Chapter 12
Dynamical Analysis of Quantum Annealing

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Abstract Quantum annealing aims to provide a faster method than classical computing for finding the minima of complicated functions, and it has created increasing interest in the relaxation dynamics of quantum spin systems. Moreover, problems in quantum annealing caused by first-order phase transitions can be reduced via appropriate temporal adjustment of control parameters, and in order to do this optimally, it is helpful to predict the evolution of the system at the level of macroscopic observables. Solving the dynamics of quantum ensembles is nontrivial, requiring modeling of both the quantum spin system and its interaction with the environment with which it exchanges energy. An alternative approach to the dynamics of quantum spin systems was proposed about a decade ago. It involves creating stochastic proxy dynamics via the Suzuki-Trotter mapping of the quantum ensemble to a classical one (the quantum Monte Carlo method), and deriving from this new dynamics closed macroscopic equations for macroscopic observables using the dynamical replica method. In this chapter, we give an introduction to this approach, focusing on the ideas and assumptions behind the derivations, and on its potential and limitations.

12.1 Quantum Ensembles and Their Dynamics

We imagine an ensemble of K independent quantum systems $|\psi^\alpha\rangle$, labeled by $\alpha = 1 \ldots K$, all with the same Hamiltonian but distinct initial conditions. Making a measurement of an observable A in this ensemble means randomly picking one of the K systems, with equal probabilities, and measuring A in the selected system. The average of the observable A can then be written as $\langle A\rangle = \text{Tr}(\rho A)$, where ρ, the density matrix, is the Hermitian nonnegative definite operator $\rho = K^{-1}\sum_{\alpha=1}^{K} |\psi^\alpha\rangle\langle\psi^\alpha|$,

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with $\mathrm{Tr}(\rho) = 1$. Since ρ is Hermitian it has a complete basis of eigenstates $\{|k\rangle\}$. Its eigenvalues w_k, which are nonnegative and normalized according to $\sum_k w_k = 1$, can be interpreted as probabilities. We can now write $\langle A\rangle = \sum_n a_n \sum_k w_k |\langle k|n\rangle|^2$. Hence the probability of measuring eigenvalue a_n of observable A in the ensemble is $P_n = \sum_k w_k |\langle k|n\rangle|^2$, where $|\langle k|n\rangle|^2$ is the probability of observing a_n in eigenstate k of the density matrix, and w_k is the probability of finding the ensemble in eigenstate k.

The evolution of the density matrix follows from the evolution of the states $|\psi^\alpha\rangle$, each governed by the Schrödinger equation, giving $\frac{\mathrm{d}}{\mathrm{d}t}\rho = (\mathrm{i}\hbar)^{-1}[H,\rho]$. The solution is $\rho = \mathrm{e}^{-\mathrm{i}Ht/\hbar}\rho_{t=0}\,\mathrm{e}^{\mathrm{i}Ht/\hbar}$. In particular, it follows using the eigenbasis $\{|E\rangle\}$ of H that

$$\langle H\rangle = \sum_E \langle E|\mathrm{e}^{-\mathrm{i}Ht/\hbar}\rho_{t=0}\,\mathrm{e}^{\mathrm{i}Ht/\hbar}H|E\rangle \;=\; \langle H\rangle_{t=0}. \tag{12.1}$$

At equilibrium $[H,\rho] = 0$. The density matrix can therefore be diagonalized simultaneously with H, that is, $\rho = \sum_E f(E)|E\rangle\langle E|$. The values of $f(E)$ define the type of equilibrium ensemble at hand. In the canonical ensemble we have $f(E) = \exp(-\beta E)/\mathcal{Z}(\beta)$, so

$$\rho = \frac{1}{\mathcal{Z}(\beta)}\sum_E \mathrm{e}^{-\beta E}|E\rangle\langle E| \;=\; \frac{1}{\mathcal{Z}(\beta)}\mathrm{e}^{-\beta H}. \tag{12.2}$$

The quantum partition function $\mathcal{Z}(\beta)$ follows from $\mathrm{Tr}(\rho) = 1$: $\mathcal{Z}(\beta) = \mathrm{Tr}(\mathrm{e}^{-\beta H})$. The free energy and the average internal energy are given by $\mathcal{F} = -\beta^{-1}\log\mathcal{Z}(\beta)$ and $\mathcal{E} = -\frac{\partial}{\partial\beta}\log\mathcal{Z}(\beta)$. The expectation values of operators become $\langle A\rangle = \mathcal{Z}(\beta)^{-1}$ $\mathrm{Tr}(\mathrm{e}^{-\beta H}A)$. Note that if the systems of the ensemble evolve strictly according to the Schrödinger equation, there cannot be generic evolution of ρ toward the equilibrium form in Eq. (12.2). For any initial density operator with $\langle H\rangle_{t=0} \neq \mathcal{E}$ this is ruled out by Eq. (12.1). Since the state in Eq. (12.2) describes the result of equilibration of quantum systems in a heat bath with which they can exchange energy, a correct description of the dynamics requires a Hamiltonian that also describes the degrees of freedom of the heat bath.

This is the first obstacle in the analysis of the dynamics of quantum ensembles: it is difficult even to write down the correct microscopic dynamical laws. A similar situation occurs also in the classical setting. Without a heat bath we have a micro-canonical ensemble with conserved energy. Deriving the Gibbs-Boltzmann distribution from the joint dynamics of the system and heat bath requires us to connect deterministic trajectories to invariant measures via ergodic theory and to subsequently derive the form of these measures, which has so far proven possible for only a handful of models.

The approach followed in [1] was to circumvent ensembles altogether and solve the Schrödinger equation for small systems in which a decaying longitudinal field acts as quantum noise (which is indeed what happens in quantum annealing). In classical systems one often *defines* the pain away. One constructs an intuitively reasonable stochastic process that evolves toward the Gibbs-Boltzmann state, usually of the Markov Chain Monte Carlo (MCMC) form. This process is studied as a proxy for the dynamics of the original system. The price paid is that one cannot be sure to what extent the stochastic dynamics are close to those of the original system. The MCMC equations are not even unique, since there are many choices that evolve to the Gibbs-Boltzmann state. The same dynamics strategy can be applied to quantum systems if the latter can be mapped to classical ones. This is achieved by the Suzuki-Trotter formalism [4].

12.2 Quantum Monte Carlo Dynamics

In order to apply quantum annealing to optimization problems formulated in terms of binary variables, one needs spin-$\frac{1}{2}$ particles [1]. These are labeled by $i = 1 \ldots N$, with Pauli matrices $\{\sigma_i^x, \sigma_i^y, \sigma_i^z\}$. In the standard representation of σ^z-eigenstates:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

In quantum annealing one chooses Hamiltonians of the form $H = H_0 + H_1$, in which H_0 is obtained by replacing the classical spins $\sigma_i = \pm 1$ in an Ising Hamiltonian by the matrices σ_i^z and a second part H_1 that acts as a form of quantum noise[1]:

$$H_0 = -\sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z - h\sum_i \sigma_i^z, \qquad H_1 = -\Gamma\sum_i \sigma_i^x. \tag{12.3}$$

H_0 represents the quantity to be minimized in our optimization problem. The classical state achieving this minimum follows from the quantum ground state of the system upon moving the parameters Γ and β^{-1} adiabatically slowly to zero and is hence obtained from the partition function $\mathcal{Z}(\beta) = \mathrm{Tr}(\mathrm{e}^{-\beta H_0 - \beta H_1})$. For excellent reviews of the physics and the applications of the above types of quantum spin systems with transverse fields, we refer to [2, 3].

The Suzuki-Trotter procedure [4] allows us to convert the above quantum problem into a classical one using the operator identity

$$\mathrm{e}^{A+B} = \lim_{M\to\infty}\left(\mathrm{e}^{A/M}\mathrm{e}^{B/M}\right)^M. \tag{12.4}$$

From now on we assume that A and B are Hermitian operators, and we write the basis of eigenstates of A as $\{|n\rangle\}$. We then obtain after some simple manipulations:

[1] For simplicity, we choose H_0 here to be quadratic in the spins, and the external field to be uniform, but this is not essential.

$$\mathrm{Tr}(\mathrm{e}^{A+B}) = \lim_{M\to\infty} \sum_{n_1 \ldots n_M} \mathrm{e}^{\sum_{k=1}^{M} a_{n_k}/M} \prod_{k,\ \mathrm{mod}(M)} \langle n_k | \mathrm{e}^{B/M} | n_{k+1} \rangle. \tag{12.5}$$

