Dynamic Monte Carlo Study of the Two-Dimensional Quantum XY Model

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Abstract. – We present a dynamic Monte Carlo study of the Kosterlitz-Thouless phase transition for the spin-1/2 quantum XY model in two-dimensions. The short-time dynamic scaling behaviour is found and the dynamical exponent $\theta$, $z$ and the static exponent $\eta$ are determined at the transition temperature.

The existence and the nature of the phase transition in the quantum XY model is a long-standing problem. In 1973, Kosterlitz and Thouless explained what is now called the Kosterlitz-Thouless (KT) phase transition in the classical XY model, in terms of topological order, characterized by an exponentially divergent spatial correlation length and susceptibility $\xi$. General universality arguments suggest that the same KT transition may occur in the quantum XY model $\xi$. However, a quantitative determination of the critical exponents and the transition temperature with Monte Carlo methods is very difficult since one suffers from critical slowing down.

Due to the exponential divergence of the correlation length at the transition temperature $T_{KT}$ and the fact that the system remains critical below $T_{KT}$, numerical simulations of critical systems with a KT transition are more difficult than those with a second order phase transition. The situation is even more severe for quantum spin systems with a KT transition. A standard approach to the quantum XY model is the quantum Monte Carlo (QMC) method where the Suzuki–Trotter transformation is used to transform the quantum system to a classical one $\xi$. For the 2-dimensional spin-1/2 quantum XY model, Loh, Scalapino and Grant first estimated the KT transition temperature between $T_{KT} = 0.4 - 0.5$ [3]. The authors of refs. $\xi$ improved the results with extensive QMC simulations on lattices up to $128^2$. With a loop-cluster algorithm $\xi$ which is often more efficient than the conventional QMC methods, Harada and Kawashima recently measured the helicity modulus for temperatures between $T = 0.2 - 0.60$, and determined rather accurately the transition temperature $T_{KT} = 0.3423(2)$ on the lattice $64^2$. In this loop-cluster algorithm a loop is formed by spin-pairs on the interacting plaquettes and all spins on the loop are flipped.
simultaneously to overcome critical slowing down. However, up to now it is still difficult to
determine the critical exponents in equilibrium accurately. For example, the critical exponent
\( \eta \) has been given as \( \eta = 0.25 \pm 0.01 \) in ref. \[4\], and \( \eta = 0.290 \pm 0.09 \) or \( \eta = 0.276 \pm 0.014 \) in
ref. \[5\]. These values differ from each other.

On the other hand, in recent years much progress has been made in critical dynamics.
Traditionally it was believed that universal scaling behaviour only exists in equilibrium or in
the long-time regime of the dynamic evolution. However, for classical magnetic systems, it
was discovered that universal scaling behaviour emerges already in the macroscopic short-time
regime \[14, 15, 16, 17, 18, 19, 20, 21, 22\]. Important is that new independent exponents must
be introduced to describe the dependence of the scaling behaviour on the initial conditions,
or specify the scaling behaviour of special dynamic observables. More interestingly, based on
the short-time dynamic scaling form, static exponents and the dynamic exponent \( z \) originally
defined in equilibrium or in the long-time regime of the dynamic evolution can be extracted
already from the universal short-time behaviour \[19, 23, 24\]. This provides a possible new way
out of critical slowing down.

In this paper, we investigate whether there exists universal short-time dynamic scaling
behaviour in quantum spin systems, taking the spin-1/2 quantum XY model in two dimensions
as an example. We determine the new exponent \( \theta \) and the dynamic exponent \( z \) as well as the
static exponent \( \eta \) from the power law behaviour of the observables at the beginning of the
time evolution.

The spin-1/2 quantum XY model is defined by the Hamiltonian
\[
\hat{H} = -J \sum_{<ij>} [s^x_i \cdot s^x_j + s^z_i \cdot s^z_j],
\]
where \( <ij> \) stands for nearest-neighbour pairs on a 2-dimensional lattice, \( s^x_i \) and \( s^z_i \) are
spin operators defined on each lattice site, which can be expressed by the Pauli matrices as
\( (s^x_i, s^z_i) = \frac{1}{2} (\sigma^x, \sigma^z) \).

