2D XXZ Model ground state Properties using an analytic Lanczos Expansion

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We develop the formalism for calculating arbitrary expectation values for any extensive lattice Hamiltonian system using a new analytic Lanczos expansion, or plaquette expansion, and a recently proved exact theorem for ground state energies. The ground state energy, staggered magnetisation and the excited state gap of the 2D anisotropic antiferromagnetic Heisenberg Model are then calculated using this expansion for a range of anisotropy parameters and compared to other moment based techniques, such as the $t$-expansion, and spin-wave theory and series expansion methods. We find that far from the isotropic point all moment methods give essentially very similar results, but near the isotropic point the plaquette expansion is generally better than the others.

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I. INTRODUCTION

In this work we employ a very recent addition to the range of moment methods available now to the problem of the $s = 1/2$ antiferromagnetic Heisenberg model on a square lattice. These other methods are based essentially on linked-cluster expansions and include the $t$-expansion \[7\], the connected moment expansion (CMX) \[8\], and the coupled-cluster expansion \[8\], \[9\]. The method we use is based on the Lanczos method,

$$\hat{H}|\psi_n\rangle = \beta_n|\psi_{n-1}\rangle + \alpha_n|\psi_n\rangle + \beta_{n+1}|\psi_{n+1}\rangle,$$

starting with a trial state $|\psi_n\rangle$, whereby approximate yet analytic expressions for the Lanczos coefficients $\alpha_n(N)$ and $\beta_n^2(N)$ can be found at an arbitrary Lanczos step $n$ in terms of low order cumulants, denoted by $c_n$ $n = 1, \ldots$. This expansion, also called the “plaquette expansion” \[8\], \[9\], is actually an expansion of the exact coefficients about the infinite size limit, that is in $1/N$. Furthermore in the combined limit of complete Lanczos convergence $n \to \infty$ and the thermodynamic limit $N \to \infty$ scaled Lanczos coefficients emerge in terms of $z = n/N$, taken to the lowest three orders

$$\begin{align*}
\alpha(z) &\equiv \lim_{n,N \to \infty} \alpha_n(N) \\
&= c_1 + z \left[ \frac{c_3}{c_2} \right] + z^2 \left[ \frac{3c_3^2 - 4c_2c_3c_4 + c_2^2c_6}{4c_2^2} \right] + O(z^3), \\
\beta^2(z) &\equiv \lim_{n,N \to \infty} \beta_n^2(N) \\
&= z c_2 + z^2 \left[ \frac{c_2^2c_4 - c_3^2}{2c_2^2} \right] + z^3 \left[ \frac{21c_2c_3^2c_4 - 12c_3^2c_5 - 4c_2^2c_3^2 - 6c_2^2c_3c_5 + c_3^2c_6}{12c_2^3} \right] + O(z^4). 
\end{align*}$$

In Ref \[9\] it was found that the ground-state energy density in the bulk limit to be given in general by

$$\epsilon_0 = \inf_z [\alpha(z) - 2\beta(z)] \equiv \inf_z \epsilon(z).$$

All these moment methods use the same input data, a sequence of connected moments up to some cut-off order, yet have rather different treatments of these so that it is of interest to compare them with each other. This work is the logical extension of Ref \[8\] which compared the $t$-expansion and the connected moments expansion with the coupled-cluster method, series expansions and spin-wave theory for the same model. In this work we have used the same set of cumulants as in the above work, up to the 15th order, and an additional set taken to the same order. However the interest of this work is not just confined to a discussion of the relative merits of the various methods, but also to demonstrate the contribution of moment methods to an understanding of the planar antiferromagnetic Heisenberg model.

II. GROUND STATE AVERAGES FOR ANALYTIC LANCZOS EXPANSION

Most previous applications of the plaquette expansion have been to the energy spectrum, notably the ground state energy \[8\], \[10\], \[11\] and the mass gap \[12\]. Two earlier examples of the application of the expansion to other averages were the calculation of the staggered magnetisation of the isotropic 2D Heisenberg model \[13\], \[14\]. In these works the staggered magnetisation was extracted from the full nonlinear magnetic field dependence of the ground state energy for a system in a transverse external field. Here we take this approach to its logical conclusion and establish the formalism to describe an ground state average of an arbitrary operator $\hat{V}$. Our approach is quite simple, we “piggy-back” our operator $\hat{V}$ onto our Hamiltonian, by tagging it with a variable $\lambda$, and apply the earlier results and theorems to this new Hamiltonian.

