Introduction

This document aims to explain the numerical solution of the Born-Markov master equation, for a transverse-field XY model, close to the XY-XX crossover. First is an explanation of the model, the eigenstates of the unperturbed case, which have a spin-subspace structure which allows for quick exact diagonalisation. Then the perturbative corrections are derived, and the numerical algorithm is described.

Hamiltonian

The system of interest is a spin-$\frac{1}{2}$ chain of length N coupled to a set of N independent thermal environments, one for each spin. The system is modelled using an (anti-)ferromagnetic Hamiltonian, describing nearest-neighbour interactions with hopping strength $-J$. There is also an external magnetic field, whose magnitude is characterised by a constant g. Finally, there is pair-creation and annihilation induced by a small pertubative factor $\lambda \ll J, g$.

It is of interest to calculate the 'eigenoperators' $A(\omega)$ of this system. This allows for the modelling of the evolution of the system under the infulence of the thermal environments, with a Born-Markov master equation. This however, requires knowing the eigenstates of the system, $|\epsilon\rangle$. Now the Hamiltonian of the system will be described.

The spins are modelled using Pauli operators σ^μ, $\mu = x, y, z, +, -$ and so the system is described by a Hamiltonian

$$\begin{aligned} H &= H_0 + \lambda \hat{V} \\ &= -J \sum_n (\sigma_n^+ \sigma_{n+1}^- + \sigma_n^- \sigma_{n+1}^+) + gS^z + \lambda \sum_n (\sigma_n^+ \sigma_{n+1}^+ + \sigma_n^- \sigma_{n+1}^-), \end{aligned} \tag{1}$$

where $S^z = \sum_n \sigma_n^z$. The sum over n takes all values of the site label with the inclusion of periodic boundary conditions. Since the total z-projection spin operator S^z commutes with the unperturbed Hamiltonian $[H_0, S^z] = 0$, we may order the eigenstates in terms of their spin-sector. Let $|\epsilon_{r,i_r}^{(0)}\rangle$ denote the ${i_r}^{\text{th}}$ eigenstate with r up-spins of the unperturbed Hamiltonian. Then we have:

$$H_0 |\epsilon_{r,i_r}^{(0)}\rangle = \epsilon_{r,i_r}^{(0)} |\epsilon_{r,i_r}^{(0)}\rangle, \qquad S^z |\epsilon_{r,i_r}^{(0)}\rangle = (2r - N) |\epsilon_{r,i_r}^{(0)}\rangle. \tag{2}$$

The label r runs from 0 to N, giving a total of $N + 1$ spin-sectors. In each subsector, there are r up-spins distributed on a chain of N spins, which gives an ${}^N C_r$-dimensional space, where ${}^N C_r$ is the binomial coefficient $N!/(N - r)!r!$. Therefore, i_r runs from 1 to ${}^N C_r$.

Consider the configuration basis, ordered in terms of the total z-spin projection, which for $N = 3$ is

$$|000\rangle, |100\rangle, |010\rangle, |001\rangle, |110\rangle, |101\rangle, |011\rangle, |111\rangle. \tag{3}$$

Let $|\{\sigma\}\rangle$ denote one such configuration-basis state. Then in this basis, H_0 takes a

block-diagonal form:

$$\langle\{\sigma\}|H_0|\{\sigma'\}\rangle = \begin{pmatrix} -3g & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -g & -J & -J & 0 & 0 & 0 & 0 \\ 0 & -J & -g & -J & 0 & 0 & 0 & 0 \\ 0 & -J & -J & -g & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & g & -J & -J & 0 \\ 0 & 0 & 0 & 0 & -J & g & -J & 0 \\ 0 & 0 & 0 & 0 & -J & -J & g & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3g \end{pmatrix}. \tag{4}$$

The eigenvectors of this matrix can be found by diagonalising the four sub-blocks of the matrix.

Perturbation theory

Next, the perturbative corrections to the eigenstates of the unperturbed Hamiltonian are calculated to give an approximation to the full perturbed model.