Application to $A = -\beta H_0$ and $B = -\beta H_1$, where the relevant basis is that of the joint eigenstates of all $\{\sigma_i^z\}$, that is, $|s_1, \ldots, s_N\rangle = |s_1\rangle \otimes \ldots \otimes |s_N\rangle$, with $s_i = \pm 1$ and $\sigma_i^z |s_1, \ldots, s_N\rangle = s_i |s_1, \ldots, s_N\rangle$, gives $\mathcal{Z}(\beta) = \lim_{M\to\infty} \mathcal{Z}_M(\beta)$, where

$$\begin{aligned}
\mathcal{Z}_M(\beta) &= \sum_{\{s_{ik}=\pm 1\}} \mathrm{e}^{(\beta/M)\sum_{k=1}^{M}[\sum_{i<j} J_{ij} s_{ik} s_{jk} + h \sum_i s_{ik}]} \prod_{k,\ \mathrm{mod}(M)} \prod_{i=1}^{N} \langle s_{ik} | \mathrm{e}^{(\beta\Gamma/M)\sigma_i^x} | s_{i,k+1} \rangle \\
&= \mathrm{e}^{\frac{1}{2} NM \log[\frac{1}{2}\sinh(2\beta\Gamma/M)]} \\
&\quad \times \sum_{\{s_{ik}=\pm 1\}} \mathrm{e}^{(\beta/M)\sum_{k=1}^{M}[\sum_{i<j} J_{ij} s_{ik} s_{jk} + h \sum_i s_{ik}] + B \sum_{k,\mathrm{mod}(M)} \sum_i s_{ik} s_{i,k+1}}.
\end{aligned} \tag{12.6}$$

in which $B = -\frac{1}{2} \log \tanh(\beta\Gamma/M)$. Thus the partition function of the N-spin quantum system is mapped (apart from a constant) onto the limit $M \to \infty$ of that of a classical Ising model with NM spins $\boldsymbol{s} = \{s_{ik}\}$, with Hamiltonian $H(\boldsymbol{s})$ and asymptotic free energy density $f = \lim_{N\to\infty} \lim_{M\to\infty} f_{N,M}$:

$$\begin{aligned}
H(\boldsymbol{s}) &= -\frac{1}{M} \sum_{k=1}^{M} \sum_{i<j} J_{ij} s_{ik} s_{jk} - \frac{h}{M} \sum_{k=1}^{M} \sum_{i} s_{ik} \\
&\quad - \frac{B}{\beta} \sum_{k,\mathrm{mod}(M)} \sum_{i} s_{ik} s_{i,k+1},
\end{aligned} \tag{12.7}$$

$$\begin{aligned}
f_{N,M} &= -\frac{M}{2\beta} \log\left[\frac{1}{2}\sinh(2\beta\Gamma/M)\right] \\
&\quad - \frac{1}{\beta N} \log \sum_{\{s_{ik}=\pm 1\}} \mathrm{e}^{\frac{\beta}{M}\sum_{k=1}^{M}[\sum_{i<j} J_{ij} s_{ik} s_{jk} + h \sum_i s_{ik}] + B \sum_{k,\mathrm{mod}(M)} \sum_i s_{ik} s_{i,k+1}}.
\end{aligned} \tag{12.8}$$

The new system in Eq. (12.8), for $M \to \infty$ equivalent to the original quantum one, lends itself to constructing a stochastic dynamics. We first write the Suzuki-Trotter Hamiltonian in the standard form of NM interacting Ising spins in an external field:

$$H(\boldsymbol{s}) = -\frac{1}{2} \sum_{ik,j\ell} s_{ik} J_{ik,j\ell} s_{j\ell} - \theta \sum_{ik} s_{ik}, \tag{12.9}$$

$$J_{ik,j\ell} = \frac{1}{M} \delta_{k\ell} J_{ij} (1 - \delta_{ij}) + \frac{B}{\beta} \delta_{ij} (\delta_{k,\ell+1} + \delta_{\ell,k+1}), \qquad \theta = h/M. \tag{12.10}$$

The conventional Glauber dynamics by which this classical system evolves toward the equilibrium state with the above Hamiltonian is, after switching to continuous time [5] and denoting by $p_t(\boldsymbol{s})$ the probability of finding the system in state $\boldsymbol{s}$ at time t:

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} p_t(\boldsymbol{s}) = \sum_{i=1}^{N} \sum_{k=1}^{M} \Big\{ p_t(F_{ik}\boldsymbol{s}) w_{ik}(F_{ik}\boldsymbol{s}) - p_t(\boldsymbol{s}) w_{ik}(\boldsymbol{s}) \Big\}, \tag{12.11}$$

$$w_{ik}(\boldsymbol{s}) = \frac{1}{2}[1 - s_{ik} \tanh(\beta h_{ik}(\boldsymbol{s}))], \qquad h_{ik}(\boldsymbol{s}) = \sum_{j\ell} J_{ik,j\ell} s_{j\ell} + \theta. \tag{12.12}$$

This master equation describes a process where at each step a site $i \in \{1, \ldots, N\}$ and a Trotter slice $k \in \{1, \ldots, M\}$ are picked at random, followed by an attempt to flip the spin s_{ik}. The $w_{ik}(\boldsymbol{s})$ denote transition rates for $s_{ik} \to -s_{ik}$. F_{ik} is an operator that flips spin s_{ik} and leaves all others invariant. The parameter τ defines time units such that the average duration of a single spin update is τ/N. Working out the local fields $h_{ik}(\boldsymbol{s})$ gives

$$h_{ik}(\boldsymbol{s}) = \frac{1}{M} \sum_{j \neq i} J_{ij} s_{jk} + \frac{B}{\beta}(s_{i,k+1} + s_{i,k-1}) + h/M. \tag{12.13}$$

The process in Eqs. (12.11, 12.12) is suitable for numerical simulation and defines the quantum Monte Carlo dynamics for the ensemble with Hamiltonian given by Eq. (12.3) provided we take $M \to \infty$. When applied to quantum annealing models, some authors have called it ‘simulated quantum annealing’. The definition in Eqs. (12.11, 12.12), however, is not unique. Many alternative stochastic processes evolve toward the same Gibbs-Boltzmann state (see, e.g., [6]).

12.3 Dynamical Replica Analysis

The remaining challenge is to extract formulae describing the evolution of relevant macroscopic quantities from Eqs. (12.11, 12.12). This was addressed in [7–10] using the so-called dynamical replica method (DRT) [12–14]. In this chapter, we deviate from the definitions in [7–10] and stay closer to the original DRT ideas.

The dynamics (12.11, 12.12) imply that expectation values $\langle G(\boldsymbol{s})\rangle = \sum_{\boldsymbol{s}} p_t(\boldsymbol{s}) G(\boldsymbol{s})$ evolve according to:

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \langle G(\boldsymbol{s}) \rangle = \sum_{i=1}^{N} \sum_{k=1}^{M} \sum_{\boldsymbol{s}} p_t(\boldsymbol{s}) w_{ik}(\boldsymbol{s}) \Big[G(F_{ik}\boldsymbol{s}) - G(\boldsymbol{s}) \Big]. \tag{12.14}$$

To study the joint dynamics of a set of L observables $\boldsymbol{\Omega}(\boldsymbol{s}) = (\Omega_1(\boldsymbol{s}), \ldots, \Omega_L(\boldsymbol{s}))$ we substitute $G(\boldsymbol{s}) = \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{s})]$. Now $\langle G(\boldsymbol{s}) \rangle = P_t(\boldsymbol{\Omega})$, and

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} P_t(\boldsymbol{\Omega}) = \sum_{i=1}^{N} \sum_{k=1}^{M} \sum_{\boldsymbol{s}} p_t(\boldsymbol{s}) w_{ik}(\boldsymbol{s}) \Big[\delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(F_{ik}\boldsymbol{s})] - \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{s})] \Big]. \tag{12.15}$$

If the observables $\Omega_\mu(\boldsymbol{s})$ are $\mathcal{O}(1)$ and macroscopic in nature, their susceptibility to single spin flips $\Delta_{jk\mu}(\boldsymbol{s}) = \Omega_\mu(F_{ik}\boldsymbol{s}) - \Omega_\mu(\boldsymbol{s})$ will be small. We can then define $\boldsymbol{\Delta}_{jk} = (\Delta_{jk1}(\boldsymbol{s}), \ldots, \Delta_{jkL}(\boldsymbol{s})) \in \mathbb{R}^L$, and expand (12.15) in a distributional sense, that is,

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \int \mathrm{d}\boldsymbol{\Omega}\; P_t(\boldsymbol{\Omega}) G(\boldsymbol{\Omega}) = \int \mathrm{d}\boldsymbol{\Omega}\; G(\boldsymbol{\Omega}) \sum_{\ell \geq 1} \frac{(-1)^\ell}{\ell!} \frac{\partial^\ell}{\partial \Omega_{\mu_1} \ldots \partial \Omega_{\mu_\ell}}$$
$$\times \left\{ \sum_{\mu_1=1}^{L} \cdots \sum_{\mu_\ell=1}^{L} \sum_{i=1}^{N} \sum_{k=1}^{M} \left\langle w_{ik}(\boldsymbol{s}) \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{s})] \Delta_{ik\mu_1}(\boldsymbol{s}) \ldots \Delta_{ik\mu_\ell}(\boldsymbol{s}) \right\rangle \right\}. \quad (12.16)$$

We thereby arrive at the following Kramers-Moyal expansion

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} P_t(\boldsymbol{\Omega}) = \sum_{\ell \geq 1} \frac{(-1)^\ell}{\ell!} \sum_{\mu_1=1}^{L} \cdots \sum_{\mu_\ell=1}^{L} \frac{\partial^\ell}{\partial \Omega_{\mu_1} \ldots \partial \Omega_{\mu_\ell}} \left\{ P_t(\boldsymbol{\Omega}) F^{(\ell)}_{\mu_1 \ldots \mu_\ell}[\boldsymbol{\Omega}; t] \right\}, \quad (12.17)$$

with

$$F^{(\ell)}_{\mu_1 \ldots \mu_\ell}[\boldsymbol{\Omega}; t] = \left\langle \sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\boldsymbol{s}) \Delta_{ik\mu_1}(\boldsymbol{s}) \ldots \Delta_{ik\mu_\ell}(\boldsymbol{s}) \right\rangle_{\boldsymbol{\Omega};t}, \quad (12.18)$$

$$\langle f(\boldsymbol{s}) \rangle_{\boldsymbol{\Omega};t} = \frac{\sum_{\boldsymbol{s}} p_t(\boldsymbol{s}) \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{s})] f(\boldsymbol{s})}{\sum_{\boldsymbol{s}} p_t(\boldsymbol{s}) \delta[\boldsymbol{\Omega} - \boldsymbol{\Omega}(\boldsymbol{s})]}. \quad (12.19)$$

Asymptotically, that is, for $N, M \to \infty$, only the first term of Eq. (12.17) survives if

$$\lim_{N,M \to \infty} \sum_{\ell \geq 2} \frac{1}{\ell!} \sum_{\mu_1=1}^{L} \cdots \sum_{\mu_\ell=1}^{L} \sum_{i=1}^{N} \sum_{k=1}^{M} \left\langle |\Delta_{ik\mu_1}(\boldsymbol{s}) \ldots \Delta_{ik\mu_\ell}(\boldsymbol{s})| \right\rangle_{\boldsymbol{\Omega};t} = 0. \quad (12.20)$$

If all $\Delta_{ik\mu}(\boldsymbol{s})$ scale similarly, that is, $\exists \tilde{\Delta}_{N,M}$ such that $\Delta_{ik\mu}(\boldsymbol{s}) = \mathcal{O}(\tilde{\Delta}_{N,M})$ for $N, M \to \infty$, then Eq. (12.17) retains only its first term if $\lim_{N,M\to\infty} L \tilde{\Delta}_{N,M} \sqrt{NM} = 0$. In that case it reduces to a Liouville equation describing deterministic evolution of $\boldsymbol{\Omega}$:

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \Omega_\mu = \left\langle \sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\boldsymbol{s}) \Delta_{ik\mu}(\boldsymbol{s}) \right\rangle_{\boldsymbol{\Omega};t}. \quad (12.21)$$

If $\lim_{N,M\to\infty} L \tilde{\Delta}_{N,M} \sqrt{NM} > 0$, we can no longer ignore the fluctuations in our observables $\boldsymbol{\Omega}(\boldsymbol{s})$, which limits our choice of observables.