Consider the exact ground state energy of the new Hamiltonian $\hat{H} + \lambda \hat{V}$, namely $\epsilon(\lambda)$ and with exact ground state wavefunction $|\Psi_{\lambda}\rangle$.

$$\epsilon(\lambda) = \langle \Psi_{\lambda}|\hat{H} + \lambda \hat{V}|\Psi_{\lambda}\rangle,$$

then the Hellmann-Feynman theorem gives the ground state average as
\[\langle \hat{V} \rangle = \left. \frac{d}{d\lambda} \epsilon(\lambda) \right|_{\lambda=0}.\] (5)

So we need only evaluate the first order change in \(\lambda\) in any quantity. Because we are assuming all quantities thus derived are analytic in some small neighbourhood of \(\lambda = 0\) we require the overlap of the new ground state wavefunction with the original is nonzero, \(\langle \Psi_0 | \Psi_\lambda \rangle \neq 0\).

The new Hamiltonian \(H_\lambda\) will generate a new sequence of Lanczos coefficients \(\alpha_n(\lambda)\) and \(\beta_n^2(\lambda)\) from some suitable trial state \(|\psi_0\rangle\) and these in turn will have analytic expansions

\[
\begin{align*}
\alpha_n(\lambda) &= \alpha_n + \lambda \delta^V \alpha_n + O(\lambda^2) \\
\beta_n^2(\lambda) &= \beta_n^2 + \lambda \delta^V \beta_n^2 + O(\lambda^2),
\end{align*}
\]

where \(\delta^V \alpha_n\) and \(\delta^V \beta_n^2\) define the first order shifts in \(\alpha_n\) and \(\beta_n^2\) in the presence of the operator \(\hat{V}\). In the interests of clarity a symbol without an argument of \(\lambda\) is assumed to be the case where \(\lambda = 0\). Furthermore we consider models where the extensive scaling property when the Lanczos iteration number \(n\) and the system size \(N\) both tend to infinity with \(z = n/N\) fixed applies to the Lanczos coefficients,

\[
\begin{align*}
\alpha_n(\lambda) \xrightarrow{n,N \to \infty} \alpha(z) + \lambda \delta^V \alpha(z) + O(\lambda^2) \\
\beta_n^2(\lambda) \xrightarrow{n,N \to \infty} \beta_0^2(z) + \lambda \delta^V \beta_0^2(z) + O(\lambda^2).
\end{align*}
\]

Then the exact ground state theorem can be applied in the form

\[\epsilon(\lambda) = \inf_z \left\{ \alpha(\lambda, z) - 2[\beta^2(\lambda, z)]^{1/2} \right\},\] (6)

and one can show that

\[\langle \hat{V} \rangle = v(z)\big|_{z=\bar{z}},\] (7)

where our new \(z\)-function \(v(z)\) is

\[v(z) = \delta^V \alpha(z) - \frac{\delta^V \beta^2(z)}{\beta(z)},\] (8)

and \(\bar{z}\) is the \(z\)-value of the minima in \(e(z) = \alpha(z) - 2\beta(z)\) if it exists. The new quantities in this, our central result, are the first order shifts in the Lanczos coefficients, and these will now be found in terms of moments.

As is fundamental in the Lanczos process we need to find the moments of the new Hamiltonian with respect to our trial state, and the first order shifts of these \(T_n\), by

\[\langle (\hat{H}_\lambda)^n \rangle = \langle \hat{H}^n \rangle + \lambda T_n + O(\lambda^2),\] (9)

and it is found that \(T_n\) is given by a sum of distributed generalised moments,

\[T_n = \sum_{k=0}^{n-1} (\hat{H}^{n-1-k} \hat{V} \hat{H}^k),\] (10)

when \(n > 1\). The first member, \(T_0 = 0\). This result can be proven from the recurrence relation \(T_{n+1} = \langle \hat{H} \hat{T}_n \rangle + \langle \hat{V} \hat{H}^n \rangle\) or from the generating function

\[\sum_{n=0}^{\infty} w^n T_n = w\left( \frac{1}{1 - w\hat{V}} - \frac{1}{1 - w\hat{H}} \right).\] (11)

From this point we go to the connected parts of these moments, with a first order shift denoted by \(S_n\),

\[\langle (\hat{H}_\lambda)^n \rangle_c = \langle \hat{H}^n \rangle_c + \lambda S_n + O(\lambda^2).\] (12)

