Assignment 2: Annealing

Ph 50 - Fall 2015

Due: 26 November 2015

Please submit your solutions in class or by e-mail to achatwin@caltech.edu

Problem 1: Annealing Ice Cream

Should you anneal ice cream? Tastes are subjective, so please describe why or why not.

Problem 2: Annealing a Single Spin

In class, we saw that the Hamiltonian for a single spin-1/2 in the presence of a constant, weak magnetic field in the z direction and a time-varying transverse magnetic field in the x direction is given by

$$\hat{H}(t) = -J\hat{\sigma}_z - g(t)\hat{\sigma}_x \, . \tag{1}$$

J and $g(t)$ both have units of energy and reflect the strength of the magnetic fields. $\hat{\sigma}_z$ and $\hat{\sigma}_x$ are 2×2 matrices:

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{2}$$

The state, or wavefunction, of the spin can be represented by a 2-component vector,

$$|\psi(t)\rangle \equiv \begin{pmatrix} \alpha(t) \\ \beta(t) \end{pmatrix}, \tag{3}$$

where $|\alpha(t)|^2$ (resp. $|\beta(t)|^2$) gives the probability of finding the spin pointing in the positive (resp. negative) z direction at time t. The state evolves according to the Schrödinger equation

$$i\hbar \frac{d}{dt}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle, \tag{4}$$

which has a unique solution given an initial state $|\psi(0)\rangle$. Collecting all of the definitions so far, we see that Eq. (4) just describes a system of two differential equations:

$$i\hbar\,\dot{\alpha}(t) = -J\alpha(t) - g(t)\beta(t) \tag{5}$$

$$i\hbar\,\dot{\beta}(t) = -g(t)\alpha(t) + J\beta(t) \tag{6}$$

A dot above a function denotes a derivative with respect to t.

To anneal the spin, one should choose $g(t)$ such that $g(0)$ is very large compared to J and such that $g(t)$ slowly decreases to zero. Then, at $t = 0$ we have that $\hat{H}(0) \approx -g(0)\hat{\sigma}_x$. We initialize the spin in the ground state of $-g(0)\hat{\sigma}_x$, or in other words, the eigenvector with the smallest eigenvalue. This state is

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{7}$$

or $\alpha(0) = \beta(0) = 1/\sqrt{2}$.

In this problem, you will compute an exact solution for $\alpha(t)$ and $\beta(t)$ for a particular choice of $g(t)$. You are welcome to solve the system of differential equations (5), (6) using symbolic algebra software, but I will step you through the solution in case you would like to practice some techniques for solving systems of coupled differential equations by hand.

(a) Lets first reduce the system of ordinary differential equations (ODEs) to a single second-order differential equation for $\alpha(t)$. To do this, start by taking a derivative with respect to t of both sides of Eq. (5). Then, use Eqs. (5) and (6) to eliminate β and $\dot{\beta}$ from the resulting equation. Given an initial condition $\{\alpha(0), \beta(0)\}$, what is the initial condition for $\alpha(t)$ and $\dot{\alpha}(t)$?

(b) Next, lets choose $g(t) = g_0\, e^{-Jt/\hbar}$. Use this choice to simplify your ODE for $\alpha(t)$. I suggest organizing your ODE in the form $\ddot{\alpha}(t) + c_1(t)\dot{\alpha}(t) + c_0(t)\alpha(t) = 0$.

(c) To make this ODE look more familiar, change to a new dependent variable $x = g(t)/J = (g_0/J)\, e^{-Jt/\hbar}$ and write down an ODE for $\alpha(x)$.

(d) What is the general solution of this ODE? If this ODE doesn't quite look familiar yet, let $\alpha(x) = \sqrt{x}A(x)$ and write down the ODE for $A(x)$.

(Hint: It's ok for Bessel functions to have an imaginary order...)

(e) What is the asymptotic behaviour of the general solution for $|\alpha(x)|^2$ as $x \to 0^+$ (*i.e.*, as $t \to \infty$)? At this point you may want to have Mathematica or Maple assist you with your calculations.

(Hint 1: I recommend using the Bessel J and Bessel Y functions to write down the general solution for $\alpha(x)$, *i.e.*, write $\alpha(x) = C_1(\text{term containing } J) + C_2(\text{term containing } Y)$. You may find the following asymptotic forms helpful,

$$J_q(z) \sim \frac{1}{\Gamma(q+1)}\left(\frac{z}{2}\right)^q \qquad Y_q(z) \sim -\frac{\Gamma(q)}{\pi}\left(\frac{2}{z}\right)^q, \tag{8}$$

which are valid for small $|z|$.)

(Hint 2: You should find that $|\alpha(x)|^2 \to (\text{some constant})$ as $x \to 0^+$.)

(f) Recall that in this case, the goal of annealing is to obtain, with high probability, the ground state of $H_0 \equiv -J\hat{\sigma}_z$, *i.e.*, the state $\binom{1}{0}$. Does annealing succeed? How does the answer depend on g_0 and J?

(Hint 1: Be careful, the initial value of $d\alpha/dx$ is not the same as the initial value of $d\alpha/dt$.)

(Hint 2: In this question you are being asked to analyze $|\alpha(x)|^2$ as $x \to 0^+$, now for the given initial condition (7). This part can get pretty harrowing, so I will let you decide how you would like to carry out your analysis to extract useful information. If you are looking for inspiration, here is what I did:

- Given the initial condition (7), I used Maple to solve for C_1 and C_2, expressing the answer in terms of $\epsilon \equiv J/g_0$.
- Next, I expanded $|\alpha(x \to 0^+)|^2$ for both small and large ϵ. For this, you may find the following pseudo-asymptotic forms helpful,

$$J_q(z) \sim \sqrt{\frac{2}{\pi z}}\cos\left(z - \frac{q\pi}{2} - \frac{\pi}{4}\right) \qquad Y_q(z) \sim \sqrt{\frac{2}{\pi z}}\sin\left(z - \frac{q\pi}{2} - \frac{\pi}{4}\right) \tag{9}$$

which are valid for large $|z|$.)