Equation (12.21) is closed if $\sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\boldsymbol{s}) \Delta_{ik\mu}(\boldsymbol{s})$ is a function of $\boldsymbol{\Omega}(\boldsymbol{s})$ only (which would simply drop out). If this is not the case, we close Eq. (12.21) using a maximum entropy argument: we approximate $p_t(\boldsymbol{s})$ in Eq. (12.21) by a form that assumes that all micro-states with the same value for $\mathbf{\Omega}(\mathbf{s})$ are equally likely. Now Eq. (12.21) becomes

$$\tau \frac{\mathrm{d}}{\mathrm{d}t}\Omega_\mu = \frac{\sum_{\mathbf{s}} \delta[\mathbf{\Omega} - \mathbf{\Omega}(\mathbf{s})] \sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\mathbf{s}) \Delta_{ik\mu}(\mathbf{s})}{\sum_{\mathbf{s}} \delta[\mathbf{\Omega} - \mathbf{\Omega}(\mathbf{s})]}. \tag{12.22}$$

Within the replica formalism [16, 17], this closed equation can also be written as

$$\tau \frac{\mathrm{d}}{\mathrm{d}t}\Omega_\mu = \lim_{n\to 0} \sum_{\mathbf{s}^1 \ldots \mathbf{s}^n} \left(\prod_{\alpha=1}^{n} \delta[\mathbf{\Omega} - \mathbf{\Omega}(\mathbf{s}^\alpha)] \right) \sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\mathbf{s}^1) \Delta_{ik\mu}(\mathbf{s}^1). \tag{12.23}$$

The accuracy of Eq. (12.22) depends on our choice for the observables $\Omega_\mu(\mathbf{s})$. We want them to be $\mathcal{O}(1)$, obeying $\lim_{N,M\to\infty} L\tilde{\Delta}_{N,M}\sqrt{NM} = 0$, and such that the probability equipartitioning assumption is as harmless as possible. Including $H(\mathbf{s})/N$ and $N^{-1} \log p_0(\mathbf{s})$ in our set of observables ensures that equipartitioning holds for $t \to 0$ and $t \to \infty$. If we have disorder in the couplings $\{J_{ij}\}$, and for $N \to \infty$ our observables are self-averaging with respect to its realization, we can average over the disorder.[2] This gives

$$\tau \frac{\mathrm{d}}{\mathrm{d}t}\Omega_\mu = \lim_{n\to 0} \sum_{\mathbf{s}^1 \ldots \mathbf{s}^n} \overline{\left(\prod_{\alpha=1}^{n} \delta[\mathbf{\Omega} - \mathbf{\Omega}(\mathbf{s}^\alpha)] \right) \sum_{i=1}^{N} \sum_{k=1}^{M} w_{ik}(\mathbf{s}^1) \Delta_{ik\mu}(\mathbf{s}^1)}. \tag{12.24}$$

For the system in Eq. (12.8) and the typical initial conditions in quantum annealing, there are two natural and simple routes for choosing the observables in the DRT method,[3] all involving the normalized distinct energy contributions in Eq. (12.27):

- *Trotter slice-dependent observables*
  We choose, for $k = 1 \ldots M$ (mod M),

$$E_k(\mathbf{s}) = -\frac{1}{N}\sum_{i<j} J_{ij} s_{ik} s_{jk}, \quad m_k(\mathbf{s}) = \frac{1}{N}\sum_i s_{ik}, \quad \mathcal{E}_k(\mathbf{s}) = \frac{1}{N}\sum_i s_{ik} s_{i,k+1}. \tag{12.25}$$

  Now $L = 3M$, and the susceptibilities of the observables to single spin flips are, using $\sum_j J_{ij} s_{jk} = \mathcal{O}(1)$ for all k (required for an extensive Hamiltonian):

$$\Delta_{ik} E_q(\mathbf{s}) = 2N^{-1} \delta_{qk} s_{ik} \sum_{j\neq i} J_{ij} s_{jk} = \mathcal{O}(N^{-1}), \tag{12.26}$$

$$\Delta_{ik} m_q(\mathbf{s}) = -2N^{-1} \delta_{qk} s_{ik} = \mathcal{O}(N^{-1}), \tag{12.27}$$

$$\Delta_{ik} \mathcal{E}_q(\mathbf{s}) = -2N^{-1} s_{ik} (\delta_{qk} s_{i,k+1} + \delta_{k,q+1} s_{i,k-1}) = \mathcal{O}(N^{-1}). \tag{12.28}$$

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[2] Without disorder one does not need the replica formalism yet and can work directly with (12.22).

[3] One can always add further observables, or split the present ones into distinct contributions. This generally improves the accuracy of the theory provided $\lim_{N,M\to\infty} L\tilde{\Delta}_{N,M}\sqrt{NM} = 0$ still holds.

Hence $\tilde{\Delta}_{N,M} = N^{-1}$, so deterministic evolution requires that $M \ll N^{\frac{1}{3}}$ as $M, N \to \infty$. Hence, on choosing Eq. (12.25) we can no longer take $M \to \infty$ before $N \to \infty$, which would have been the correct order, and must rely on these limits commuting.[4]

- *Trotter slice-independent observables*
  These are simply averages over all Trotter slices of the previous set in Eq. (12.25), that is,

$$E(\mathbf{s}) = \frac{1}{M}\sum_{k=1}^{M} E_k(\mathbf{s}), \quad m(\mathbf{s}) = \frac{1}{M}\sum_{k=1}^{M} m_k(\mathbf{s}), \quad \mathcal{E}(\mathbf{s}) = \frac{1}{M}\sum_{k=1}^{M} \mathcal{E}_k(\mathbf{s}). \tag{12.29}$$

Hence $L = 3$, and the spin-flip susceptibilities come out as

$$\Delta_{ik} E(\mathbf{s}) = 2(NM)^{-1} s_{ik} \sum_{j \neq i} J_{ij} s_{jk} = \mathcal{O}((NM)^{-1}), \tag{12.30}$$

$$\Delta_{ik} m(\mathbf{s}) = -2(NM)^{-1} s_{ik} = \mathcal{O}((NM)^{-1}), \tag{12.31}$$

$$\Delta_{ik} \mathcal{E}(\mathbf{s}) = -2(NM)^{-1} s_{ik}(s_{i,k+1} + s_{i,k-1}) = \mathcal{O}((NM)^{-1}). \tag{12.32}$$

Now $\tilde{\Delta}_{N,M} = 1/NM$. Deterministic evolution requires $\lim_{N,M\to\infty} (NM)^{-\frac{1}{2}} = 0$, which is always true. We can therefore take our two limits in any desired order without having to worry about fluctuations in our macroscopic observables.

12.4 Simple Examples

We illustrate the previous approach by application to simple models. We investigate the commutation of the limits $N \to \infty$ and $M \to \infty$, and the link between stationary states of the dynamical equations and the equilibrium theory. We start with the simplest case of non-interacting spins in a uniform x field, followed by non-interacting spins in uniform x and z fields and ferromagnetically interacting quantum systems.

12.4.1 Non-interacting Quantum Spins in a Uniform x Field

This is the simplest case of Eq. (12.8), where $h = J_{ij} = 0$ for all (i, j). Although this specific model is physically trivial, it is still instructive since it already reveals many general features of the more general dynamical theory. The statics analysis gives

$$\mathcal{Z}_M(\beta) = \left\{ \mathrm{e}^{\frac{1}{2} M \log[\frac{1}{2}\sinh(2\beta\Gamma/M)]} \mathrm{Tr}(\boldsymbol{K}^M) \right\}^N, \tag{12.33}$$

with a 2×2 transfer matrix of the one-dimensional Ising chain:

[4] The assumption that the order of the limits $N \to \infty$ and $M \to \infty$ can be changed is also made in equilibrium studies such as [15], where steepest descent integration is used as $N \to \infty$ for fixed M.

$$\boldsymbol{K} = \begin{pmatrix} e^{B} & e^{-B} \\ e^{-B} & e^{B} \end{pmatrix}, \quad \text{eigenvalues:}\ \lambda_+ = 2\cosh(B),\ \ \lambda_- = 2\sinh(B). \tag{12.34}$$

After some rewriting and insertion of the definition of B we obtain:

$$\begin{aligned} \mathcal{Z}_M(\beta) &= \left\{ e^{\frac{1}{2}M\log[\frac{1}{2}\sinh(2\beta\Gamma/M)]} 2^M [\cosh^M(B) + \sinh^M(B)] \right\}^N \\ &= [2\cosh(\beta\Gamma)]^N. \end{aligned} \tag{12.35}$$

This gives the correct free energy density $f_{N,M} = -\frac{1}{\beta}\log[2\cosh(\beta\Gamma)]$.