This connected part, or cumulant, has the standard generating function.
\[
\frac{d}{d\lambda} \log \langle e^{iH_{\lambda}} \rangle \bigg|_{\lambda=0} = \sum_{n=1}^{\infty} \frac{t^n}{n!} S_n ,
\]
and the standard recurrence relation with the moments
\[
T_{n+1} = \sum_{k=0}^{n} \binom{n+1}{k} \langle \hat{H}^k \rangle S_{n+1-k} ,
\]
for \( n \geq 0 \). In effect what this reduces \( S_n \) to is a sum similar to Eq. [13] except now it is over the connected parts of the distributed generalised moments, namely \( \langle \hat{H}^{n-v} V \hat{H}^v \rangle \). It is these moments which are actually directly calculated. Finally, in the extensive many-body problem the connected moments have a size dependence via the coefficients
\[
S_n = \delta c_n N .
\]

The expression for \( T_n \) (see Eq. [10]) or \( S_n \) in terms of the distributed generalised moments bears some similarity with the ones appearing in the \( t \)-expansion (see Equation 2.10 in Ref [8]), in that exactly the same averages occur, but that here the binomial coefficient is absent. This is because the Lanczos process is one where the Hamiltonian \( \hat{H} \) generates new states in an enlarging state space, akin to a geometrical progression, and geometrical generating functions and convolutions arise. In contrast the \( t \)-expansion employs an exponentially mapped state \( e^{-\frac{1}{2} t \hat{H} / \psi_0} \) and therefore exponential generating functions and convolutions appear.

It should be noted that all the foregoing is exact, given that a system is solvable in this sense and all the moments, and Lanczos coefficients are analytically known. However for many non-trivial models one has knowledge only of the first say, \( 2r \) moments which give terms of \( z^0, \ldots, z^{r-1} \) in \( \alpha(z) \) and \( z, \ldots, z^{r} \) in \( \beta^2(z) \), or \( 2r + 1 \) moments which give terms in \( \alpha(z) \) from \( z^0, \ldots, z^{r} \) and terms in \( \beta^2(z) \) from \( z, \ldots, z^{r} \). In the even case, with \( 2r \) moments, we define the truncation order as \( r \) and this is a natural ordering as there are equal numbers of terms in \( \alpha \) and \( \beta^2 \) coefficients, and in the odd case \( 2r + 1 \) the truncation order is still \( r \), but is not a natural order, but termed supplemented, in having one more term, namely a \( z^r \) in \( \alpha(z) \).

Given the shifted cumulant coefficients \( \delta c_n \), and therefore the shifted moments \( T_n \) there exists a number of algorithms for generating the shifted Lanczos coefficients, and one of the more robust and efficient ones is briefly described in the Appendix. The first few terms in the Lanczos coefficients are given by

\[
\delta^V \alpha(z) = \delta c_1 + z \left( -\delta c_2 \frac{c_3}{c_2} + \delta c_1 \frac{1}{c_2} \right)
+ \frac{1}{2} z^2 \left( \delta c_2 \left[ -6 \frac{c_3}{c_2} + 6 \frac{c_3 c_4}{c_2} - \frac{c_5}{c_2} \right] + \delta c_3 \left[ \frac{9 c_3}{2 c_2} - \frac{2 c_4}{c_2} \right] + \delta c_4 \left[ - \frac{2 c_4}{c_2} \right] + \delta c_5 \left[ \frac{1}{2 c_2} \right] \right)
+ O(z^3) ,
\]
\[
\delta^V \beta^2(z) = z \delta c_2
+ \frac{1}{2} z^2 \left( \delta c_2 \left[ -2 \frac{c_3}{c_2} + \frac{c_4}{c_2} \right] + \delta c_3 \left[ - \frac{2 c_3}{c_2} + \delta c_4 \left[ \frac{1}{c_2} \right] \right] \right)
+ \frac{1}{6} z^3 \left( \delta c_2 \left[ \frac{30}{2} \frac{c_3}{c_2} - 4 \frac{c_4}{c_2} + \frac{6 c_3 c_4}{c_2} - \frac{c_5}{c_2} \right] + \delta c_3 \left[ -4 \frac{c_3}{c_2} + 21 \frac{c_3 c_4}{c_2} - 3 \frac{c_5}{c_2} \right] \right)
+ \delta c_4 \left[ \frac{21}{2} \frac{c_3}{c_2} - 4 \frac{c_4}{c_2} \right] + \delta c_5 \left[ - \frac{3 c_3}{c_2} + \delta c_6 \left[ \frac{1}{2 c_2} \right] \right]
+ O(z^4) .
\]