To begin, we note that the unperturbed eigenstates form a complete state and so any state in the system space may be expressed as a superposition

$$|\psi\rangle = \sum_{r=0}^{N} \sum_{i_r=1}^{{}^{N}C_r} a_{r,i_r} |\epsilon^{(0)}_{r,i_r}\rangle, \tag{5}$$

where the a_{r,i_r} are complex numbers. This principle of superposition must also apply to the eigenstates of the perturbed Hamiltonian too:

$$|\epsilon_{n,i_n}\rangle = \sum_{r} \sum_{i_r} a^{n,i_n}_{r,i_r} |\epsilon^{(0)}_{r,i_r}\rangle. \tag{6}$$

In this expression the symbol a^{n,i_n}_{r,i_r} is represented as a perturbation series

$$a^{n,i_n}_{r,i_r} = \delta^n_r \delta^{i_n}_{i_r} + \lambda a^{n,i_n,(1)}_{r,i_r} + \lambda^2 a^{n,i_n,(2)}_{r,i_r} + \mathcal{O}(\lambda^3). \tag{7}$$

Similarly the perturbed eigenenergies can be written

$$\epsilon_{n,i_n} = \epsilon^{(0)}_{n,i_n} + \lambda \epsilon^{(1)}_{n,i_n} + \lambda^2 \epsilon^{(2)}_{n,i_n} + \mathcal{O}(\lambda^3). \tag{8}$$

Perturbation theory allows the calculation of the terms $a^{n,i_n,(m)}_{r,i_r}$ and $\epsilon^{(m)}_{n,i_n}$ in terms of the unperturbed eigenenergies and unperturbed eigenstates. Without going into the full derivation (which is simply a term-by-term equation of the Schrödinger equation using the perturbation series), the perturbative corrections are found to be, at first order:

$$\epsilon^{(1)}_{n,i_n} = \langle \epsilon^{(0)}_{n,i_n} | \hat{V} | \epsilon^{(0)}_{n,i_n} \rangle, \qquad a^{n,i_n,(1)}_{r,i_r} = \frac{\langle \epsilon^{(0)}_{r,i_r} | \hat{V} | \epsilon^{(0)}_{n,i_n} \rangle}{\epsilon^{(0)}_{n,i_n} - \epsilon^{(0)}_{r,i_r}}. \tag{9}$$

The remainder of this section will involve rewriting these expressions – particularly the first order correction to the wavefunctions – in terms of the subspace structure, so that a matrix form may be written down.

Rewriting perturbative correction

Let us first devide up the perturbative term in the Hamiltonian into two operators:

$$\hat{V} = \sum_n (\sigma_n^+ \sigma_{n+1}^+ + \sigma_n^- \sigma_{n+1}^-) = \hat{\Sigma}^{(+2)} + \hat{\Sigma}^{(-2)}, \tag{10}$$

where we have defined $\hat{\Sigma}^{(+2)} \equiv \sum_n \sigma_n^+ \sigma_{n+1}^+$ and $\hat{\Sigma}^{(-2)} \equiv \sum_n \sigma_n^- \sigma_{n+1}^-$. Clearly $\hat{\Sigma}^{(+2)}$ will take a state lying in the r-spin subspace to the $(r+2)$-spin subspace and $\hat{\Sigma}^{(-2)}$ will take an r-spin state to an $(r-2)$-spin state. More precisely:

$$\hat{V}|\epsilon_{r,i_r}^{(0)}\rangle = \sum_{i_{r-2}}^{{}^N C_{r-2}} c_{i_{r-2}} |\epsilon_{r-2,i_{r-2}}^{(0)}\rangle + \sum_{i_{r+2}}^{{}^N C_{r+2}} c_{i_{r+2}} |\epsilon_{r+2,i_{r+2}}^{(0)}\rangle. \tag{11}$$

Now, since the unperturbed eigenstates are an orthonormal set, we have that

$$\langle \epsilon_{n,i_n}^{(0)} | \epsilon_{r,i_r}^{(0)} \rangle = \delta_r^n \delta_{i_r}^{i_n}, \tag{12}$$

which implies immediately that $\langle \epsilon_{n,i_n}^{(0)} | \hat{V} | \epsilon_{r,i_r}^{(0)} \rangle = 0$ so there is *no* energy correction at first order for this perturbation.

