The Quantum Compass Model on the Square and Simple Cubic Lattices

J. Oitmaa and C. J. Hamer
School of Physics, The University of New South Wales, Sydney 2052, Australia.

We use high-temperature series expansions to obtain thermodynamic properties of the quantum compass model, and to investigate the phase transition on the square and simple cubic lattices. On the square lattice we obtain evidence for a phase transition, consistent with recent Monte Carlo results. On the simple cubic lattice the same procedure provides no sign of a transition, and we conjecture that there is no finite temperature transition in this case.

PACS numbers: PACS Indices: 05.30.-d, 75.10.-b, 75.10.Jm, 75.30.Cr, 75.30.Kz

I. INTRODUCTION

Quantum compass models are spin models in which the nearest-neighbour exchange coupling has the form $J_\alpha S_\alpha^i S_\alpha^j$ where $\alpha = (x, y, z)$ depends on the direction of the particular link or bond. This then implies a coupling between the spin space and the physical space of the lattice. Such models were first introduced, and have been regularly employed, to describe orbital ordering in various transition metal compounds [1–4], and references therein.

Such models also have applicability to models of superconducting arrays [5, 6] and it has been argued that such arrays can provide fault-tolerant qubits for quantum information systems.

Compass models can be defined in various ways, depending on the underlying lattice. Exact solutions have been obtained for a 1-dimensional alternating (xx),(zz) model [8] and for a 2-leg ladder [9]. A remarkable solution has also been found for the honeycomb lattice with (xx), (yy) and (zz) couplings along the three independent lattice directions [10]. As far as we are aware, no other exact solutions exist.

In the present paper we consider the spin-1/2 quantum compass model on the simple cubic lattice, with Hamiltonian

$$H = J_x \sum_{<ij>} \sigma_i^x \sigma_j^x + J_y \sum_{<ik>} \sigma_i^y \sigma_k^y + J_z \sum_{<il>} \sigma_i^z \sigma_l^z$$  (1)

where the $\sigma^\alpha_i$ are Pauli operators, and the sums are, respectively, over lattice bonds along the x,y,z directions. We will also consider the square lattice version, where the last term in (1) is omitted.

As is well known [8], this model possesses a number of unusual gauge-like symmetries. As a consequence each energy state has a macroscopic degeneracy and, consequently, there is no conventionally ordered magnetic phase at any temperature. However it has been pointed out that a state of orientational or ‘nematic’ order is possible, in which the nearest neighbour bonds of lowest energy lie predominantly along a specific lattice direction. In the isotropic case of equal interactions $(J_x = J_y = J_z)$ this represents a spontaneous symmetry breaking. Consequently there may be a critical point at a temperature $T_c$, above which the system is disordered, with no preferred direction.

Recent quantum Monte Carlo studies of the isotropic 2-dimensional model [11–13] have found strong evidence for a finite temperature critical point with $kT_c/J = 0.234$ (in our units) with a critical exponent $\nu \simeq 0.97$, consistent with 2D Ising behaviour. The same authors [13] also identified a transition in the corresponding classical model, but we do not consider the classical case in the present work. As far as we are aware, no investigation of the occurrence of such a critical point, or its value, has been reported in the 3-dimensional case.

The goal of the present work is to attempt to answer this question. We employ the method of high-temperature series expansions, which has proven successful in the past [14] in obtaining accurate values for critical temperatures and exponents in a wide variety of classical and quantum models. The basic idea is to expand the Boltzmann factor $e^{-\beta H}$ in the partition function in powers of $\beta = 1/kT$

$$Z = Tr\{e^{-\beta H}\} = \sum_{r=0}^\infty \frac{(-1)^r}{r!} Tr(H^r) \beta^r$$  (2)

The coefficients in this series can be evaluated in a number of (related) ways. We use a linked cluster approach [15] in which $lnZ$ is evaluated, as a series in $\beta$, on a sequence of finite connected clusters of increasing size, and the cluster contributions are combined appropriately to give the bulk free energy in the form

$$-\beta F = \frac{1}{N} lnZ = ln2 + \sum_{r=2}^\infty a_r (J_x, J_y, J_z) \beta^r$$  (3)

with the $a_r$ being multinomial expressions of degree $r$ in the $J$’s. From this one can immediately obtain a corresponding series for the specific heat.
However the specific heat has, in most cases, only a weak singularity and is not well suited to estimation of critical properties. Including an external field which couples to the order parameter \( D \),

\[
H = H_0 - hD
\]  