Lastly we report some similar results to the above for the excited state gap, which was first found at the level of the first order plaquette expansion in Ref [12], and has been generalised in Ref. [13]. The connected moments for the excited (triplet) state \( c_n^I N \) are related to the ground (singlet) state cumulants \( c_n^S N \) by
\[
c_n^P N = c_n^S N + \delta^S c_n .
\]
One can define shifted Lanczos coefficients by
\[
\delta^G \alpha(z) = \lim_{n,N \to \infty} N \left\{ \alpha_n^P(N) - \alpha_n^S(N) \right\}
\]
\[
\delta^G \beta^2(z) = \lim_{n,N \to \infty} N \left\{ [\beta_n^P(N)]^2 - [\beta_n^S(N)]^2 \right\} ,
\]
\[
.\]
\[
.\]
and there is an analogous exact result for the triplet gap

$$g = m(z)|_{z = z},$$

(19)

where the gap function $m(z)$ is defined as

$$m(z) = \delta^G \alpha(z) - \frac{\delta^G \beta^2(z)}{\beta(z) .}

(20)

The shifted cumulants $\delta^G c_n$ can be found from the equivalent $t$-expansion function $R(t)$ via

$$\log R(t) \equiv \log \frac{\langle \psi_P^0 | e^{-tH} | \psi_P^0 \rangle}{\langle \psi_S^0 | e^{-tH} | \psi_S^0 \rangle} = \sum_{n=1}^{\infty} \frac{(-t)^n}{n!} \delta c_n .

(21)

III. APPLICATION TO THE 2D XXZ HEISENBERG MODEL

We apply the plaquette expansion formalism to the $s = 1/2$ anisotropic antiferromagnetic Heisenberg Model on a square lattice, with the usual Hamiltonian

$$H = \sum_{\langle i,j \rangle} \left[ S_x^i S_x^j + x (S_y^i S_y^j + S_z^i S_z^j) \right],

(22)

where $x = 0$ denotes the Ising Model and $x = 1$ the isotropic antiferromagnetic Heisenberg Model. For the trial ground state we take the “natural” and commonly employed choice of the eigenstate to $x = 0$ problem, the classical Neel state, and for the excited triplet trial state a state with one spin of the Neel state flipped. We have used the cumulants $I_n$ and $R_n$ in Ref. [8], and generated a new set of staggered magnetisation cumulants to an order equivalent to that used in the above reference. From these we have generated the Lanczos coefficients and the staggered magnetisation Lanczos coefficients up to 7th order, and the triplet gap Lanczos coefficients up to 5th order. All new cumulants and the Lanczos coefficients are displayed in the Appendix.

Using these cumulants the ground state energy density $\gamma_0$, the staggered magnetisation $M$ and triplet gap $G$ have been computed for a set of anisotropy parameters and for all truncation orders up to the maximum, by evaluation at the minima of $e(z)$. This is the simplest way of analysing the plaquette expansion and is free from any biasing and assumptions, so it is the preferred option. Given more understanding of the convergence properties of the plaquette expansion a more sophisticated analysis or extrapolation strategy may be employed, and we refer the reader to Ref [11] for a discussion of this issue. The results for the ground state energy density, the staggered magnetisation and the excited state gap are displayed in Table I, Table II, and Table III respectively. Depending on the order and anisotropy parameter, the minima in the ground state energy function $e(z)$, could be complex, usually close to the positive real axis, however. In these cases we took the real part of the function computed at the complex minima, and these are marked with a asterix(*). To treat the case of no real minima properly some form of extrapolation would be needed but we do not pursue this issue here for several reasons. Firstly, a real minima exists for all the data at the highest order ($r = 7$), which is the most important, at least for the ground state energy and magnetisation. Secondly there is some continuity at a given order, between the data where a real minima exists and that data where it is complex. As the anisotropy parameter varies through these regions the minima shifts off slightly from the real axis but nonetheless remains close. There is also a second number appended to each data entry of the tables, and that is the difference between that value computed using the natural ordering and the supplemented ordering. This is the most unbiased estimate we have for indicating the systematic error in our expansion although there are no rigorous results to say that this difference somehow bounds the error - it is at best semi-quantitative.

The plaquette expansion results display two trends - one where as the truncation order increases we find substantial and systematic improvement in the averages, at least over the region where a real minima exists, and another as the anisotropy parameter increases from zero, where we find rapidly increasing errors, although the extent of this is dependent on the particular quantity. The ground state energy density is the most accurate, then the staggered magnetisation, and the triplet gap is the worst.
IV. COMPARISON OF THE METHODS

Taking the highest order plaquette expansion results, we have tabulated these against the other methods in Table IV, Table V and Table VI.

