Stochastic Approach to Non-Equilibrium Quantum Spin Systems

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We investigate a stochastic approach to non-equilibrium quantum spin systems based on recent insights linking quantum and classical dynamics. Exploiting a sequence of exact transformations, quantum expectation values can be recast as averages over classical stochastic processes. We illustrate this approach for the quantum Ising model by extracting the Loschmidt amplitude and the magnetization dynamics from the numerical solution of stochastic differential equations. We show that dynamical quantum phase transitions are accompanied by clear signatures in the associated classical distribution functions, including the presence of enhanced fluctuations. We demonstrate that the method is capable of handling integrable and non-integrable problems in a unified framework, including those in higher dimensions.

Recent experimental advances in cold atomic gases [1-7] have catalyzed widespread interest in the non-equilibrium dynamics of isolated quantum many-body systems [8]. Questions ranging from the nature of thermalization [9-12] to the growth of entanglement following a quantum quench [13] have attracted considerable theoretical attention. In one dimension, the availability of analytical techniques based on integrability has led to fundamental insights into the role of conservation laws and the Generalized Gibbs Ensemble (GGE) [14-17]. Significant advances have also been made using machine-learning algorithms [22, 23] by exploiting novel representations of the quantum wavefunction.

In this manuscript, we explore a rather different approach to non-equilibrium systems based on an exact mapping between quantum spin dynamics and classical stochastic processes [24-26]. By a sequence of exact transformations, stochastic differential equations (SDEs) can be derived whose solutions yield quantum expectation values. We show that this approach can be turned into a viable tool for exploring quantum many-body dynamics in both integrable and non-integrable settings, including higher dimensions.

**Stochastic Formalism.**— The method is readily illustrated by considering the quantum Hamiltonian

\[ \hat{H} = \sum_{ij} J_{ij}^{ab} \hat{S}_i^a \hat{S}_j^b + \sum_i h_i^a \hat{S}_i^a, \tag{1} \]

where the spin operators \( \hat{S}_j^a \) on site \( j \) obey the commutation relations \([\hat{S}_j^a, \hat{S}_j^b] = i\delta_{j,ij} e^{abc} \hat{S}_j^c\) and we set \( \hbar = 1 \). Here \( J_{ij}^{ab} \) is the exchange interaction and \( h_i^a \) is an applied magnetic field with arbitrary orientation. The dynamics of the model is governed by the time evolution operator

\[ \hat{U}(t_f, t_i) = \mathbb{T} \exp \left( -i \int_{t_i}^{t_f} dt \hat{H}(t) \right), \tag{2} \]

between initial and final times \( t_i \) and \( t_f \), where \( \hat{H}(t) \) can be time-dependent and \( \mathbb{T} \) denotes time ordering. The operator \( \hat{U} \) is non-trivial, due to the interactions in \( \hat{H} \), the non-commutativity of the spin operators, and the time-ordering. However, \( \hat{U} \) can be expressed in an alternative form by means of a sequence of exact transformations [24-26]. To begin with, the interactions can be decoupled using Hubbard–Stratonovich transformations [27, 28] over auxiliary variables \( \phi_j^a \):

\[ \hat{U} = \mathbb{T} \int \mathcal{D}\phi \exp \left( -i S - i \int_{t_i}^{t_f} dt \sum_j (\phi_j^a \hat{S}_j^a + h_j^a \hat{S}_j^a) \right), \tag{3} \]

where \( \mathcal{D}\phi \equiv \prod_j \mathcal{D}\phi_j^a \) and the normalization factors have been absorbed into the measure. Eq. (3) describes decoupled spins interacting with stochastic magnetic fields \( \phi_j^a \) governed by the Gaussian action

\[ S = \frac{1}{4} \int_{t_i}^{t_f} dt \sum_{ij} (J^{-1})^{ij}_{ab} \phi_i^a \phi_j^b. \tag{4} \]