(4)

where we now write the original Hamiltonian \( \hat{H} \) as \( H_0 \), allows calculation of a high temperature series for a generalized ‘susceptibility’

\[
\chi = \frac{1}{\beta} \lim_{N \to 0} \frac{\partial^2}{\partial h^2} \left( \frac{1}{N} \ln Z \right)
\]  

(5)

The order parameter \( D \) was introduced \([13]\) for the 2-dimensional model as

\[
D_{2d} = J_x \sum_{<ij>} \sigma_i^x \sigma_j^x - J_y \sum_{<ik>} \sigma_i^y \sigma_k^y
\]  

(6)

because the use of the expression in \( (3) \) to obtain

\[
\text{with bonds. We generalize this for the 3-dimensional model as}
\]

\[
D_{3d} = 2J_x \sum_{<ij>} \sigma_i^x \sigma_j^x - J_y \sum_{<ik>} \sigma_i^y \sigma_k^y
\]  

(7)

Normally the calculation of the susceptibility would be somewhat involved, since \( H_0 \) and \( D \) do not commute. However, in the present model, we can simply combine the two terms into a Hamiltonian of the original form \([11]\), with \( J_x \to J_x(1-h), J_y \to J_y(1-h), J_z \to J_z(1+2h) \) and use the expression in \( (3) \) to obtain

\[
\beta \chi = \sum_{r=2}^{\infty} c_r (J_x, J_y, J_z) \beta^r
\]  

(8)

where the \( c_r \) are again multinomials of degree \( r \) in the \( J \)'s. The susceptibility series is expected to show a strong divergence at the critical point and hence should be more amenable to analysis.

Another quantity which is expected to show a strong divergence is the fluctuation in the order parameter

\[
Q = < D^2 > - < D >^2.
\]  

(9)

For the classical model this quantity is identical to \( \chi \), but this is not the case for the quantum model.

In the following sections we will present the series and our analysis for the 2-d case (Section \( \text{IV} \)) and 3-d case (Section \( \text{III} \)). Our conclusions are summarized in Section \( \text{V} \).

### II. THE SQUARE LATTICE

To test the effectiveness of the high-temperature series approach for the present model, we first investigate the square lattice case, where previous results exist \([11, 13]\).

We use a linked cluster method \([15]\) based on connected clusters (‘graphs’). To obtain a series for \( (\ln Z)/N \) correct to order \( \beta^{24} \), as we have done, requires the enumeration of clusters with up to 12 bonds. It is a special feature of this model that each bond must be used an even number of times to give a nonzero trace. There are 4423 topologically distinct clusters with 12 or fewer bonds, embeddable on the square lattice. This gives rise to 751663 distinct graphs with 2 bond types \( (x \text{ and } y) \). However the vast majority of these do not contribute, and the final irreducible list of contributing graphs numbers 60127. We give below the leading terms in the partition function series

\[
\frac{1}{N} \ln Z = \ln 2 + \frac{1}{2}(x^2 + y^2)\beta^2 - \frac{1}{12}(x^4 + 8x^2y^2 + y^4)\beta^4
\]

\[
+ \frac{1}{45}(x^6 + y^6) + 30(x^4y^2 + x^2y^4)\beta^6 - \frac{1}{2520}(17(x^8 + y^8) + 1736(x^6y^2 + x^2y^6) + 4344x^4y^4)\beta^8
\]

\[
+ \frac{1}{14175}(31x^{10} + y^{10}) + 5570(x^8y^2 + x^2y^8) + 40500(x^6y^4 + x^4y^6)\beta^{10}
\]

\[
- \frac{1}{935560}(691x^{12} + y^{12}) + 241800(x^{10}y^2 + x^2y^{10}) + 3426402(x^8y^4 + x^4y^8) + 7679480x^6y^6)\beta^{12} \cdots
\]  

(10)

where \( x \equiv J_x, y \equiv J_y \). Note that only even powers of \( \beta \) occur. This is a feature of all series for this model.

