\tag{9}
$$

where we work in the basis $\{\sigma^z\} = \{\sigma_1^z, \ldots, \sigma_N^z\}$ of the z spin components. Instead of a function f depending on x and t in Eq. (7), we now have to act with the Hamiltonian on the wave function, which is easy to do when we work in the matrix form of the Schrödinger equation.

Thus, instead of the scalar x in Eq. (8) we now work with vectors Ψ_n with 2^N components $\Psi_n(a)$ at time-step n, each element a of the vector representing the weight of a basis state in the bit representation ($a = 0$ corresponding to all down spins etc.). To integrate one time step we have to carry out the following operations corresponding to Eq. (8):

$$
\begin{aligned}
\phi_1 &= \Delta_t H(t_n)\Psi_n, \\
\phi_2 &= \Delta_t H(t_{n+1/2})[\Psi_n + \phi_1/2], \\
\phi_3 &= \Delta_t H(t_{n+1/2})[\Psi_n + \phi_2/2], \\
\phi_4 &= \Delta_t H(t_{n+1})[\Psi_n + \phi_3], \\
\Psi_{n+1} &= \Psi_n + \frac{1}{6}(\phi_1 + 2\phi_2 + 2\phi_3 + \phi_4),
\end{aligned}
\tag{10}
$$

where $\phi_1, \ldots, \phi_4$ are also vectors with 2^N elements. For each step we have to carry out four multiplications of the Hamiltonian matrix (at three different time points) with a vector.

Starting program for non-random ferromagnet

The program given to you with this assignment carries out the RK integration for a system with all ferromagnetic couplings $J_{ij} = 1$. The input data, read from the file `read.in` are: The number of spins N, the total time T, the RK time step Δ_t, and the frequency f_w at which output data should be written to a file. The format is two lines as follows:

N
T, δ_t, f_w

The output data are written to `res.dat` on lines with $t, P_s(t), E_s(t)$ for times t separated by w_f steps of size Δ_t. P_s is the probability of the system being in the classical $s = 1$ ground state (i.e., the state with the lowest Ising energy), which can be interpreted as the success rate of the
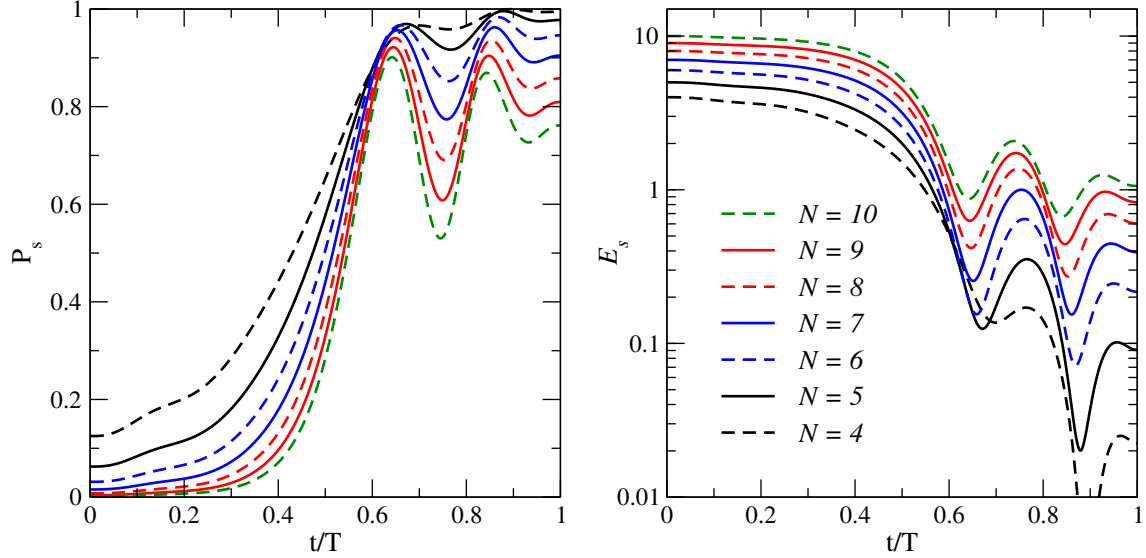
Figure 2: Sucess rate (left) and excess energy (right) in annealing processes with velocity $v = 1/10$ for systems with different number of spins N.

optimization. E_s is the excess Ising energy above the lowest value, which is another measure of the efficiency of the optimization procedure. We would certainly be interested in these quantities at the end of the process, $t = T$, but it is also interesting to look at their behaviors throughout the simulation.

Programming task

You should modify the program so that it can study systems with couplings distributed according to Eq. (6). Use the random number generateor we have used in past assignments. Since the results will depend strongly on the coupling realization, the program should average over realizations. As always in such cases, we should calculate error bars for the averages and you are given the program used to compute averages based on bin averages to be generated by your program. The input format for `read.in` should now be:

N,a
T, δ_t, f_w
`bins,reps`

where a is the parameter in the probability distribution, `bins` is the number of bins to be generated, and `reps` is the number of random instances of the couplings to be run for each bin. The output file with bin data should be called `res.dat` and it should be in the same format as the output file from the starting program, but now with bin averages instead of the results from the single run.

Investigations

<u>Part 1</u>

As always, we have to check convergence with the time step Δ_t. To do this, use the starting program and repeat calculations such as those illustrated in Fig. 2 for $N = 8$. Use two different

total integration times; $T = 10$ ($v = 0.1$) and $T = 100$ ($v = 0.01$) and vary Δ_t. Show figures illustrating poor performance when Δ_t is too large and convergence as Δ_t is reduced.

Part 2

Use your own program and carry out calculations for $a = 0$, $1/4$, and $1/2$. Note that for $a = 0$ the system is a random ferromagnet, so it is different from part 1. You have to check how many repetitions and bins you need in order for the error bars to be reasonably small (you can keep `bins=20` and vary `reps`). The way you carry out the investigation is open eneded. You should investigate different system sizes and velocities, and based on this work draw some conclusions on the efficiency of quantum annealing to reach the ground state. The computing time increases very quickly as a function of N and this will limit how far you can go in size. Just do whatever you can with your resources.

In addition to plots showing behaviors over the whole annealing path ($s \in [0, 1]$ as in Fig. 2), you should also focus on the final point $s = 1$, which is the point of main interest in quantum computing (the ability of the system to reach the classical ground states, i.e., the solutions of corresponding optimization problems). Produce plots of the success probability and the excess energy versus the system size N for different velocities and verrsus the velocity for different system sizes.