Equivalently,

\[ \hat{U}(t_f, t_i) = \langle \mathbb{T} e^{-i \int_{t_i}^{t_f} dt \sum_j \Phi_j^a(t) \hat{S}_j^a} \rangle_\phi, \tag{5} \]

where \( \Phi_j^a \equiv \phi_j^a + h_j^a \) and the average \( \langle \ldots \rangle_\phi \) is taken with the action in Eq. (4). This can be further simplified as the time-ordered exponential in Eq. (5) can be directly expressed as a group element [24-26] using the Wei–Norman–Kolokolov decomposition for SU(2) [29, 30]:

\[ \hat{U}(t_f, t_i) = \langle \prod_j \xi_j^a(t_f) \hat{S}_j^a \xi_j^b(t_i) \xi_j^c(t_i) \hat{S}_j^c \rangle_\phi, \tag{6} \]

where \( \hat{S}_j^\pm = \hat{S}_j^x \pm i \hat{S}_j^y \). The coefficients \( \xi_j^a \) are referred to as disentangling variables [26] and are related to the
original $\Phi_j^\alpha$ via
\begin{align}
    i\dot{\xi}_j^+ &= \Phi_j^+ + \Phi_j^x \xi_j^+ - \Phi_j^- \xi_j^{+2}, \\
    i\dot{\xi}_j^- &= \Phi_j^- - 2\Phi_j^x \xi_j^+, \\
    i\dot{\xi}_j^x &= \Phi_j^x \exp(\xi_j^x),
\end{align}

where $\xi_j^\alpha(t_i) = 0$. These equations are non-linear SDEs for the complex variables $\xi_j^\alpha$, where the Hubbard–Stratonovich variables $\phi_j^\alpha$ represent Gaussian form. Indeed, the SDEs can be put in the canonical form [31]:
\begin{equation}
    \frac{d\xi}{dt} = A^a_i(\{\xi\}) + \sum_{j} B_{ij}^{ab}(\{\xi\}) \phi_j^b,
\end{equation}

where $A^a_i$ and $B_{ij}^{ab}$ are the drift and diffusion coefficients respectively with $\{\xi\} = (\xi_j^x, \xi_j^\pm)$, and $\phi_j^b$ are delta-correlated white noise variables obtained by diagonalizing the action in Eq. (4) [32]. These exact transformations allow one to recast quantum dynamics in terms of SDEs, where quantum expectation values are replaced by averages over classical processes. This method has been applied to the thermodynamics of a single cluster of quantum spins [24] and to the dynamics of a single spin coupled to a photonic waveguide [26]. Here, we show that this novel approach can be applied to both integrable and non-integrable lattice spin models, including those in higher dimensions. In the numerical solution of non-linear SDEs using the Euler scheme may have divergent trajectories where the stochastic variables, such as $\xi_j^\pm(t)$, grow without bound [33]. Throughout this manuscript we present results obtained from the non-divergent trajectories. In evaluating quantum expectation values we retain more than 99% of the realizations at the stopping time. In plotting the associated classical variables for large system sizes, we typically retain more than 90% of the trajectories.

Loschmidt Amplitude.— A natural quantity to study using the stochastic formalism is the Loschmidt amplitude $A(t)$, defined as the probability amplitude to return to an initial state $|\psi(0)\rangle$ after time $t$:
\begin{equation}
    A(t) = \langle \psi(0)| \hat{U}(t, 0)|\psi(0)\rangle.
\end{equation}

In order to provide explicit results, we first examine the quantum Ising model in a transverse field $\Gamma$
\begin{equation}
    \hat{H}_1 = -J \sum_{j=1}^N \hat{S}_j^z \hat{S}_{j+1}^z - \Gamma \sum_{j=1}^N \hat{S}_j^z,
\end{equation}

where $N$ is the number of lattice sites. We consider ferromagnetic interactions $J > 0$ and impose periodic boundary conditions; in the numerical simulations below we set $J = 1$ and measure time in units of $J$. We take $|\psi(0)\rangle = \otimes_j |\downarrow\rangle \equiv |\downarrow\rangle$ with all spins down, corresponding to a ferromagnetic initial state. For this initial state, the Loschmidt amplitude is given by
\begin{equation}
    A(t) = \left\langle \prod_{j=1}^N \exp\left(-\frac{\xi_j^z(t)}{2}\right) \right\rangle_\phi,
\end{equation}