Next, we turn to the macroscopic dynamical equations in Eq. (12.21). Since $J_{ij} = 0$, the order parameters $E_k(\boldsymbol{s})$ and $E(\boldsymbol{s})$ are always zero. The two dynamical routes give:

- *Trotter slice-dependent observables*

  The observables are $\{m_k(\boldsymbol{s}), \mathcal{E}_k(\boldsymbol{s})\}$, and we are forced to take $N \to \infty$ before $M \to \infty$. Using identities such as $\tanh[B(s+s')] = \frac{1}{2}(s+s')\tanh(2B)$ we obtain:

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} m_k = -m_k + \frac{1}{2}(m_{k+1} + m_{k-1})\tanh(2B), \tag{12.36}$$

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}_k = \tanh(2B)[1 + \frac{1}{2}(C_k + C_{k+1})] - 2\mathcal{E}_k, \tag{12.37}$$

  in which, using the equivalence of the N sites i, we have the 2-slice correlators:

$$C_k = \frac{\sum_{\boldsymbol{s}} \left[\prod_q \delta[m_q - m_q(\boldsymbol{s})]\delta[\mathcal{E}_q - \mathcal{E}_q(\boldsymbol{s})] \right] s_{1,k-1}s_{1,k+1}}{\sum_{\boldsymbol{s}} \left[\prod_q \delta[m_q - m_q(\boldsymbol{s})]\delta[\mathcal{E}_q - \mathcal{E}_q(\boldsymbol{s})] \right]}. \tag{12.38}$$

  One can compute these for $N \to \infty$ with fixed M via steepest descent integration:

$$C_k = \frac{\sum_{s_1\ldots s_M} e^{\sum_q (x_q s_q + y_q s_q s_{q+1})} s_{k-1}s_{k+1}}{\sum_{s_1\ldots s_M} e^{\sum_q (x_q s_q + y_q s_q s_{q+1})}}, \tag{12.39}$$

  in which $\boldsymbol{x} = (x_1, \ldots, x_M)$ and $\boldsymbol{y} = (y_1, \ldots, y_M)$ are to be solved from

$$m_k = \frac{\partial \log Z}{\partial x_k}, \quad \mathcal{E}_k = \frac{\partial \log Z}{\partial y_k}, \quad Z(\boldsymbol{x}, \boldsymbol{y}) = \sum_{s_1\ldots s_M} e^{\sum_q (x_q s_q + y_q s_q s_{q+1})}. \tag{12.40}$$

- *Trotter slice-independent observables*

  In this case, we only have $m(\boldsymbol{s})$ and $\mathcal{E}(\boldsymbol{s})$, and working out Eq. (12.21) gives

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} m = -m[1 - \tanh(2B)], \quad \tau \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E} = (1 + C)\tanh(2B) - 2\mathcal{E}, \tag{12.41}$$

with

$$C = \frac{\sum_{s} \delta[m - m(s)]\delta[\mathcal{E} - \mathcal{E}(s)]s_{1,1}s_{1,3}}{\sum_{s} \delta[m - m(s)]\delta[\mathcal{E} - \mathcal{E}(s)]}. \tag{12.42}$$

Calculating the 2-slice correlator C using steepest descent results in

$$C = \frac{\sum_{s_1 \ldots s_M} e^{\frac{1}{M}\sum_q (x s_q + y s_q s_{q+1})} s_1 s_3}{\sum_{s_1 \ldots s_M} e^{\frac{1}{M}\sum_q (x s_q + y s_q s_{q+1})}}, \tag{12.43}$$

$$m = \frac{\partial \log Z}{\partial x}, \qquad \mathcal{E} = \frac{\partial \log Z}{\partial y}, \qquad Z(x, y) = \sum_{s_1 \ldots s_M} e^{\frac{1}{M}\sum_q (x s_q + y s_q s_{q+1})}. \tag{12.44}$$

If at time zero the m_k and $\mathcal{E}_k$ in Eqs. (12.36, 12.37) are independent of k, this will remain true at all times[5] and the dynamics in Eqs. (12.36, 12.37) simplifies to Eq. (12.41). Computing C involves solving a one-dimensional Ising model with a constant external field, whereas computing C_k requires solving heterogeneous spin chain models in equilibrium for arbitrary coupling constants and fields. This is the second reason, in addition to the issue with limits, for why it is preferable to work with Trotter slice-independent observables.

For non-interacting spins with $h \neq 0$ the analysis is similar. Here $f = \lim_{M\to\infty} f_{N,M} = -\beta^{-1} \log[2\cosh(\beta\sqrt{\Gamma^2 + h^2})]$, with equilibrium magnetisation

$$m = -\partial f/\partial h = \tanh(\beta\sqrt{h^2 + \Gamma^2}) \frac{h}{\sqrt{h^2 + \Gamma^2}}, \tag{12.45}$$

and the Trotter slice-independent observables are predicted to obey

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} m = \frac{1}{2}(1 - C)\tanh(\beta h/M) + \frac{1}{2} Q_+(1 + C) - m(1 - Q_-), \tag{12.46}$$

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E} = (1 + C)Q_- + 2Q_+ m - 2\mathcal{E}, \tag{12.47}$$

with $Q_\pm = \frac{1}{2}[\tanh(\beta h/M + 2B) \pm \tanh(\beta h/M - 2B)]$. Since $\lim_{h\to 0} Q_+ = 0$ and $\lim_{h\to 0} Q_- = \tanh(2B)$, Eqs. (12.46,12.47) indeed revert back to Eq. (12.41) for $h \to 0$. We inspect the fixed-points of Eqs. (12.46, 12.47) after having also added spin interactions in the next section. Clearly, since $\lim_{M\to\infty} Q_+ = \lim_{M\to\infty}(1 - Q_-) = 0$ the relaxation time of the system diverges for $M \to \infty$, with closer inspection revealing that $\mathrm{d}m/\mathrm{d}t = \mathcal{O}(M^{-2})$. This makes physical sense: for large M, hence large B, the Trotter slices increasingly prefer identical states, so state changes (in a single slice) become rare as they require the mounting energetic costs of breaking the Trotter symmetry.

[5] In [7, 8, 10] this is called the static approximation.

12.4.2 Ferromagnetic z-interactions and Uniform x and z Fields

We now choose $h \neq 0$, $\Gamma \neq 0$, and $J_{ij} = J_0/N$ for all $i \neq j$, so that the quantum Hamiltonian is $H = -(J_0/N)\sum_{i<j}\sigma_i^z\sigma_j^z - \sum_i(h\sigma_i^z + \Gamma\sigma_i^x)$. This is known as the Husimi-Temperley-Curie-Weiss model in a transverse field [11]. In the statics, after some simple manipulations and using the short-hand $\mathrm{D}z = (2\pi)^{-\frac{1}{2}}\mathrm{e}^{-\frac{1}{2}z^2}\mathrm{d}z$, we find:

$$\mathcal{Z}_M(\beta) = \mathrm{e}^{\frac{1}{2}NM\log[\frac{1}{2}\sinh(2\beta\Gamma/M)]-\frac{1}{2}\beta J_0} \times \int\Big[\prod_{k=1}^{M}\mathrm{D}z_k\Big]\Big\{\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}\Big(z_k\sqrt{\frac{M}{\beta J_0 N}}\Big)\Big\}^N, \tag{12.48}$$

with the non-symmetric transfer matrix

$$\boldsymbol{K}(x) = \begin{pmatrix} \mathrm{e}^{B+\beta h/M+\beta J_0 x/M} & \mathrm{e}^{-B+\beta J_0 x/M} \\ \mathrm{e}^{-B-\beta J_0 x/M} & \mathrm{e}^{B-\beta h/M-\beta J_0 x/M}\end{pmatrix} = \mathrm{e}^{x(\beta J_0/M)\sigma^z}\boldsymbol{K}(0). \tag{12.49}$$

We first turn to the statics of the model. It is not immediately clear whether or not the limits $N, M \to \infty$ in Eq. (12.48) commute. Upon taking the limit $N \to \infty$ first, one obtains via steepest descent integration:

$$\lim_{N\to\infty} f_{N,M} = -\frac{M}{2\beta}\log\Big[\frac{1}{2}\sinh\Big(\frac{2\beta\Gamma}{M}\Big)\Big] -\frac{1}{\beta}\mathrm{extr}_{\boldsymbol{x}}\Big\{\log\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}(x_k) - \frac{\beta J_0}{2M}\boldsymbol{x}^2\Big\}. \tag{12.50}$$

We find the derivatives of the quantity $\Psi(\boldsymbol{x})$ to be extremized, with $\overline{\delta}_{ab} = 1-\delta_{ab}$:

$$\frac{\partial\Psi}{\partial x_q} = \frac{\beta J_0}{M}\Big\{\frac{\mathrm{Tr}\prod_{k=1}^{M}(\overline{\delta}_{kq}\mathbf{I}+\delta_{kq}\sigma^z)\boldsymbol{K}(x_k)}{\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}(x_k)} - x_q\Big\}, \tag{12.51}$$

$$\frac{\partial^2\Psi}{\partial x_q\partial x_r} = \Big(\frac{\beta J_0}{M}\Big)^2\Big\{\frac{\mathrm{Tr}\prod_{k=1}^{M}(\overline{\delta}_{kq}\mathbf{I}+\delta_{kq}\sigma^z)(\overline{\delta}_{kr}\mathbf{I}+\delta_{kr}\sigma^z)\boldsymbol{K}(x_k)}{\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}(x_k)} - \frac{\mathrm{Tr}\prod_{k=1}^{M}(\overline{\delta}_{kq}\mathbf{I}+\delta_{kq}\sigma^z)\boldsymbol{K}(x_k)}{\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}(x_k)}\frac{\mathrm{Tr}\prod_{k=1}^{M}(\overline{\delta}_{kr}\mathbf{I}+\delta_{kr}\sigma^z)\boldsymbol{K}(x_k)}{\mathrm{Tr}\prod_{k=1}^{M}\boldsymbol{K}(x_k)}\Big\} - \frac{\beta J_0}{M}\delta_{qr}. \tag{12.52}$$