By the checkerboard decomposition \[6, 8\] with the Suzuki-Trotter formula we express the
partition function as
\[
Z = \text{Tr}[\exp(-\beta \hat{H})] = \lim_{m \to \infty} \text{Tr}[\exp(-\epsilon \hat{H}_1)\exp(-\epsilon \hat{H}_2)\exp(-\epsilon \hat{H}_3)\exp(-\epsilon \hat{H}_4)]^m.
\]
Here \( \beta = 1/T \) is the inverse temperature, \( \epsilon = \beta/m \) and the set of \( \hat{H}_i \) arises from a decom-
position of \( \hat{H} \) as defined in ref. \[10\]. Since the coupling constant \( J \) can be absorbed into
the temperature, we put \( J = 1 \) in our later discussions. Now we insert complete sets of
eigenstates \( |+1\rangle \) and \(|-1\rangle \) of \( \sigma^z \) between each factor of \( \exp(-\epsilon \hat{H}_i) \) to map the 2-dimensional
quantum system to an induced (2+1)-dimensional classical system with Ising-like variables
\( s(i, r) = \pm 1/2 \),
\[
Z = \sum_{s(i,r)=\pm 1/2} \exp[-S(\{s(i,r)\})].
\]
Here \( r \) labels the slices in the artificial third dimension which has total \( 4m \) layers. \( S(\{s(i,r)\}) \)
consists of the four-spin interaction associated with the \( r \)-like plaquettes, which are called in-
teracting plaquettes. Each interacting plaquette is bounded by four non-interacting plaquettes
to form a checkerboard lattice \[23\]. The interacting plaquette weights are determined by the
products of the transfer matrix
\[
\exp[-S_p(s_1, s_2; s_3, s_4)] = <s_1, s_2|\exp[\frac{\epsilon}{4}(\sigma^x_i \cdot \sigma^x_j + \sigma^z_i \cdot \sigma^z_j)]|s_3, s_4>,
\]
where
for each plaquette configuration \(C_p(s_1, s_2; s_3, s_4)\) with \(s_1\) and \(s_2\) locating on a \(r\)th-slice, and \(s_3\) and \(s_4\) on the \((r+1)\)th-slice \([12]\). Actually \(S(\{s(i, r)\}) = \sum_p S_p(s_1, s_2; s_3, s_4)\) and the sum is over all possible interacting plaquetts \(p\). A calculation of the transfer matrix \(\exp[-S_p(s_1, s_2; s_3, s_4)]\) leads to the form

\[
\exp\left(\frac{\epsilon}{4}\right) \begin{pmatrix}
\cosh\left(\frac{\epsilon}{4}\right) & 0 & 0 & \sinh\left(\frac{\epsilon}{4}\right) \\
0 & \exp\left(-\frac{\epsilon}{4}\right) \cosh\left(\frac{\epsilon}{4}\right) & \exp\left(-\frac{\epsilon}{4}\right) \sinh\left(\frac{\epsilon}{4}\right) & 0 \\
0 & \exp\left(-\frac{\epsilon}{4}\right) \sinh\left(\frac{\epsilon}{4}\right) & \exp\left(-\frac{\epsilon}{4}\right) \cosh\left(\frac{\epsilon}{4}\right) & 0 \\
0 & 0 & 0 & \cosh\left(\frac{\epsilon}{4}\right)
\end{pmatrix}.
\]

The states of the spin-pair \((s_1, s_2)\) for the row index and \((s_3, s_4)\) for the column index are arranged in a sequence of \((+, +), (+, -), (-, +), (-, -)\). The elements of the matrix (up to an overall constant) can be interpreted as the Boltzmann weights of the configurations for the induced classical spin system. The zero elements indicate that only a part of the spin configurations is allowed.