where the disentangling variables $\xi_j^z$ satisfy the SDEs (7) with the appropriate model specific coefficients. The amplitude (11) can be obtained by averaging over different realizations of the stochastic process. In Fig. 1 we plot the associated rate function $\lambda(t) = -N^{-1} \ln |A(t)|^2$, for unitary evolution in a non-zero transverse field. For quenches across a quantum critical point, $\lambda(t)$ is known to exhibit sharp peaks, corresponding to dynamical quantum phase transitions (DQPTs) in the thermodynamic limit [34–36]. Fig. 1 shows that the SDE method is able to resolve these peaks for a quantum quench across the critical point at $\Gamma_c = J/2$. The SDE results are in excellent agreement with exact diagonalization (ED) results obtained via the QuSpin package [37]. Remarkably, the presence of the DQPTs is reflected in the disentangling variables themselves. In Fig. 2 we plot the time evolution of the distribution of $\chi^a(t) \equiv N^{-1} \sum_j \xi_j^a(t)$ with $a = z, x$, as suggested by Eq. (11). It can be seen in Fig. 2(a) that both the average value and the width of the distribution of $\chi^a(t)$ have smooth maxima in the vicinity of the DQPTs, as further illustrated in the inset. Likewise, Im $\chi^z(t)$ shows pronounced signatures close to the DQPTs, as indicated in Fig. 2(b); these features become less visible with increasing $N$, and the overall phase of the argument of Eq. (11) becomes uniformly distributed over $[-\pi, \pi]$ due to its scaling with $N$. Further insight into the location of the DQPTs can be obtained from the SDEs. From Eq. (7) it can be seen that the turning points...
The stochastic approach can also be applied to other physical observables including the magnetization. Following a quench from an initial state $|\psi(0)\rangle$, the local magnetization evolves according to

$$
\langle \hat{S}_z(t) \rangle = \langle \psi(0) | \hat{U}(t) \hat{S}_z(0) \hat{U}(t) | \psi(0) \rangle.
$$

The forwards and backwards time-evolution operators can be decoupled by independent Hubbard–Stratonovich variables, $\phi_i$ and $\phi_i^*$, with corresponding disentangling variables $\xi_i(\phi)$ and $\xi_i^*(\phi)$. For a quantum quench starting in the ferromagnetic ground state $|\psi(0)\rangle = |\uparrow\rangle$ with $\Gamma = 0$, and time-evolving with $\Gamma \neq 0$, one obtains

$$
\langle \hat{S}_z(t) \rangle = \left\langle f_i \left( \xi(t), \xi^*(t) \right) \right\rangle_{\phi, \phi^*}.
$$

The distribution of $\text{Re} \chi(t)$ for the quantum Ising model following a quantum quench from $\Gamma = 0$ to $\Gamma = 16$, with $N = 7$. (a) The distribution of $\text{Re} \chi(t)$ shows smooth maxima and increased fluctuations in the vicinity of the Loschmidt peaks (dashed lines at $t = 0.39, 1.18, 1.96, 2.75$ obtained by ED). Inset: the average value and width of the distribution of $\text{Re} \chi(t)$ increases on approaching the Loschmidt peaks as illustrated for the first peak. (b) The distribution of $\text{Im} \chi(t)$ also shows signatures in the vicinity of the Loschmidt peaks. (c) Time-evolution of $\text{Im} \chi(t)$ for $N = 7, 25$, and $50$. The zeros of $\text{Im} \chi(t)$ occur in proximity to the turning points of $\lambda(t)$.
The dynamics of these variables can be tracked to larger system sizes as shown in Fig. 5(c) for the 10 x 10 system. This provides a novel handle on the dynamics of higher-dimensional quantum many-body systems. As found in 1D, the time evolution of the classical average $\langle \chi^2 \rangle$ and its turning points are strikingly independent of $N$. This, together with the form of Eq. (11), suggests the possibility of developing a classical large deviation approach to quantum dynamics in future work.

Conclusions.— In this manuscript we have explored the dynamics of non-equilibrium quantum spin systems via an exact mapping to classical stochastic processes. We have shown that this approach can handle the dynamics of integrable and non-integrable systems, including those in higher dimensions. This novel approach provides a valuable handle on challenging problems out of equilibrium and provides fundamental links between quantum and classical dynamics. There are many directions for future research including comparison with tensor network and machine learning approaches, and the development of enhanced numerical sampling techniques for the SDEs.

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