In Trotter-symmetric solutions $x_k = m$ for all k, these derivatives simplify to

$$\frac{\partial \Psi}{\partial x_q} = \frac{\beta J_0}{M}\left\{\frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^M(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]} - m\right\}, \tag{12.53}$$

$$\frac{\partial^2 \Psi}{\partial x_q \partial x_r} = \left(\frac{\beta J_0}{M}\right)^2 \left\{\frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^{|q-r|}(m)\sigma^z \boldsymbol{K}^{M-|q-r|}(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]} - \left(\frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^M(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]}\right)^2\right\} - (\beta J_0/M)\delta_{qr}. \tag{12.54}$$

and m is the solution of

$$m = \frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^M(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]}. \tag{12.55}$$

Trotter symmetry-breaking bifurcations occur when $\mathrm{Det}[(\beta J_0/M)\boldsymbol{A} - \mathbf{I}] = 0$, where

$$A_{qr} = \frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^{|q-r|}(m)\sigma^z \boldsymbol{K}^{M-|q-r|}(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]} - m^2. \tag{12.56}$$

We introduce the symmetric matrix $\boldsymbol{Q}(m) = \mathrm{e}^{-\frac{1}{2}m(\beta J_0/M)\sigma^z}\boldsymbol{K}(m)\mathrm{e}^{\frac{1}{2}m(\beta J_0/M)\sigma^z}$, with eigenvalues $\lambda_\pm(x)$ and orthogonal eigenbasis $|\pm\rangle$. Now for any $\ell \in \mathbb{N}$ we have

$$\boldsymbol{K}^\ell(m) = \mathrm{e}^{\frac{1}{2}m(\beta J_0/M)\sigma^z}\Big(\lambda_+^\ell(m)|+\rangle\langle+| + \lambda_-^\ell(m)|-\rangle\langle-|\Big)\mathrm{e}^{-\frac{1}{2}m(\beta J_0/M)\sigma^z}, \tag{12.57}$$

and hence, with the short-hand $\sigma^z_{ab} = \langle a|\sigma^z|b\rangle$ and $\phi = \lambda_-(m)/\lambda_+(m) \in (-1, 1)$:

$$\frac{\mathrm{Tr}[\sigma^z \boldsymbol{K}^M(m)]}{\mathrm{Tr}[\boldsymbol{K}^M(m)]} = \frac{\sigma^z_{++} + \sigma^z_{--}\phi^M}{1 + \phi^M}, \tag{12.58}$$

$$A_{qr} = \frac{\sigma^{z2}_{++} + \left[\phi^{|q-r|} + \phi^{M-|q-r|}\right]|\sigma^z_{+-}|^2 + \phi^M \sigma^{z2}_{--}}{1 + \phi^M} - m^2. \tag{12.59}$$

Since $\boldsymbol{A}$ has a Toeplitz form, we know its eigenvalues:

$$k = 1 \ldots M: \quad a_k = \frac{|\sigma^z_{+-}|^2}{1+\phi^M}\frac{(1-\phi^M)(1-\phi^2)}{1+\phi^2 - 2\phi\cos(2\pi(k-1)/M)}. \tag{12.60}$$

Finally we need to diagonalize $\boldsymbol{Q}(m)$ for large M. This gives:

$$\boldsymbol{Q}(m) = \begin{pmatrix} \mathrm{e}^{B+\beta(h+J_0 m)/M} & \mathrm{e}^{-B} \\ \mathrm{e}^{-B} & \mathrm{e}^{B-\beta(h+J_0 m)/M} \end{pmatrix} \tag{12.61}$$

$$\lambda_\pm(m) = \mathrm{e}^{B\pm\frac{\beta}{M}\sqrt{(h+J_0 m)^2+\Gamma^2}+\mathcal{O}(M^{-2})}, \tag{12.62}$$

$$\lim_{M\to\infty} |\pm\rangle = \frac{1}{C_\pm(m)}\Big(\Gamma, -(h+J_0 m) \pm \sqrt{(h+J_0 m)^2+\Gamma^2}\Big), \tag{12.63}$$

$$C_\pm(m) = \sqrt{2}\Big[(h+J_0 m)^2+\Gamma^2 \mp (h+J_0 m)\sqrt{(h+J_0 m)^2+\Gamma^2}\Big]^{\frac{1}{2}}. \tag{12.64}$$

It follows that

$$\phi = \mathrm{e}^{-\frac{2\beta}{M}\sqrt{(h+J_0 m)^2+\Gamma^2}+\mathcal{O}(M^{-2})}. \tag{12.65}$$

Hence $\lim_{M\to\infty}\phi=1$, $\lim_{M\to\infty}\phi^M = \exp[-2\beta\sqrt{(h+J_0 m)^2+\Gamma^2}]$, $\lim_{M\to\infty}\sigma^z_{++} = -\lim_{M\to\infty}\sigma^z_{--} = (h+J_0 m)/\sqrt{(h+J_0 m)^2+\Gamma^2}$, and $\lim_{M\to\infty}\sigma^z_{+-} = \Gamma/\sqrt{(h+J_0 m)^2+\Gamma^2}$. The equation for the magnetization m and the eigenvalues of $\boldsymbol{A}$ thereby become

$$m = \frac{(h+J_0 m)\tanh[\beta\sqrt{(h+J_0 m)^2+\Gamma^2}]}{\sqrt{(h+J_0 m)^2+\Gamma^2}}, \tag{12.66}$$

$$a_k = \frac{\Gamma^2\tanh[\beta\sqrt{(h+J_0 m)^2+\Gamma^2}]}{(h+J_0 m)^2+\Gamma^2}\Big[1+2\lim_{M\to\infty}\frac{1-\cos(2\pi(k-1)/M)}{1-\phi^2}\Big]^{-1}. \tag{12.67}$$

Since all a_k are bounded for large M, the condition $\beta J_0 a_k/M = 1$ for bifurcations away from the Trotter-symmetric state are never met, indicating that the state described by Eq. (12.66) is the physical one. The free energy density $f = \lim_{M\to\infty}\lim_{N\to\infty} f_{N,M}$ is

$$\begin{aligned} f &= \frac{1}{2}J_0 m^2 - \lim_{M\to\infty}\left\{\frac{M}{2\beta}\log\Big[\frac{1}{2}\sinh\Big(\frac{2\beta\Gamma}{M}\Big)\Big] + \frac{1}{\beta}\log\Big(\lambda_+^M(m)+\lambda_-^M(m)\Big)\right\} \\ &= \frac{1}{2}J_0 m^2 - \frac{1}{\beta}\log\Big[2\cosh\Big(\beta\sqrt{(h+J_0 m)^2+\Gamma^2}\Big)\Big]. \end{aligned} \tag{12.68}$$

Extremizing the expression in Eq. (12.68) over m reproduces Eq. (12.66).

We return to Eq. (12.48), and now seek to take the Trotter limit $M\to\infty$ first. The complexities are all in the evaluation for large M of the quantity

$$Z_M = \int\Big[\prod_{k=1}^{M}\mathrm{D}z_k\Big]\left\{\mathrm{Tr}\Big[\prod_{k=1}^{M}\mathrm{e}^{z_k\sqrt{\frac{\beta J_0}{MN}}\sigma^z}\begin{pmatrix}\mathrm{e}^{B+\beta h/M} & \mathrm{e}^{-B} \\ \mathrm{e}^{-B} & \mathrm{e}^{B-\beta h/M}\end{pmatrix}\Big]\right\}^N. \tag{12.69}$$

This can be analyzed using random field Ising chain techniques [18]. Alternatively, we can use the fact that in summations of the form $\sum_k z_k$, each z_k effectively scales as $\mathcal{O}(M^{-\frac{1}{2}})$, enabling us to use $\mathrm{e}^{-B} = \sqrt{\tanh(\beta\Gamma/M)}$ and a modified version of the Trotter identity, viz. $\prod_{k\le M}\big(\mathrm{e}^{u_k/M}\mathrm{e}^{v/M}\big) = \mathrm{e}^{M^{-1}\sum_{k\le M}u_k+v}$, to derive

$$Z_M = e^{NMB} \int \Big[\prod_{k=1}^{M} \mathrm{D}z_k\Big] \Big\{ \mathrm{Tr}\Big[\prod_{k=1}^{M} e^{z_k\sqrt{\frac{\beta J_0}{MN}}\sigma^z}\Big(\mathbf{I}+\frac{\beta}{M}(h\sigma^z+\Gamma\sigma^x)+\mathcal{O}(\frac{1}{M^2})\Big)\Big]\Big\}^N$$
$$= \sqrt{\beta J_0 N} e^{NMB} \int \frac{\mathrm{d}m}{\sqrt{2\pi}} e^{-\frac{1}{2}\beta J_0 N m^2} \Big\{\mathrm{Tr}\, e^{\beta(h+J_0 m)\sigma^z+\beta\Gamma\sigma^x+\mathcal{O}(M^{-1})}\Big\}^N. \quad (12.70)$$

The free energy density $f = \lim_{N\to\infty} \lim_{M\to\infty} f_{N,M}$ then becomes

$$f = -\frac{1}{\beta}\mathrm{extr}_m \Big\{ \log\big(e^{\beta\mu_+(m)} + e^{\beta\mu_-(m)}\big) - \frac{1}{2}\beta J_0 m^2 \Big\}, \quad (12.71)$$

in which $\mu_\pm(m)$ are the eigenvalues of the matrix $\boldsymbol{L}(m) = (h+J_0 m)\sigma^z+\Gamma\sigma^x$:

$$\boldsymbol{L}(m) = \begin{pmatrix} h+J_0 m & \Gamma \\ \Gamma & -(h+J_0 m)\end{pmatrix}, \quad \mu_\pm(m) = \pm\sqrt{(h+J_0 m)^2+\Gamma^2}. \quad (12.72)$$