From this result we can obtain the susceptibility

\[
\chi/\beta = (x^2 + y^2) - \frac{1}{3}(3x^4 + y^4) - 8x^2y^2)\beta^2 + \frac{2}{3}((x^6 + y^6) - 2(x^4y^2 + x^2y^4))\beta^4
\]

\[
- \frac{1}{315}(119(x^8 + y^8) + 1376(x^6y^2 + x^2y^6) - 4344x^4y^4)\beta^6
\]

\[
+ \frac{1}{14175}(2790(x^{10} + y^{10}) + 144820(x^8y^2 + x^2y^8) - 243000(x^6y^4 + x^4y^6))\beta^8 \cdots
\]  

(11)
The higher order terms were evaluated numerically. In Table I we show the full series for the isotropic case $J_x = J_y$. The expansion variable is $K = \beta J$.

We have attempted to analyse these series using standard Padé approximant methods. Our discussion is confined to the $\chi$ series, as this (together, possibly, with $Q$) is expected to have a strong singular behaviour at the critical point. The first point to make about the series in $\beta^2$ is the regular alternation in sign. This reflects the presence of a dominant singularity on the negative $\beta^2$ axis (i.e. the imaginary $\beta$ axis). In fact there appears to be a whole string of such imaginary poles in the Dlog Padé approximants. This, in itself, is not so unusual. Recall that the exact result for the 1D Ising model has poles at $\beta J = \pm i(n + 1/2)\pi$.

However these interfering singularities mask the expected physical singularity on the real positive $\beta$ axis. One possible strategy to overcome this is to use an Euler transformation of the form $y = x/(1 + ax)$, $(x = K^2)$, which has the effect of compressing the positive real axis and expanding the region $-1/a < x < 0$ of the negative real axis. The use of such transformations is well known in the field of critical phenomena, as are the possible pitfalls.

To provide the reader with some insight into the analytic structure of the $\chi$ series we discuss the location of poles of Dlog Padé approximants to the series for $\beta J^2/\chi$ before and after the Euler transformation (with $a = 2.0$). The original series in $x = \beta^2$ has very consistent poles at $x \approx -0.28, -0.32, -0.46$, with less consistent poles much further from the origin. The transformed series shows images of these at $y = -0.65, -0.9$ as well as poles on the positive real axis at $y = 0.47, 0.54$. The last of these corresponds to a large negative value $x \approx -6.8$, whereas $y = 0.47$ corresponds to $x = 7.8$, or a physical critical value $kT_c/J \approx 0.34$. In Table II we show the estimates of $y_c$ and the exponent $\gamma$ at various orders. As can be seen, these are quite consistent at $y_c \approx 0.473$ and $\gamma \approx 0.52$. However, this critical temperature is much higher than the Monte Carlo estimate 0.234 and the corresponding exponent is much lower than the expected Ising value of 1.75. Therefore we can only conclude that, while the Dlog Padé analysis provides evidence for a physical critical point, the numerical estimates cannot be taken with any confidence. We comment further on this in the conclusions.

An alternative approach to analysing our series data is to evaluate the susceptibility itself at temperatures above $T_c$, using Padé approximants, and to plot the inverse susceptibility $\chi^{-1}$ versus $T$. In Figure 1 we plot both $\beta/\chi$, obtained directly from the series and $1/\chi$ versus temperature. Both curves clearly approach zero at $T_c \approx 0.25$, a value consistent with the Monte Carlo estimates [12, 13], and considerably below our Dlog Padé results. It is not possible to obtain accurate exponent estimates from this procedure, but if we fit our data points

| $p$ | $\frac{1}{\chi}(\beta J^2)$ | $Q$ |
|-----|-----------------|-----|
| 0   | 0.693147180560D+00 | 0.200000000000D+01 |
| 2   | 0.100000000000D+01 | 0.666666666666D+00 |
| 4   | -0.133333333333D+01 | -0.120000000000D+02 |
| 6   | 0.137777777778D+01 | 0.132382287013D+03 |
| 8   | -0.282935079370D+01 | -0.849650736643D+02 |
| 10  | 0.650455026455D+01 | 0.245585890085D+03 |
| 12  | -0.160518048207D+01 | -0.730131587978D+03 |
| 14  | 0.416028785294D+01 | 0.221467773923D+04 |
| 16  | -0.111781974764D+01 | -0.681447081860D+04 |
| 18  | 0.308758184039D+01 | 0.212139054331D+05 |
| 20  | -0.871688240896D+01 | -0.664573373818D+05 |
| 22  | 0.250506394206D+01 | 0.210941032291D+06 |
| 24  | -0.730521400959D+01 |           |
FIG. 1: Estimated values of the inverse susceptibility $\beta/\chi$ (circles) and $\chi^{-1}$ (squares) as functions of temperature $T$ for the 2D quantum compass model ($J=1$).

with a simple form $1/\chi = a(T - T_c)^\gamma$ together with the Monte Carlo critical point $T_c = 0.234$ we obtain $\gamma \simeq 1.3$, which is at least a good deal closer to the expected Ising value.