Updating schemes based on the transfer matrix must satisfy the ergodicity and detailed balance condition. Due to the facts that any allowed configurations can be achieved by flipping pairs of spins on plaquette edges from an allowed configuration and each spin is shared by two interacting plaquettes \([6]\), it follows immediately that one should flip a closed loop of spins, i.e. change the signs of all spins on the loop simultaneously. Practically, we adopt the updating procedure introduced in refs. \([8, 13]\) in our simulations. A complete Monte Carlo sweep procedure starts from an ordered state \((m_0 = 1)\) \([22, 23]\). In this dynamic process, it is believed that at the transition temperature \(T_{KT}\) or below, there exists a dynamic scaling form, e.g. for the \(k\)th moment of the magnetization,

\[
M^{(k)}(t) = b^{-kn/2} M^{(k)}(b^{-z}t, b^{-1}L),
\]

which sets in right after a microscopic time scale \(t_{mic}\). This time scale can depend on initial conditions, algorithms or other microscopic details. In simulations of classical spin systems \(t_{mic} \sim 100\) Monte Carlo time steps is observed. If a Monte Carlo time step is considered to be a typical microscopic time unit, this is reasonable.

Starting from all spins up, we have performed the simulations with the Metropolis algorithm at the transition temperature \(T_{KT} = 0.3423\) \([11]\). Lattice sizes are taken to be \(L^2 \times 4m = 64^2 \times 120\) and \(L^2 \times 4m = 32^2 \times 120\). Samples for average are over 1 000 for \(L = 64\) and 2 000 for \(L = 32\). Statistic errors are estimated by dividing the samples into three groups. We measure the magnetization defined as

\[
M(t) = \frac{1}{L^2 \times 4m} \sum_{(i, r)} s(i, r, t)
\]

and its second moment. From the scaling form in \([8]\), it is easy to deduce that the magnetization decays by a power law

\[
M(t) \sim t^{-\eta/2z}.
\]

Such a power law decay has actually been known for a long time in the long-time regime of the dynamic evolution, but now it is expected to hold also in the macroscopic short-time regime. To
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determine the dynamic exponent \( z \) independently and further confirm the short-time dynamic scaling, we introduce a dynamic Binder cumulant \( U(t, L) = M^{(2)}/M^2 - 1 \). Simple finite size scaling analysis shows

\[
U(t, L) \sim t^{d/z}.
\]  

(9)

This behaviour of the Binder cumulant is a typical behaviour in the short-time regime, where the non-equilibrium spatial correlation length is very small.

![Fig. 1](image1.png)

**Fig. 1.** – The time evolution of the magnetization for \( L = 64 \) and \( L = 32 \) by starting from ordered state is plotted in double-log scale.

![Fig. 2](image2.png)

**Fig. 2.** – The time evolution of the cumulant for \( L = 64 \) and \( L = 32 \) by starting from ordered state is plotted in double-log scale.

In fig. 1 the time evolution of \( M(t) \) is plotted in double-log scale. The solid line is that for \( L = 64 \) and the circles for \( L = 32 \). One can see that until 1000 Monte Carlo steps, there is no visible finite size effect for these lattice sizes. Here the microscopic time scale \( t_{\text{mic}} \sim 100 \). In the figure we have skipped data for \( t \) smaller than 200. From the slope of \( M(t) \) in the time interval [200, 1000] we measure the critical exponent \( \eta/2z = 0.0522(6) \) for \( L = 64 \) and for \( L = 32 \) we get \( \eta/2z = 0.0518(7) \). Within the statistic errors, they coincide.

From the measured \( M(t) \) and \( M^{(2)}(t) \) we calculate the Binder cumulant \( U(t) \) which is plotted in fig. 2. It is interesting that the curves of \( U(t) \) exhibit short-wave fluctuations, which have not been observed in classical spin systems [22, 23]. However, the short-wave fluctuations do not affect so much the long-wave behaviour and a clear power law behaviour is seen in the figure. From the slopes of the curves, we measure the critical exponent \( d/z = 0.85(3) \) for \( L = 64 \) and \( d/z = 0.86(3) \) for \( L = 32 \). With the results of \( L = 64 \), we get the critical exponent \( z = 2.35(8) \). Taking \( z \) as input, from the measured value of \( \eta/2z = 0.0522(6) \) we obtain \( \eta = 0.245(8) \). Compared with the results from simulations in equilibrium, our value of the exponent \( \eta \) supports \( \eta = 0.25 \pm 0.01 \) in ref. [4] but is smaller than \( \eta = 0.29 \pm 0.09 \) or \( \eta = 0.276 \pm 0.014 \) given in ref. [5]. This suggests that the exponent \( \eta \) in this quantum XY model takes a classical value \( \eta = 1/4 \).
In the short-time regime of the dynamic evolution, there are plenty of new phenomena. To describe all these phenomena, the static exponents together with the dynamic exponent \( z \) are in general not sufficient. Another interesting and important dynamic process is the relaxation starting from a high temperature initial state with a small initial magnetization \( m_0 \). It has been shown analytically and observed numerically in classical spin systems, that after a microscopic time scale \( t_{\text{mic}} \), the magnetization undergoes surprisingly a power law initial increase \[ M(t) \sim m_0^\theta. \] (10)