We now recover Eqs. (12.66, 12.68), so the limits $N\to\infty$ and $M\to\infty$ can be interchanged:

$$f = \mathrm{extr}_m \Big\{ \frac{1}{2} J_0 m^2 - \frac{1}{\beta}\log\Big[2\cosh\Big(\beta\sqrt{(h+J_0 m)^2+\Gamma^2}\Big)\Big]\Big\}. \quad (12.73)$$

We next turn to the DRT dynamics. The energy and the usual initial conditions can once more be expressed in terms of $\{m_k, \mathcal{E}_k\}$ (slice-dependent observables) or $(m, \mathcal{E})$ (slice-independent ones). We define the short-hand $Q_\pm(m) = \frac{1}{2}\tanh(\beta(J_0 m+h)/M+2B) \pm \frac{1}{2}\tanh(\beta(J_0 m+h)/M-2B) \in (-1, 1)$. Upon inserting Eqs. (12.27, 12.28) and Eqs. (12.31, 12.32) into Eq. (12.21), with the fields $h_{ik}(\boldsymbol{s}) = M^{-1}[h+J_0 m_k(\boldsymbol{s})] + (B/\beta)(s_{i,k+1}+s_{i,k-1}) + \mathcal{O}(N^{-1})$, and using expressions such as $\tanh[a+b(s+s')] = \frac{1}{4}(1+s)(1+s')\tanh(a+2b) + \frac{1}{4}(1-s)(1-s')\tanh(a-2b) + \frac{1}{2}(1-ss')\tanh(a)$, one finds the following descriptions:

- *Trotter slice-dependent observables*
  Our observables are $m_q(\boldsymbol{s}) = N^{-1}\sum_i s_{i,q}$ and $\mathcal{E}_q(\boldsymbol{s}) = N^{-1}\sum_i s_{i,q}s_{i,q+1}$, for $q = 1\ldots M$, and we must take the limit $N\to\infty$ before $M\to\infty$. We note that

$$\tanh(\beta h_{ik}(\boldsymbol{s})) = \frac{1}{2}(1+s_{i,k+1}s_{i,k-1})Q_+(m_k(\boldsymbol{s})) + \frac{1}{2}(s_{i,k+1}+s_{i,k-1})Q_-(m_k(\boldsymbol{s}))$$
$$+\frac{1}{2}(1-s_{i,k+1}s_{i,k-1})\tanh(\beta(h+J_0 m_k(\boldsymbol{s}))/M), \quad (12.74)$$

  so with the correlators C_k in Eq. (12.39) the dynamical laws take the form

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}m_q = \frac{1}{2}(1+C_q)Q_+(m_q) + \frac{1}{2}(m_{q+1}+m_{q-1})Q_-(m_q) - m_q + \frac{1}{2}(1-C_q)\tanh\left(\frac{\beta}{M}(h+J_0m_q)\right), \tag{12.75}$$

$$\begin{aligned}\tau\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}_q =& \frac{1}{2}(m_{q+1}+m_{q-1})Q_+(m_q) + \frac{1}{2}(1+C_q)Q_-(m_q) \\ &+\frac{1}{2}(m_q+m_{q+2})Q_+(m_{q+1}) + \frac{1}{2}(1+C_{q+1})Q_-(m_{q+1}) \\ &+\frac{1}{2}(m_{q+1}-m_{q-1})\tanh\left(\frac{\beta}{M}(h+J_0m_q)\right) \\ &+\frac{1}{2}(m_q-m_{q+2})\tanh\left(\frac{\beta}{M}(h+J_0m_{q+1})\right) - 2\mathcal{E}_q.\end{aligned} \tag{12.76}$$

For slice-independent initial conditions, where $m_k = m$ and $\mathcal{E}_k = \mathcal{E}$, this becomes

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}m = \frac{1}{2}(1+C)Q_+(m)+mQ_-(m)-m+\frac{1}{2}(1-C)\tanh\left(\frac{\beta}{M}(h+J_0m)\right), \tag{12.77}$$

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E} = 2mQ_+(m) + (1+C)Q_-(m) - 2\mathcal{E}, \tag{12.78}$$

with the correlator C in Eq. (12.43).

- *Trotter slice-independent observables*
  For the choice $(m, \mathcal{E})$ there is no constraint on the order of limits, but the quantities $m_k(\boldsymbol{s})$ appearing inside $\tanh(\beta h_{ik}(\boldsymbol{s}))$ can no longer be replaced by deterministic macroscopic observables, but must now be calculated. Using Trotter slice permutation symmetry wherever possible, one finds

$$\begin{aligned}\tau\frac{\mathrm{d}}{\mathrm{d}t}m =& \frac{1}{2M}\sum_{k=1}^{M}\Big\langle[1+C_k(\boldsymbol{s})]Q_+(m_k(\boldsymbol{s})) + [m_{k+1}(\boldsymbol{s})+m_{k-1}(\boldsymbol{s})]Q_-(m_k(\boldsymbol{s})) \\ &+[1-C_k(\boldsymbol{s})]\tanh(\beta(h+J_0m_k(\boldsymbol{s}))/M)\Big\rangle_{m,\mathcal{E}} - m,\end{aligned} \tag{12.79}$$

$$\begin{aligned}\tau\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E} =& \frac{1}{M}\sum_{k=1}^{M}\Big\langle[m_{k+1}(\boldsymbol{s})+m_{k-1}(\boldsymbol{s})]Q_+(m_k(\boldsymbol{s}))\Big\rangle_{m,\mathcal{E}} \\ &+\frac{1}{M}\sum_{k=1}^{M}\Big\langle[1+C_k(\boldsymbol{s})]Q_-(m_k(\boldsymbol{s}))\Big\rangle_{m,\mathcal{E}} - 2\mathcal{E},\end{aligned} \tag{12.80}$$

with $C_k(\boldsymbol{s}) = N^{-1}\sum_i s_{i,k+1}s_{i,k-1}$. For large M and N, and in view of the interchangeability of the limits $M\to\infty$ and $N\to\infty$ in the equilibrium calculation, we may anticipate (and can indeed show) that we can neglect the fluctuations in the values of $\{m_k(\boldsymbol{s})\}$ and simply replace $m_k(\boldsymbol{s}) \to m(\boldsymbol{s}) + o(1)$ in the right-hand sides of the above equations, upon which these simplify to Eqs. (12.77, 12.78).

12.5 Link Between Statics and Dynamics

We now show that for $M \to \infty$, the stationary state of Eqs. (12.77, 12.78) reproduces the equilibrium result in Eq. (12.66) as expected. The fixed-point equations of Eqs. (12.77, 12.78) are

$$m = \frac{1}{2}(1+C)Q_+(m) + mQ_-(m) + \frac{1}{2}(1-C)\tanh\left(\frac{\beta}{M}(h+J_0 m)\right), \tag{12.81}$$

$$\mathcal{E} = mQ_+(m) + \frac{1}{2}(1+C)Q_-(m), \tag{12.82}$$

with the correlator $C = C(m, \mathcal{E}) \in (-1, 1)$ to be solved from

$$C = \frac{\sum_{s_1 \ldots s_M} e^{\sum_{k=1}^{M}(xs_k + ys_k s_{k+1})} s_1 s_3}{\sum_{s_1 \ldots s_M} e^{\sum_{k=1}^{M}(xs_k + ys_k s_{k+1})}}, \tag{12.83}$$

$$m = \frac{1}{M}\frac{\partial \log Z}{\partial x}, \qquad \mathcal{E} = \frac{1}{M}\frac{\partial \log Z}{\partial y}, \qquad Z(x, y) = \sum_{s_1 \ldots s_M} e^{\sum_{k=1}^{M}(xs_k + ys_k s_{k+1})}. \tag{12.84}$$

We compute $Z(x, y)$ via the transfer matrix $\boldsymbol{K}(x, y)$ with elements $K_{ss'} = e^{\frac{1}{2}x(s+s')+yss'}$. This gives $Z(x, y) = \lambda_+^M(x, y) + \lambda_-^M(x, y)$, where $\lambda_\pm(.)$ are the eigenvalues of $\boldsymbol{K}(.)$,

$$\lambda_\pm(x, y) = e^y\left(\cosh(x) \pm \sqrt{\sinh^2(x) + e^{-4y}}\right). \tag{12.85}$$

For the equilbrium values of $(m, \mathcal{E})$, Eq. (12.84) are solved by

$$x = \beta(h+J_0 m)/M, \qquad y = B = -\frac{1}{2}\log\tanh\left(\frac{\beta\Gamma}{M}\right), \quad \text{so } e^{-4y} = \tanh^2\left(\frac{\beta\Gamma}{M}\right). \tag{12.86}$$

This claim is confirmed by substituting these as ansätze into the expressions given in the appendix. The key ingredient $\phi = \lambda_-/\lambda_+$ of our formulae then becomes

$$\log\phi = -\frac{2\beta}{M}\sqrt{(h+J_0 m)^2 + \Gamma^2} + \mathcal{O}(M^{-3}). \tag{12.87}$$

Hence for $M \to \infty$ the formulae for m and $\mathcal{E}$ in Eq. (12.84) become

$$m = \frac{(h+J_0 m)\tanh[\beta\sqrt{(h+J_0 m)^2 + \Gamma^2}]}{\sqrt{(h+J_0 m)^2 + \Gamma^2}}, \qquad \mathcal{E} = 1. \tag{12.88}$$

in which we recognize (12.66). For large M one finds $Q_+(m) = \mathcal{O}(M^{-3})$ and $Q_-(m) = 1 - 2(\beta\Gamma/M)^2 + \mathcal{O}(M^{-3})$, so expansion of the fixed-point equations gives

$$m = M(1-C)\frac{h+J_0 m}{4\beta\Gamma^2} + \mathcal{O}(M^{-1}), \tag{12.89}$$

$$\mathcal{E} = \frac{1}{2}(1+C)[1-2(\beta\Gamma/M)^2] + \mathcal{O}(M^{-3}). \tag{12.90}$$