Thus we conclude that the series approach does confirm the existence of a finite temperature critical point in the isotropic 2D model, and corroborates the presumably more accurate Monte Carlo results.

III. THE SIMPLE CUBIC LATTICE

We now turn to the 3-dimensional model, where no previous results exist. We use the same approach as for the 2D case, and compute series for the same quantities. The leading terms of the series for $\ln Z$ are

$$\frac{1}{N} \ln Z = \ln 2 + \frac{1}{2} (x^2 + y^2 + z^2) \beta^2 - \frac{1}{12} (x^4 + y^4 + z^4 + 8(x^2y^2 + x^2z^2 + y^2z^2)) \beta^4$$
$$+ \frac{1}{45} (x^6 + y^6 + z^6 + 30(x^4y^2 + x^4z^2 + x^2y^4 + y^4z^2 + y^2z^4 + z^4y^2) + 120x^2y^2z^2) \beta^6$$
$$- \frac{1}{2520} (17(x^8 + y^8 + z^8) + 1376(x^6y^2 + x^6z^2 + y^6z^2 + y^6z^2 + z^6y^2) + 4344(x^4y^4 + x^4z^4 + y^4z^4)$$
$$+ 14176(x^4y^2z^2 + y^4x^2z^2 + z^4x^2y^2)) \beta^8$$
$$+ \frac{1}{14175} (31(x^{10} + y^{10} + z^{10}) + 5570(x^8y^2 + x^8z^2 + y^8x^2 + y^8z^2 + z^8x^2 + z^8y^2))$$
$$+ 40500(x^6y^4 + y^6x^4 + x^6z^4 + y^6z^4 + z^6x^4 + y^6z^4) + 120320(x^6y^2z^2 + y^6x^2z^2 + z^6x^2y^2)$$
$$+ 297200(x^4y^4z^2 + x^4y^2z^4 + x^4y^4z^2)) \beta^{10} + \ldots$$

(12)

where $x \equiv J_x, y \equiv J_y, z \equiv J_z$.

The susceptibility corresponding to the order parameter $D_{3d}$ (equation (7)) can be obtained by the substitution $J_x \rightarrow J_x(1 - \lambda), J_y \rightarrow J_y(1 - \lambda), J_z \rightarrow J_z(1 + 2\lambda)$ in (1). This definition, of course, introduces a preferred direction $z$. However in the isotropic limit the resulting series is unaffected by this.

We have evaluated the series numerically, up to order $\beta^{20}$, and the coefficients are shown in Table III.

As for the 2D case, the series are dominated by singularities on the negative $\beta^2$ axis. However, in contrast to the 2D case, Euler transformations yield no indica-
TABLE III: Series coefficients for the isotropic 3D Compass Model

| p   | \(\frac{1}{\ln Z}\) | \(\chi/(\beta J^2)\) | Q     |
|-----|----------------------|------------------------|-------|
| 0   | 0.693147180560D+00   | 0.600000000000D+01     | 0.600000000000D+01 |
| 2   | 0.150000000000D+01   | -0.600000000000D+01    | 0.180000000000D+02 |
| 4   | -0.250000000000D+01  | 0.200000000000D+02     | -0.760000000000D+02 |
| 6   | 0.673333333333D+01   | -0.810476190476D+02    | 0.377466666667D+03 |
| 8   | -0.253440476190D+02  | 0.200000000000D+02     | -0.760000000000D+02 |
| 10  | 0.107871111111D+03   | -0.178751576719D+04    | 0.110779369318D+05 |
| 12  | -0.496475097002D+03  | 0.915575874989D+04     | -0.62867973726D+05 |
| 14  | 0.241283362972D+04   | -0.48688476086D+05     | 0.363814737295D+06 |
| 16  | -0.122062709687D+05  | 0.266451000791D+06     | -0.213714381541D+07 |
| 18  | 0.636830117143D+05   |                           | 0.127041779973D+08 |
| 20  | -0.340463327677D+06  |                           |                   |

FIG. 2: Estimated values of the inverse susceptibility \(\beta/\chi\) (circles) and \(\chi^{-1}\) (squares) as functions of temperature \(T\) for the 3D quantum compass model \((J=1)\).