The exponent \( \theta \) is a new independent critical exponent, which can not be expressed in terms of other known exponents.

In order to measure the critical exponent \( \theta \), we must prepare an initial state of random configurations but with a small initial magnetization \( m_0 \). In the high temperature limit of the transfer matrix in eq. (5), the four elements proportional to \( \sinh(\epsilon) \) vanish and only the four equal-weighted non-zero diagonal elements remain, which correspond to the interacting plaquettes of \( C_p(s_1, s_2; s_3, s_4) = (+; +; +; +), (-; -; -; -), (+; +; +; -) \) and \((-; +; -; +)\). Therefore, we first put randomly \( s^z_i = \frac{1}{2} \) with a probability of \( p = (m_0 + 1)/2 \) and \( s^z_i = -\frac{1}{2} \) with a probability of \( 1 - p \) respectively on the first layer \((r = 1)\) of the \( L^2 \times 4m \) lattice. Then we copy this configuration to all other \( r - 1 \) layers. This procedure gives the required initial random configuration.

The simulations have been performed with a lattice size \( L = 64 \) and total samples over 4 000. It is well known that the microscopic time scale \( t_{\text{mic}} \) in this case is small, typically less than 20 Monte Carlo time steps \([16, 17, 21, 23]\). Therefore we stop updating at \( t = 150 \). In fig. 3, the time evolutions of \( M(t) \) are plotted in log-log scale. After about 30 Monte Carlo steps, the curves show a nice power law behaviour. From the slope of the curves, we measure the critical exponent \( \theta = 0.18(1) \) for \( m_0 = 0.01 \), and \( 0.18(2) \) for \( m_0 = 0.005 \). Rigorously speaking, the exponent \( \theta \) is defined in the limit \( m_0 \to 0 \). However, within statistical errors our results for \( m_0 = 0.01 \) and \( 0.005 \) show already no difference. Therefore an extrapolation of \( \theta \) to the limit \( m_0 = 0 \) is not necessary here. In conclusions, for the first time we have investigated the short-time critical dynamics of the quantum spin system taking the two-dimensional spin \( 1/2 \) quantum XY model as an example. Universal power law behaviour of the magnetization and

![Fig. 3. – The time evolution of the magnetization for \( L = 64 \) with \( m_0 = 0.01 \) and \( m_0 = 0.005 \) is plotted in double-log scale.](image-url)
the Binder cumulant is found and the new critical exponent $\theta$, the dynamic exponent $z$ and the static exponent $\eta$ are determined at the transition temperature $T_{KT} = 0.3423$. The measured exponent $\eta = 0.245(8)$ agrees very well with $\eta = 0.244(5)$ obtained for the classical XY model \cite{22} and also with the theoretical prediction $\eta = 0.25$. However, the exponent $\theta = 0.18(2)$ and the dynamic exponent $z = 2.35(8)$ are apparently different from $\theta = 0.250(1)$ and $z = 1.96(4)$ for the classical XY model \cite{21,22}. These results indicate that the quantum XY model and the classical XY model are in a same static universality class but in a different dynamic universality class. As an alternative approach, our simulations pave a way for a systematic application of the short-time dynamic scaling to quantum spin systems.

For quantum spin systems, besides the stochastic relaxational dynamics there exists a true dynamics described by the Heisenberg equation of motion. It is challenging whether the short-time dynamic scaling can be found also there.

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