Phase diagram of the 3D quantum anisotropic XY model—A quantum Monte Carlo calculation

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In this work we apply the stochastic series expansion quantum Monte Carlo method to study the quantum phase transition of the spin 1 three-dimensional XY model with easy-plane anisotropy D. We simulate this model in cubic lattices \((L \times L \times L)\) with \(L \in (4,24)\) and periodic boundary condition. Using finite size scaling we obtained the phase diagram for the model, the critical exponent \(z = 0.50(1)\) and the quantum critical point \(D_c = 9.795(3)\). Using a low temperature expansion for the magnetic susceptibility we obtained \(z = 0.59(1)\).

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1. Introduction

Classic order–disorder transitions are characterized as a change in the balance between the ordering arising from minimizing energy and the disordering arising from maximizing entropy, both driven by the temperature of the system. The expression quantum phase transition (QPT) is widely used when a transition takes place at temperature \(T = 0\), i.e., at any point of non-analyticity of the ground state energy of the system under investigation [1,2]. Classical transitions are driven by thermal fluctuations while QPT are driven by quantum fluctuations at a transition point \(T_c\). An interesting result obtained was a slight increase in \(T_c\) for \(D < D_c\) where \(D_c\) is the correlation length and \(\xi\) the correlation length and \(z\) the dynamical critical exponent. This model has been studied by Pires and Costa [3] using the SCHA and the bond operator formalism in the small and large D phases respectively. The authors obtained the entire \(T_c \times D\) critical diagram using SCHA formalism. It was found that as \(D\) approaches \(D_c\) from above the energy gap vanishes continuously as \(T \approx (D - D_c)^{1/2}\). They obtained: \(B = 1\) for \(a = J_2/J_1 = 0\), \(B = 0.6\) for \(0 < a < 1\), \(B = 0.5\) for \(a = 1\) and \(B = 0\) for \(J_2/J_1 = 0\). The value \(B = 0.5\) is in agreement with the work of Wang and Wang [4].

An expression for the gap as a function of temperature was obtained as \(m^2 = c_0 + c_1 T^{1/2} e^{-c_2/T} [3]\) where \(c_0\), \(c_1\) and \(c_2\) are constants that depend on \(D\) and \(J_2/J_1\). The phase diagram obtained by Pires and Costa is pictured in Fig. 2 in a plot \(T_c \times D\) as a solid line. An interesting result obtained was a slight increase in \(T_c\) with increasing \(D\) for small \(D\). A more pronounced effect was observed by Wang and Wang [4] and by Wang and Wong [5] using the bond operator and the series expansion method respectively. This effect can also be seen in the Heisebeng model [4–6]. As it is well known, the SCHA is a reasonable semi-classical approximation to calculate the transition temperature and low-temperature...
2. Quantum Monte Carlo—results

In our Quantum Monte Carlo (QMC) simulations of the Hamiltonian \( H \) we use the code developed by the ALPS group [11] which is based on the Stochastic Series Expansion (SSE) [12] and use the directed loop update scheme developed by Sandvik [13] implemented with an optimal-local stochastic matrix for the algorithm [14]. The SSE approach is based on the high temperature expansion of the partition function up to order \( M \), being a generalization of Handscomb’ algorithm [15] used to study the ferromagnetic Heisenberg model. The SSE method does not bear from usual convergence difficulties found in the Suzuki–Trotter formulation [16,17].

Thermodynamical quantities, such as the total energy \( \langle E \rangle \), susceptibility \( \langle \chi \rangle \) and spin stiffness \( \langle r \rangle \) are straightforwardly obtained as derivatives of the free energy. The spin stiffness in particular can be defined as the increase in the free energy due to imposing a twist in the boundary condition on the order parameter [18]. In the simulation the spin stiffness is given by the “winding numbers”, i.e., the net spin current across the periodic boundaries in the directions \( x \) and \( y \) (for simulations performed in the \( z \) quantization axis). In analogy with the superfluid density of a boson system [19,20] one can demonstrate that [21]

\[
\rho = \frac{\partial^2 E(\theta)}{\partial \theta^2} |_{\theta = 0} = \frac{\langle W^2 \rangle + \langle W^2 \rangle}{2N\beta},
\]

where \( E(\theta) \) is the internal energy per spin, \( \beta \) is the inverse temperature and \( W_x \) and \( W_y \) are the winding numbers.