The first equation implies that $C = 1-\tilde{C}/M$ for $M \to \infty$, with $\tilde{C} = \mathcal{O}(1)$. In turn, this gives $\mathcal{E} = 1-\frac{\tilde{C}}{2M}+\mathcal{O}(M^{-2})$. What is left in our proof is to show that m obeys

$$m = \frac{h+J_0 m}{4\beta\Gamma^2}\lim_{M\to\infty} M(1-C). \tag{12.91}$$

We hence compute the correlator C to order M^{-1}, using the identities in the appendix:

$$\begin{aligned}
C &= \langle+|\sigma^z|+\rangle^2 + \frac{\cosh\left[(\frac{1}{2}M-2)\log\phi\right]}{\cosh\left[\frac{1}{2}M\log\phi\right]}\left(1-\langle+|\sigma^z|+\rangle^2\right) \\
&= \frac{(h+J_0 m)^2}{(h+J_0 m)^2+\Gamma^2} + \frac{\cosh[\beta(1-4/M)\sqrt{(h+J_0 m)^2+\Gamma^2}]}{\cosh[\beta\sqrt{(h+J_0 m)^2+\Gamma^2}]} \\
&\times \frac{\Gamma^2}{(h+J_0 m)^2+\Gamma^2} + \mathcal{O}\left(\frac{1}{M^2}\right) \\
&= 1-\frac{1}{M}\tanh\left[\beta\sqrt{(h+J_0 m)^2+\Gamma^2}\right]\frac{4\beta\Gamma^2}{\sqrt{(h+J_0 m)^2+\Gamma^2}} + \mathcal{O}\left(\frac{1}{M^2}\right).
\end{aligned} \tag{12.92}$$

We can now read off the value of $\tilde{C}$, and the condition in Eq. (12.91) is found to reduce to Eq. (12.66), so that it is indeed satisfied. This completes the demonstration that for large M, the macroscopic Eqs. (12.77, 12.78) indeed have the equilibrium state as their fixed-point.

12.6 Evolution on Adiabatically Separated Timescales

We return to the dynamical laws in Eqs. (12.77, 12.78). As noted earlier, these exhibit a divergent relaxation time for the magnetization for large M, suggesting that the dynamics have distinct phases. The first phase is studied by choosing $\tau = \mathcal{O}(1)$. Using

$$Q_+(m) = \frac{4\beta^3\Gamma^2(J_0 m+h)}{M^3} + \mathcal{O}(M^{-4}),\;\; Q_-(m) = 1-\frac{2\beta^2\Gamma^2}{M^2} + \mathcal{O}(M^{-4}), \tag{12.93}$$

we here find that

$$m = m_0 + \mathcal{O}(M^{-1}), \qquad \tau\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E} = 1+C(m_0,\mathcal{E}) - 2\mathcal{E} + \mathcal{O}(M^{-1}). \tag{12.94}$$

So on these timescales the magnetization does not change, whereas the Trotter energy evolves to the solution of the fixed-point equation $\mathcal{E} = \frac{1}{2} + \frac{1}{2}C(m_0, \mathcal{E})$, in which $C(m_0, \mathcal{E})$ is to be solved from the following equations according to the appendix:

$$m = -\frac{\sinh(x)\tanh[\frac{1}{2}M\log\phi]}{\sqrt{\sinh^2(x)+\mathrm{e}^{-4y}}}, \tag{12.95}$$

$$\mathcal{E} = \frac{\sinh^2(x)}{\sinh^2(x)+\mathrm{e}^{-4y}} + \frac{\cosh[(\frac{1}{2}M-1)\log\phi]}{\cosh[\frac{1}{2}M\log\phi]}\,\frac{\mathrm{e}^{-4y}}{\sinh^2(x)+\mathrm{e}^{-4y}}, \tag{12.96}$$

$$C = \frac{\sinh^2(x)}{\sinh^2(x)+\mathrm{e}^{-4y}} + \frac{\cosh[(\frac{1}{2}M-2)\log\phi]}{\cosh[\frac{1}{2}M\log\phi]}\,\frac{\mathrm{e}^{-4y}}{\sinh^2(x)+\mathrm{e}^{-4y}}, \tag{12.97}$$

with $\phi = [\cosh(x)-\sqrt{\sinh^2(x)+\mathrm{e}^{-4y}}]/[\cosh(x) + \sqrt{\sinh^2(x)+\mathrm{e}^{-4y}}]$. Inspection of these equations reveals that the correct scaling with M requires $(x, \mathrm{e}^{-2y}) = (u, v)/M$, with $u, v = \mathcal{O}(1)$. Now $\frac{1}{2}M\log\phi = -\sqrt{u^2+v^2}+\mathcal{O}(M^{-2})$, $\mathcal{E} = 1-\tilde{\mathcal{E}}/M+\mathcal{O}(M^{-2})$, and $C = 1-2\tilde{\mathcal{E}}/M+\mathcal{O}(M^{-2})$, in which (u, v) are solved from

$$m_0 = \frac{u\tanh(\sqrt{u^2+v^2})}{\sqrt{u^2+v^2}}, \qquad \tilde{\mathcal{E}} = \frac{2v^2\tanh(\sqrt{u^2+v^2})}{\sqrt{u^2+v^2}}. \tag{12.98}$$

Although the fixed-point equation for $\mathcal{E}$ is now solved to order $\mathcal{O}(M^{-1})$, computation of $\tilde{\mathcal{E}}$ requires higher orders of M^{-1}. Once $\mathcal{E} = 1-\tilde{\mathcal{E}}/M+\mathcal{O}(N^{-2})$ and $C(m, \mathcal{E}) = 1-2\tilde{\mathcal{E}}/M+\mathcal{O}(M^{-2})$, we find $\mathrm{d}m/\mathrm{d}t = \mathcal{O}(M^{-2})$ and $\mathrm{d}\mathcal{E}/\mathrm{d}t = \mathcal{O}(M^{-2})$, so nothing evolves further macroscopically on these finite timescales.

Since we need $\tau = \mathcal{O}(M^{-2})$ to probe the macroscopic evolution of the system on larger timescales, spin flips in the Trotter system are attempted on unit timescales of $\mathcal{O}(M^3N)$.[6] With the choice $\tau = M^{-2}$, and upon defining $M(1-\mathcal{E}) = \tilde{\mathcal{E}}$ and $M(1-C) = \tilde{C}$, the macroscopic laws (12.77, 12.78) become

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \frac{1}{2}\tilde{C}\beta(h+J_0m) - 2m\beta^2\Gamma^2 + \mathcal{O}\left(\frac{1}{M}\right), \tag{12.99}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathcal{E}} = 4M\beta^2\Gamma^2 - M^2(2\tilde{\mathcal{E}}-\tilde{C}) - 8\beta^3\Gamma^2m(J_0m+h) - 2\beta^2\Gamma^2\tilde{C} + \mathcal{O}\left(\frac{1}{M}\right). \tag{12.100}$$

The quantity $\tilde{C} = \tilde{C}(m, \tilde{\mathcal{E}})$ is to be solved together with (x, y) from Eqs. (12.95, 12.96, 12.97). The relevant scaling is still $(x, \mathrm{e}^{-2y}) = (u, v)/M$, with $u, v = \mathcal{O}(1)$, but according to Eq. (12.100) we now need more than just the leading order in M^{-1}. Using

$$\log\phi = -\frac{2\sqrt{u^2+v^2}}{M} + \mathcal{O}(M^{-3}), \tag{12.101}$$

[6] This reflects the high energy cost of breaking Trotter symmetry to induce magnetization changes.

the equations for $\mathcal{E}$ and C take the form $\mathcal{E} = \Xi_1(u, v)$ and $C = \Xi_2(u, v)$, where

$$\Xi_\ell(u, v) = \left[\sinh^2\left(\frac{u}{M}\right) + \frac{v^2}{M^2}\right]^{-1} \left[\sinh^2\left(\frac{u}{M}\right) + \frac{v^2}{M^2}\frac{F_\ell(u, v)}{F_0(u, v)}\right], \tag{12.102}$$

$$F_\ell(u, v) = \cosh\left[\left(\frac{1}{2}M - \ell\right)\log\phi\right]. \tag{12.103}$$

Now, after tedious but straightforward expansion in M^{-1} one finds that

$$\frac{F_\ell(u, v)}{F_0(u, v)} = 1 - \frac{2\ell\sqrt{u^2+v^2}}{M}\tanh\left(\sqrt{u^2+v^2}\right) + \frac{2\ell^2(u^2+v^2)}{M^2} + \mathcal{O}(M^{-3}). \tag{12.104}$$

Hence

$$\Xi_\ell(u, v) = 1 - \frac{2\ell v^2}{M}\frac{\tanh(\sqrt{u^2+v^2})}{\sqrt{u^2+v^2}} + \frac{2\ell^2 v^2}{M^2} + \mathcal{O}(M^{-3}). \tag{12.105}$$

It follows that the equations for $\tilde{\mathcal{E}} = M(1-\mathcal{E})$ and $\tilde{C} = M(1-C)$ take the form

$$\tilde{\mathcal{E}} = 2v^2\frac{\tanh(\sqrt{u^2+v^2})}{\sqrt{u^2+v^2}} - \frac{2v^2}{M} + \mathcal{O}(M^{-2}),\ \ \tilde{C} = 2\tilde{\mathcal{E}} - \frac{4v^2}{M} + \mathcal{O}(M^{-2}). \tag{12.106}$$

The dynamical equations then become

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \tilde{\mathcal{E}}\beta(h + J_0 m) - 2m\beta^2\Gamma^2 + \mathcal{O}\left(\frac{1}{M}\right), \tag{12.107}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathcal{E}} = 4M(\beta^2\Gamma^2 - v^2) - 8\beta^3\Gamma^2 m(J_0 m + h) - 4\beta^2\Gamma^2\tilde{\mathcal{E}} + \mathcal{O}\left(\frac{1}{M}\right). \tag{12.108}$$