Since the perturbation splits into to two terms, we shall deal with them independently. We first define the following symbols:

$$K_{r,n}^{(i_r,i_n)} = \frac{\langle \epsilon_{r,i_r}^{(0)} | \hat{\Sigma}^{(-2)} | \epsilon_{n,i_n}^{(0)} \rangle}{\epsilon_{n,i_n}^{(0)} - \epsilon_{r,i_r}^{(0)}}, \qquad M_{r,n}^{(i_r,i_n)} = \frac{\langle \epsilon_{r,i_r}^{(0)} | \hat{\Sigma}^{(+2)} | \epsilon_{n,i_n}^{(0)} \rangle}{\epsilon_{n,i_n}^{(0)} - \epsilon_{r,i_r}^{(0)}}. \tag{13}$$

With these new definitions the perturbative expansion of the eigenstates becomes:

$$|\epsilon_{n,i_n}\rangle = |\epsilon_{n,i_n}^{(0)}\rangle + \lambda \sum_r \sum_{i_r} \left(K_{r,n}^{(i_r,i_n)} + M_{r,n}^{(i_r,i_n)} \right) |\epsilon_{r,i_r}^{(0)}\rangle + \mathcal{O}(\lambda^2). \tag{14}$$

We may simplify this by noting that because $\hat{\Sigma}^{(-2)}$ and $\hat{\Sigma}^{(+2)}$ remove or add 2 spins, the tensor $K_{r,n}^{(i_r,i_n)} + M_{r,n}^{(i_r,i_n)}$ has a value of zero if $|r-n| > 2$. This is encapsulated by the following expressions:

$$K_{r,n}^{(i_r,i_n)} = \delta_{r,n-2} K_{n-2,n}^{(i_{n-2},i_n)} \qquad M_{r,n}^{(i_r,i_n)} = \delta_{r,n+2} M_{n+2,n}^{(i_{n+2},i_n)} \tag{15}$$

which leads to the introduction of the symbols

$$K_{n-2}^{(i,j)} = K_{n-2,n}^{(i_{n-2},j_n)} \qquad \text{and} \qquad M_{n+2}^{(i,j)} = M_{n+2,n}^{(i_{n+2},j_n)}. \tag{16}$$

The perturbative expansion then takes the form:

$$|\epsilon_{n,i_n}\rangle = |\epsilon_{n,i_n}^{(0)}\rangle + \lambda \left(\sum_i K_{n-2}^{(i,i_n)} |\epsilon_{n-2,i}^{(0)}\rangle + \sum_{i'} M_{n+2}^{(i',i_n)} |\epsilon_{n+2,i'}^{(0)}\rangle \right) + \mathcal{O}(\lambda^2). \tag{17}$$

Evaluating matrix elements of σ_l^-

It is required that the matrix element $\langle \epsilon_{m,i_m} | \sigma_l^- | \epsilon_{n,i_n} \rangle$ be calculated so that the terms in the master equation can be evaluated numerically. The first step is to use

the pertubative expansion of the eigenstates to express the matrix element to first order. To this end, we shall ignore the cross terms which give order λ^2 or higher.

$$\langle\epsilon_{m,i_m}|\sigma_l^-|\epsilon_{n,i_n}\rangle = \left[\langle\epsilon^{(0)}_{m,i_m}| + \lambda\left(\sum_i K^{(i,i_m)^*}_{m-2}\langle\epsilon^{(0)}_{m-2,i}| + \sum_{i'} M^{(i',i_m)^*}_{m+2}\langle\epsilon^{(0)}_{m+2,i'}|\right)\right] \times \sigma_l^-\left[|\epsilon^{(0)}_{n,i_n}\rangle + \lambda\left(\sum_i K^{(i,i_n)}_{n-2}|\epsilon^{(0)}_{n-2,i}\rangle + \sum_{i'} M^{(i',i_n)}_{n+2}|\epsilon^{(0)}_{n+2,i'}\rangle\right)\right] \tag{18}$$