To build the phase diagram we use the finite size scaling behavior of the thermodynamic functions. We have simulated systems of size \( L \times L \times L \) with periodic boundary conditions. For parameters \( D < 0.9D_c \) we used 20 000 Monte Carlo Steps (MCSs) for thermalization for even lattice sizes \( L \in [4,16] \). For \( D \approx D_c \) we used 50 000 MCS for even lattice sizes \( L \in [4,24] \). In both cases the number of configurations used for measurements was 10 times the number of MCS used for thermalization. For \( D > D_c \) we used 100 000 MCS for thermalization for even lattice sizes \( L \in [4,10] \) and around 5 000 000 MCS for measurements. Throughout this work the error bars are not shown in figures, only if they are smaller than the symbols. At the critical temperature, \( T_c \), the spin stiffness has a fixed point that scales as \( D^\nu \) (for simulations performed in \( L \times L \)) [18], where \( L \) is the linear lattice size. Plotting \( \rho L \) as a function of \( T/T_c \) we expect that all curves intercept at a fixed point \( \rho(T_c)L = \text{const.} \)

The critical temperature is obtained assuming the scaling, \( T_c \approx T_c(\infty) + A L^{-1} + O(L^{-2}) \), holds for \( D > D_c \). Slightly above the \( T \approx 0 \) line we notice a continuous drop of the spin stiffness order parameter as the anisotropy is increased from \( D < D_c \) to \( D > D_c \).

For \( D < D_c \), if we plot \( \rho(\beta,L)T \) as a function of \( |t|L^{1/\nu} \) we can choose \( \nu \) such that the results for several values of \( L \) collapse into the same curve. This procedure gives an estimate of the critical index \( \nu \). In Fig. 3 it is shown the typical behavior of the spin stiffness for \( D = 0 \) and \( x = j_2/j_1 = 1 \). The estimate obtained for the critical temperature and the critical exponent is \( k_bT_c = 2.93J \) and \( \nu = 0.66 \) respectively. The value of \( T_c \) is quite close to the one obtained by the use of the SCHA approach even though far from the bond operator result (see Fig. 2).

As observed in previous works [3–6] we can confirm an increase in \( T_c \) with increasing \( D \), for small \( D \) as seen in Fig. 2. One could argue that the increase of \( D \) from 0 slightly changes the behavior of the system from XY to planar rotator, which has a higher transition temperature. As \( D \) is increased further quantum fluctuations reduces the magnetic order, thus reducing the transition temperature until it reaches the critical value \( D_c \) at \( T = 0 \).

![Fig. 1. Croquis of the interaction arrangements used in this work.](image1.png)

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![Fig. 2. Phase diagram, \( T_c \) as a function of \( D \) for \( j_2/j_1 = 1 \). The solid line is the result obtained by Pires and Costa [3] using the self-consistent harmonic approximation. The squares represent the results of Wang and Wang [4] using the bond operator approximation. The circles are the results of the present work using QMC. As a matter of comparison we plot the results of Pan [6] for the isotropic Heisenberg model as a dashed line.](image2.png)

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![Fig. 3. Figs. a, b show the finite size scaling stiffness analysis of the spin stiffness for \( D = 0 \) and \( x = 1 \). Fig. (a) shows the fixed point for \( L \rho (T_c) \). In Fig. (b) is shown the collapse of the curves for several values of \( L \). From an analysis of these figures we obtain \( k_bT_c = 2.93J \) and \( \nu = 0.66 \).](image3.png)