What remains is to express v in terms of $(m, \tilde{\mathcal{E}})$, in leading two orders, by solving Eq. (12.106) for $\tilde{\mathcal{E}}$ alongside our equation for m. The latter is

$$m = \frac{u\tanh(\sqrt{u^2+v^2})}{\sqrt{u^2+v^2}} + \mathcal{O}(M^{-2}). \tag{12.109}$$

Equation (12.106) shows that $v = 0$ corresponds to $\tilde{\mathcal{E}} = 0$, and that $\tilde{\mathcal{E}}$ increases with v^2. On intermediate timescales $\tau = M^{-1}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}m = \mathcal{O}\left(\frac{1}{M}\right),\ \ \frac{\mathrm{d}}{\mathrm{d}t}\tilde{\mathcal{E}} = 4(\beta^2\Gamma^2 - v^2) + \mathcal{O}\left(\frac{1}{M}\right), \tag{12.110}$$

where m remains constant and $\tilde{\mathcal{E}}$ evolves toward the value for which $v = \beta\Gamma + \mathcal{O}(M^{-1})$ (which is also the equilibrium value for v). Thus, in the dynamical equations in Eqs. (12.107, 12.108) describing the process on timescales of $\tau = M^{-2}$ we must substitute $v^2 = \beta^2\Gamma^2 + \mathcal{O}(M^{-1})$. Thus, during the slow process where m evolves we always have

$$\tilde{\mathcal{E}} = 2\beta^2\Gamma^2\, m/u. \tag{12.111}$$

Upon insertion into Eq. (12.107), this results in a closed dynamical equation for m only:

$$\frac{\mathrm{d}}{\mathrm{d}t}m = 2\beta^2\Gamma^2\left(\frac{\beta(h+J_0 m)\tanh(\sqrt{u^2+\beta^2\Gamma^2})}{\sqrt{u^2+\beta^2\Gamma^2}} - m\right), \tag{12.112}$$

without requiring additional approximations, and with u to be solved from[7]

$$m = \frac{u\tanh(\sqrt{u^2+\beta^2\Gamma^2})}{\sqrt{u^2+\beta^2\Gamma^2}}. \tag{12.113}$$

In equilibrium we recover from Eqs. (12.112, 12.113) the correct equilibrium state in Eq. (12.88), with $u = \beta(J_0 m+h)$. Comparison with Eq. (10) in [7] reveals, apart from a harmless difference in time units, that the approximation of [7] (used also in [8–10]) implies replacing u *at any time* by $\beta(J_0 m+h)$. While this indeed holds in equilibrium, the approximation may be dangerous far from equilibrium.

In Fig. 12.1 we test the predictions of Eqs. (12.112, 12.113) against numerical simulations of the process in Eqs. (12.11, 12.12). The approximate co-location of the simulation curves for widely varying values of M confirms that $\tau = \mathcal{O}(1/M^2)$ (inferred from the dynamical theory) indeed captures the characteristic timescale of the macroscopic process. Second, while not showing perfect agreement with the simulation data, which is not expected in view of the probability equipartitioning assumption used to close the macroscopic dynamical equations, away from stationarity the full theory in Eqs. (12.112, 12.113) is reasonably accurate and improves upon the approximation proposed in [7].

12.7 Discussion

In this chapter we aimed to explain the basic ideas and assumptions behind the DRT strategy for deriving and closing macroscopic dynamical equations, and its application to the types of spin systems used in quantum annealing with transverse fields.

[7] For certain values of m and $\beta\Gamma$, Eq. (12.113) may have more than one solution u. In such cases the physical solution is the one with the largest absolute value.

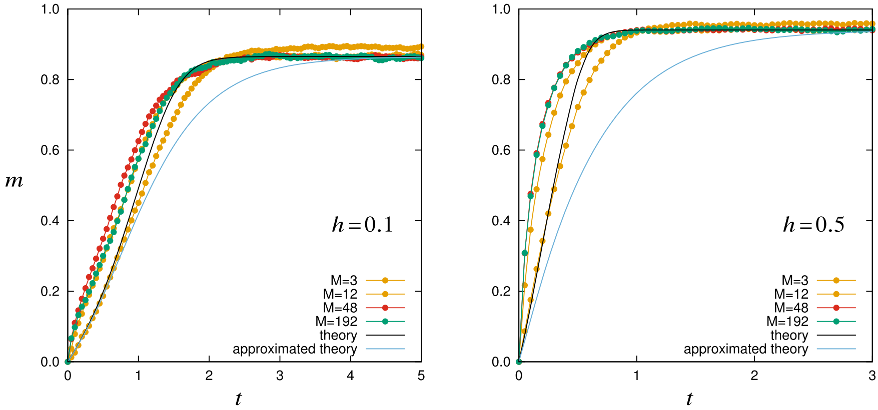

Fig. 12.1 Theory versus computer simulations of the microscopic process in Eqs. (12.11, 12.12) for the Trotter representation of the system with Hamiltonian $H = -(J_0/N)\sum_{i<j}\sigma_i^z\sigma_j^z - \sum_i(h\sigma_i^z + \Gamma\sigma_i^x)$, with $N = 10000$ and $M \in \{3, 12, 48, 192\}$. In all cases $J_0 = 1$, $T = \Gamma = 0.5$, and $\tau = 1/M^2$ (so time units correspond to NM^3 attempted moves per spin). Left figure: magnetization versus time for $h = 0.1$; right figure: the same for $h = 0.5$. The simulation data are shown as connected markers. The black curve is the theoretical prediction, that is, the solution of Eqs. (12.112, 12.113). The light blue curve is the approximated theory of [7], obtained by solving Eq. (12.112) with the equilibrium value $u = \beta(J_0 m + h)$

We focused on technicalities relating to commutation of the limits $N \to \infty$ and $M \to \infty$, the possible choices of macroscopic observables, the distinct M-dependent timescales in the evolution of the Trotter system, and on how an additional approximation made in earlier studies can be avoided, leading to a more precise dynamical theory. We have tested the theoretical predictions of the theory against numerical MCMC simulations of a ferromagnetic quantum system [11] with transverse external fields in Trotter representation and found good agreement.

Since there was no disorder in the examples used in this text, we could work with the dynamical laws in Eq. (12.22). If, in contrast, there is disorder in the problem, the macroscopic laws need to be averaged over its realization, and the main tool is Eq. (12.24). For models with random interactions, performing this disorder average is, however, relatively painless and does not make the dynamical theory significantly more complicated.

We hope that this introduction to the method may aid the development of further analytical studies of the macroscopic dynamics of quantum annealing, including models with time-dependent control parameters, more realistic quantum systems with disordered spin interactions or with interactions on finitely connected graphs, and more precise analytical descriptions in which the macroscopic dynamical observables are functions [14, 19, 20] instead of scalars.

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Appendix: Mathematical Identities

Here we list some basic properties of relevant transfer matrices and expectation values in the single-site Trotter system. The transfer matrix and its eigenvalues are

$$\boldsymbol{K} = \begin{pmatrix} e^{y+x} & e^{-y} \\ e^{-y} & e^{y-x} \end{pmatrix}, \quad \lambda_{\pm} = e^{y}\Big[\cosh(x) \pm \sqrt{\sinh^2(x) + e^{-4y}}\Big] \tag{12.114}$$

The corresponding normalized eigenvectors are

$$|+\rangle = \frac{1}{L}\Big(e^{-2y}, \sqrt{\sinh^2(x) + e^{-4y}} - \sinh(x)\Big), \tag{12.115}$$

$$|-\rangle = \frac{1}{L}\Big(\sqrt{\sinh^2(x) + e^{-4y}} - \sinh(x), -e^{-2y}\Big), \tag{12.116}$$

$$L^2 = e^{-4y} + \Big(\sqrt{\sinh^2(x) + e^{-4y}} - \sinh(x)\Big)^2. \tag{12.117}$$

From these expressions one can find $\langle\pm|\sigma^z|\pm\rangle = \pm\sinh(x)/\sqrt{\sinh^2(x)+e^{-4y}}$, and compute the following observables (with $\phi = \lambda_-/\lambda_+$):

$$\frac{\sum_{s_1\ldots s_M} s_1 \prod_{k=1}^M K_{s_k s_{k+1}}}{\sum_{s_1\ldots s_M} \prod_{k=1}^M K_{s_k s_{k+1}}} = -\frac{\sinh(x)\tanh\left[\frac{1}{2}M\log\phi\right]}{\sqrt{\sinh^2(x)+e^{-4y}}}, \tag{12.118}$$

$$\frac{\sum_{s_1\ldots s_M} s_1 s_2 \prod_{k=1}^M K_{s_k s_{k+1}}}{\sum_{s_1\ldots s_M} \prod_{k=1}^M K_{s_k s_{k+1}}} = \frac{\sinh^2(x)}{\sinh^2(x)+e^{-4y}} + \frac{\cosh\left[\left(\frac{1}{2}M-1\right)\log\phi\right]}{\cosh\left[\frac{1}{2}M\log\phi\right]}\frac{e^{-4y}}{\sinh^2(x)+e^{-4y}} \tag{12.119}$$

$$\frac{\sum_{s_1\ldots s_M} s_1 s_3 \prod_{k=1}^M K_{s_k s_{k+1}}}{\sum_{s_1\ldots s_M} \prod_{k=1}^M K_{s_k s_{k+1}}} = \frac{\sinh^2(x)}{\sinh^2(x)+e^{-4y}} + \frac{\cosh\left[\left(\frac{1}{2}M-2\right)\log\phi\right]}{\cosh\left[\frac{1}{2}M\log\phi\right]}\frac{e^{-4y}}{\sinh^2(x)+e^{-4y}} \tag{12.120}$$

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