This equation is first expanded, then the order λ^2 terms are thrown away. What results is the expression:

$$\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle + \lambda\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-\left(\sum_i K^{(i,i_n)}_{n-2}|\epsilon^{(0)}_{n-2,i}\rangle + \sum_{i'} M^{(i',i_n)}_{n+2}|\epsilon^{(0)}_{n+2,i'}\rangle\right) + \lambda\left(\sum_i K^{(i,i_m)^*}_{m-2}\langle\epsilon^{(0)}_{m-2,i}| + \sum_{i'} M^{(i',i_m)^*}_{m+2}\langle\epsilon^{(0)}_{m+2,i'}|\right)\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle,$$

which after a simple rearrangement of the bras and kets yields

$$\langle\epsilon_{m,i_m}|\sigma_l^-|\epsilon_{n,i_n}\rangle = \langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle + \lambda\Bigg(\sum_i K^{(i,i_n)}_{n-2}\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{n-2,i}\rangle + \sum_{i'} M^{(i',i_n)}_{n+2}\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{n+2,i'}\rangle + \sum_i K^{(i,i_m)^*}_{m-2}\langle\epsilon^{(0)}_{m-2,i}|\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle + \sum_{i'} M^{(i',i_m)^*}_{m+2}\langle\epsilon^{(0)}_{m+2,i'}|\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle\Bigg). \tag{19}$$

This expression can be split into cases, since σ_l^- will only talk between eigenstates living in subspaces seperated by total spin value of 1. More precisely this is expressed as $\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{n,i_n}\rangle = \delta_{n,m+1}\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{m+1,i_{m+1}}\rangle$. Instead of writing multiple Kronecker deltas on one line let us write the result as a piecewise expression:

$$\langle\epsilon_{m,i_m}|\sigma_l^-|\epsilon_{n,i_n}\rangle = \begin{cases} \text{if } n = m+1 & \langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{m+1,i_{m+1}}\rangle, \\ \text{if } n = m-1 & \sum_{i'} M^{(i',i_{m-1})}_{m+1}\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{m+1,i'}\rangle + \sum_i K^{(i,i_m)^*}_{m-2}\langle\epsilon^{(0)}_{m-2,i}|\sigma_l^-|\epsilon^{(0)}_{m-1,i_{m-1}}\rangle, \\ \text{if } n = m+3 & \sum_i K^{(i,i_{m+3})}_{m+1}\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{m+1,i}\rangle + \sum_{i'} M^{(i',i_m)^*}_{m+2}\langle\epsilon^{(0)}_{m+2,i'}|\sigma_l^-|\epsilon^{(0)}_{m+3,i_{m+3}}\rangle, \\ \text{otherwise} & 0. \end{cases} \tag{20}$$

In an attempt to lighten the notation a bit, let the following matrices be defined:

$$\tilde{\mathbf{\Sigma}}^{(l)}_m = \left[\langle\epsilon^{(0)}_{m,i_m}|\sigma_l^-|\epsilon^{(0)}_{m+1,i_{m+1}}\rangle\right], \qquad \mathbf{K}_r = [K^{(i,j)}_r], \qquad \mathbf{M}_r = [M^{(i,j)}_r]. \tag{21}$$

Which allows us to write the entries of the piecewise form above in a matrix equation, since the sums over i and i' amount to performing a matrix multiplication. Then for each pair, (m, n) we construct the following matrices:

$$\begin{array}{lll} \text{when} & n = r+1 & \tilde{\mathbf{\Sigma}}^{(l)}_m, \\ & n = m-1 & \lambda\left[\tilde{\mathbf{\Sigma}}^{(l)}_m\mathbf{M}^\top_{m+1} + \mathbf{K}^*_{r-2}\tilde{\mathbf{\Sigma}}^{(l)}_{m-2}\right], \\ & n = m+3 & \lambda\left[\tilde{\mathbf{\Sigma}}^{(l)}_m\mathbf{K}^\top_{m+1} + \mathbf{M}^*_{r-2}\tilde{\mathbf{\Sigma}}^{(l)}_{m-2}\right], \\ & \text{otherwise} & \text{nothing.} \end{array} \tag{22}$$