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Beyond the critical anisotropy $D > D_c$, we assume a low temperature expansion for the magnetic susceptibility based on an expression derived by Troyer [22]

$$\chi(L) \approx \beta^n \exp(-\beta \Delta(L)), \quad (3)$$

where $\Delta(L)$ is the gap for the finite size lattice and $\beta$ is the inverse temperature. The parameter $n$ depends on the shape of the dispersion relation. The derivative of the logarithm of the susceptibility $-\frac{\partial}{\partial \beta} \ln(\chi(L))$ provides a way to estimate the parameter $n$. At low temperature this derivative is $\Delta(L) + nT$. The slope $n$ is close to $-1$ for small systems sizes (4, 6) (see Fig. 4). In a very naive approach we can estimate the gap by supposing that $\Delta(L) \approx \Delta(\infty) + AL^m$. Solving the equation of $\chi(L)$ for $\Delta(L)$ and substituting in the previous equation with $n = -1$ we obtain

$$\Delta(L) = -T \ln(\chi(L)) = \Delta(\infty) + AL^m. \quad (4)$$

Logarithmic corrections, if present, require simulations of much larger lattice sizes than the ones performed in the present work. In Fig. 5(a) we show a plot of $-T \ln(\chi(L))$ as a function of the inverse temperature for several lattice sizes. By adjusting a straight line to the data, an estimate of the finite size gap is given by the intercept of the curve. In Fig. 5(b) we show a plot of $\Delta(L)$ as a function of inverse lattice size for several anisotropies. By adjusting a curve to the data, according to Eq. (4), an estimate of the infinite size gap is obtained.

In Figs. 6 and 7 it is shown a plot of $\ln A$ as a function of $D - D_c$ obtained by this approach. The slope of the curves provides an estimate for $B = zv$ [1].

As the anisotropy approaches the critical value $D_c$, the quantum fluctuations become stronger in such a way that the finite size scaling for the spin stiffness has to be modified to [23]

$$\rho(L,t,T) = \frac{1}{L^{d-z}} F_L(tL^z, tL^{1/z}), \quad (5)$$

where $F_L(tL^z, tL^{1/z})$ is a homogeneous function of its arguments, $t = 1 - D/D_c$ and $\xi = L^z \propto 1/T$.

Similarly, the modified finite size scaling for the uniform magnetic susceptibility is given by [23]

$$\chi(L,t,T) = \frac{L^z}{L} F_u(tL^z, tL^{1/z}). \quad (6)$$

Using Eq. (5) we can sweep $z$ and $D_c$ until a good collapse in a plot of $\rho(L,t)L^{d-z}/T$ by $T L^z$ is found. In Fig. 8 it can be seen the best collapses for $z = 1.0$ and $z = 0.5$ with $D_c = 9.8$, $z = 0.9$ and $D_c = 8.0$, $z = 0.6$ respectively. A value of $z < 1$ is obviously not the correct asymptotic behavior, and upon going to larger systems we believe that $z$ would increase to 1. A collapse can be seen in Fig. 9 for the susceptibility assuming $z = 1$.

If the temperature is low enough Eq. (5) can be used ignoring the first argument in the scaling function [24]. A plot of $\rho(L,t)L^{d-z}/T$ should produce the intended collapse as shown in Figs. 10 and 11 for $z = 1.0$ and $z = 0.5$ respectively. As usually seen in the path integral formulation, the mapping of the quantum to a classical corresponding system relates temperature with a imaginary time dimension $L \propto 1/T$ [25]. Since time and space are not equivalent, we have two correlation “lengths”, a spatial $\xi$ and a
Fig. 8. Finite size scaling stiffness analysis of the spin stiffness in a log-log plot of \(\rho(t,L) L^{d-2} / t \) by \(L^2\). It is shown the collapse of the stiffness curves for several values of \(L\). In Fig. (a) a good stiffness collapse was found with \(D=9.8\) and \(z=0.9\) for \(\tau=1.0\). In Fig. (b) a good stiffness collapse was found with \(D=8.0\) and \(z=0.66\) for \(\tau=0.5\).