The question of the existence of a thermodynamic phase transition in the quantum compass model on various lattices is of fundamental importance. The present work is, to our knowledge, the first attempt to address this problem using the technique of high-temperature series expansions, a standard method in other contexts.

The series indicate that the analytic structure of thermodynamic functions for these models is dominated by singularities on the imaginary \(\beta\) axis \((\beta = 1/kT)\). This is perhaps a reflection of the peculiar ‘1-dimensional’ nature of the couplings in the model.

Our results for the square lattice are consistent with, albeit less precise than, recent Monte Carlo results \([13]\). This demonstrates that the high-T series method does in fact work. However for the cubic lattice we find no signature of a critical point at finite \(T\), and conjecture that there is no such critical point. At first glance this appears surprising, since the normal expectation is that the ordered phase will be more robust, and hence \(T_c\) will increase, with increasing dimension. In the case of a simple antiferromagnet, for instance, the bond interactions in different directions can be satisfied simultaneously, and reinforce each other, so that the tendency to order increases with higher dimension. In the present case, however, the bond interactions in different directions pull different ways, and compete with each other, so that the tendency to order decreases with higher dimensions. In one dimension, the ‘nematic’ order parameter is non-zero at all finite temperatures; in two dimensions \(D_{2d}\) is only non-zero at low temperatures; and in three dimensions it appears that \(D_{3d}\) is actually zero at all finite temperatures. It has also been pointed out \([2, 16]\) that in this model thermal fluctuations in fact become larger with increasing dimension.

IV. DISCUSSION

but, within the numerical uncertainties, are consistent with a transition at \(T = 0\).
The series have proved difficult to analyze, because of the complex singularities, and gave rather poor estimates of the critical parameters in two dimensions. A closer investigation of the nature of these singularities may lead to more precise estimates of the critical parameters; or else higher-order series coefficients might be necessary. It is worth noting that the model has also proved difficult to analyze using finite-size scaling and Monte Carlo methods. An early Monte Carlo calculation \[11\] on lattices of up to 20 x 20 sites with periodic boundary conditions also gave a critical point about 36% too high. Wenzel et al. \[13\] showed that the use of special ‘screw periodic’ boundary conditions on lattices up to 42 x 42 was required to produce the estimates quoted earlier.

Acknowledgments

We are grateful for the computing resources provided by the Australian Partnership for Advanced Computing (APAC) National Facility.

[1] K.I. Kugel and D.I. Khomskii, Sov. Phys. Usp. 25, 231 (1982).
[2] D.I. Khomskii and M.V. Mostovoy, J. Phys. A36, 9197 (2003): M.V. Mostovoy and D.I. Khomskii, Phys. Rev. Lett. 92, 167201 (2004).
[3] J. van der Brink, New J. Phys. 6, 201 (2004).
[4] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. 102, 017205 (2009).
[5] C. Xu and J.E. Moore, Phys. Rev. Lett. 93, 047003 (2004).
[6] Z. Nussinov and E. Fradkin, Phys. Rev. B71, 195120 (2005).
[7] B. Doucot, M.V. Feigelman, L.B. Ioffe and A.S. Ioselevich, Phys. Rev. B71, 024505 (2005).
[8] W. Brzezicki, J. Dziarmaga and A.M. Oles, Phys. Rev. B75, 134415 (2007).
[9] W. Brzezicki and A.M. Oles, Phys. Rev. B80, 014405 (2009).
[10] A. Kitaev, Ann. Phys. 321, 2 (2006).
[11] T. Tanaka and S. Ishihara, Phys. Rev. Letts. 98, 256402 (2007).
[12] S. Wenzel and W. Janke, Phys. Rev. B78, 064402 (2008).
[13] S. Wenzel, W. Janke and A. Läuchli, Phys. Rev. E81, 066702 (2010).
[14] C. Domb and M.S. Green (eds.), Phase Transitions and Critical Phenomena, Vol. 3 (Academic, New York, 1974).
[15] J. Oitmaa, C. Hamer and W. Zheng, Series Expansion Methods for Strongly Interacting Lattice Models (Cambridge University Press, 2006).
[16] A. Mishra, M. Ma, F-C. Zhang, S. Guertler, L-H. Tang and S. Wán, Phys. Rev. Letts. 93, 207201 (2004).