Fig. 9. Finite size scaling collapse of susceptibility according to scaling hypothesis of Eq. (6) assuming \(z=1\) with (a) \(D_c=9.8\) for \(\tau=1.0\), (b) \(D_c=8.0\) for \(\tau=0.5\).

Fig. 10. Finite size scaling collapse of spin stiffness according to scaling hypothesis of Eq. (7) at \(k_B T=0.125\) for \(\tau=1.0\). It was found reasonable collapses for a wide range of parameters. (a) \(\tau=0.6\), \(D_c=9.79\); (b) \(\tau=0.5\), \(D_c=9.80\).

The main concern at this point is the way the \(\xi_r\) correlation. These are connected by the dynamical critical exponent \(z : \xi_r \propto L^{\zeta}\).

If a fixed aspect ratio between the imaginary time (inverse temperature) and space is set as \(const = L / L_t \propto TL^2\) then Eq. (5) reduces to
\[
\rho(L,t) L^{d-2} = F_p(const, t L^{1/\nu}).
\]

At the critical anisotropy \((t=0)\) curves for different lattice sizes should cross each other. In Fig. 12 it can be noticed that three data points with highest lattice sizes cross each other close to the same point assuming \(z=1\). Each of these three crossing points give an estimate for the critical anisotropy. Repeating this calculation for four different simulations we obtain \(D_c = 9.7945(5)\).

A precise estimative of \(D_c\) and \(\nu\) can usually be achieved by collapsing the stiffness data for different \(L\) using a correction to Eq. (7). The usual ansatz is the choice \(N(L) = 1 + c L^{-w}\) [24,26].

The corrected stiffness scaling relation is given by
\[
\rho(L,t) L^{d-2} = N(L) F_p(const, t L^{1/\nu}).
\]

The \(N(L)\) normalization factor is introduced to take into account subleading corrections to scaling. Any attempt to adjust our results with this ansatz or other ansatz [27] were fruitless, generating large error bars to the exponents. For example, the exponent \(\nu\) adjusts well for any value in the interval 0.5 and 0.6 for \(D_c\) close to 9.78 and 9.80 for a wide range of values of \(w\). The leading term itself was difficult to determine accurately, which can be seen in Fig. 13 where noticeably different values of \(\nu\) still produce fine collapses.

The main concern at this point is the way the \(N(L)\) dependence can be removed. Suppose that the scaling function \(F_p\) in Eq. (8) admits a series of expansion in \(t = 1 - D / D_c \approx 0\)
\[
\rho(L,t) L^{d-2} = N(L) F_p(0) + F_p(0) t L^{1/\nu} + O(t^{2}),
\]

and
\[
\rho(L,t) L^{d-2} \approx A(L) + B(t) L^{1/\nu}.
\]

By performing a linear fit to \(\rho(L,t) L^{d-2}\) it is then possible to obtain the independent term \(A(L) = N(L) F_p(0) \approx \rho(0) L^{d-2}\). The \(N(L)\) dependence is then eliminated by dividing \(\rho(L,t) L^{d-2}\)
Taking the average residue of a third order polynomial fit to the data around the critical anisotropy value \( D_c \) for \( n = 9.795 \). We found reasonable collapses for a wide range of \( n \) values with \( D_c = 9.794(3) \) which produced the least average error of \( n \) evaluated from Eq. (14). The error bars were calculated according to the second procedure described in the text.

\[
\rho(L) \approx 1 + \frac{F_0}{F_p} t L^{1/\nu} \approx \frac{\rho(L_T)}{\rho(L_0)},
\]

(11)

Therefore, if we plot \( \rho(L_T)/\rho(L_0) \) as a function of \( t L^{1/\nu} \) with an appropriate value for \( \nu \) and \( D_c \) curves for different values of \( L \) will collapse into the same curve. The result is shown in Fig. 14.

The error bars involved in the collapse procedure were calculated using two different methods. The first one is done by taking the average residue of a third order polynomial fit to the stiffness simulation data of the highest lattice sizes (12, 14, 16, 18, 20, 22, 24). The estimate of \( D_c \) and \( \nu \) is given by the values that produce the smallest average residue. The final result is given by the average value obtained from four independent simulations. This procedure yields the following result: \( D_c \in [9.7912, 9.7923] \), and \( \nu \in [0.485, 0.492] \). Performing a similar calculation with the uniform magnetic susceptibility we obtain \( D_c \in [9.7870, 9.7910] \) and \( \nu \in [0.505, 0.523] \). The second method for estimating the error bars depends on the error involved in the estimate of \( \nu \). Observing Eq. (10) we can expect that the slope of \( \rho L^{d+z-2} \) has the following \( L \) dependence:

\[
\left. \frac{\partial \rho(L)}{\partial t} \right|_{t=0} L^{d+z-2} \approx N(L) L^{1/\nu}.
\]

(12)

We can take its logarithm to find

\[
(d+z-2) \ln(L) + \ln \left( \left. \frac{\partial \rho(L)}{\partial t} \right|_{t=0} \right) \approx \ln(N(L)) + \ln(L) \frac{1}{\nu}.
\]

(13)

Subtracting the previous equation for different lattice sizes \( L \) and \( L' \), we obtain

\[
(d+z-2) \ln \left( \frac{L}{L'} \right) + \ln \left. \frac{\rho(L)}{\rho(L')} \right|_{t=0} \approx \ln \left( \frac{N(L)}{N(L')} \right).
\]

Isolating \( \nu \) and assuming \( \ln(N(L)) - \ln(N(L')) \approx 0 \) and \( z = 1 \) we obtain a way to estimate \( \nu \) similar to Ref. [28]

\[
\nu = \left( \frac{\ln(L) - \ln(L')}{{\ln(L)}^{1/\nu}} - \left. \frac{\ln(L) \rho(L)}{\partial t} \right|_{t=0} \right) / \left( \frac{L}{L'} \right).
\]

(14)

The best collapse is then defined by the values \( \nu \) and \( D_c \) which produce the minimum average deviation of \( \rho \) obtained using a set of couple \( (L, L') \) from the highest simulated lattice sizes (12, 14, 16, 18, 20, 22, 24). The final result is given by the average value of four independent simulations. Using this criterion we obtained \( D_c \in [9.7943, 9.7951] \), and \( \nu \in [0.4965, 0.505] \) from spin stiffness and \( D_c \in [9.7935, 9.7946] \), and \( \nu \in [0.47, 0.51] \) from susceptibility.

The final estimate is given by

\[
D_c = 9.7948(3) \quad \nu = 0.501(5),
\]

\[
D_c = 9.7941(5) \quad \nu = 0.492(2),
\]

using stiffness and susceptibility respectively.

The critical anisotropy \( D_c(\nu) \) shown in Fig. 15 can be obtained by the crossing point of \( \rho L^2 \) by \( D \) according to Eq. (7) for two different lattice sizes (14, 16). The statistical errors are smaller than systematic error due to finite size. Therefore, the error bars were estimated by the difference from the crossing from the lowest (4, 6) to the highest (14, 16) crossing points.

### 3. Conclusion

In this work we have studied the quantum phase transition in the three dimensional anisotropic XY model using a Monte Carlo numerical calculation. We found that contrary to the expected the SCHA works quite well in the whole range of anisotropy. The bond operator method that should work in the large D region does not give good results when compared to the SCHA. One possible explanation is that the SCHA works well for low temperatures and renormalizations of the harmonic interactions considered by Pires and Costa took into account thermal and quantum fluctuations while the bond operator results relied on a mean field value for...
the $t$ bosons and the global chemical potential. To obtain the critical exponent $\gamma$ we have proposed a finite size scaling that seems to work very well in the present case.

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