For the ground state energy one can see clear trends in the comparison:

- for $x < 0.5$ the $t$-expansion and CMX are slightly better than the plaquette expansion although the actual differences between them and with the series results are very small,

- for $x = 0.8$ the plaquette expansion is better than the $t$-expansion and the CMX, while for $x = 0.9$ the $t$-expansion is a slight improvement over the plaquette expansion,

- and for $x > 0.95$ the plaquette expansion is clearly better than the $t$-expansion, the CMX and 3rd order spin-wave theory, and especially so at $x = 1$.

For the staggered magnetisation one observes the following trends -

- for $x = 0.5$ the plaquette expansion is better than the $t$-expansion and the CMX,

- for $x = 0.8$ this ordering has reversed with the $t$-expansion superior to the plaquette expansion and the CMX, while for $x = 0.9$ the order gets reversed once more, and the plaquette expansion is a slight improvement over the $t$-expansion,

- and for $x \rightarrow 1.0$ the plaquette expansion stabilises on a higher value than that given by the $t$-expansion, 3rd order spin-wave theory, and the series expansion, although remaining less than the CMX result.

And for the triplet gap one finds that all moment methods give a rather high nonzero value at the isotropic point, whereas its vanishing for the spin-wave theory and series expansion is built-in. We would like to emphasise that for $x \geq 0.9$ there was no real minima at the highest order that applied in the plaquette expansion, and consequently the estimated errors grossly underestimate the true error. The trends here are -

- for $x = 0.2 \rightarrow 0.5$ the $t$-expansion is better than the CMX and the plaquette expansion,

- for $x = 0.8 \rightarrow 0.9$ the $t$-expansion is still superior to the plaquette expansion although it, in turn is better than the CMX,

- and for $x > 0.95$ the plaquette expansion is slightly better than the other moment methods but all have errors which swamp the actual values.

Finally we compare these results with the coupled-cluster results at the isotropic point. The results given in Table IV and Table V are the extrapolated results based on the first few orders of the approximation, and differ significantly from the highest order results. Both recent extrapolated ground state energies are better than either the $t$-expansion or the CMX and comparable in accuracy to the plaquette expansion energy. The extrapolated staggered magnetisations are also very close to that predicted by the plaquette expansion, probably higher than the true value.

The relatively poor performance of the $t$-expansion arises from a number of reasons. Firstly the extrapolation $t \rightarrow \infty$ is done without any knowledge of the global analytic properties of $E(t)$, and it is widely known in extrapolation work that this is perhaps the largest single source of poor convergence and inaccuracies. In contrast there is no extrapolation problem in the plaquette expansion, so long as a real minima exists. If this is not the case then some form of extrapolation of the kind employed in Ref [11] may be necessary here.

Another source of mediocre performance, and this is shared with the plaquette expansion, is the rather poor quality of trial state. The classical Neel state is usually chosen because it is simple and relatively straightforward to generate moments with, but a trial state which can generate the correct singularity structure at the isotropic point may give better results even though fewer moments may be found from it.

In summary we found good quantitative predictions from the plaquette expansion for this model but, as expected, the worst results occured near the isotropy point where a first order transition to a gapless state is expected. The plaquette expansion was clearly better at predicting the ground state energy than the other moment methods, had a slighter higher staggered magnetisation than the others, and all of the methods gave a nonzero gap at the isotropic point. We would like to emphasise that many aspects of the moment methods are still poorly understood, and that considerable scope exists for improving their accuracy.

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V. APPENDIX

Using efficient graph enumeration and calculation of the embedding constants Ref. [8], [16] we have the shift in the staggered magnetisation cumulants

\[
\begin{align*}
\delta^M_{c1} &= 1/2 \\
\delta^M_{c2} &= 0 \\
\delta^M_{c3} &= -x^2 \\
\delta^M_{c4} &= -6 x^2 \\
\delta^M_{c5} &= 10 x^4 - 27 x^2 \\
\delta^M_{c6} &= 231 x^4 - 108 x^2 \\
\delta^M_{c7} &= -266 x^6 + 3153 x^4 - 405 x^2 \\
\delta^M_{c8} &= -13382 x^6 + 33494 x^4 - 1458 x^2 \\
\delta^M_{c9} &= 12953 x^8 - 374132 x^6 + 307212 x^4 - 5103 x^2 \\
\delta^M_{c10} &= 1153345 x^8 - 7722995 x^6 + 2562205 x^4 - 17496 x^2 \\
\delta^M_{c11} &= -\frac{3998639 x^{10}}{4} + \frac{109952063 x^8}{2} - \frac{131870963 x^6}{2} + \frac{20015055 x^4}{4} - \frac{59049 x^2}{2} \\
\delta^M_{c12} &= -\frac{559451229 x^{10}}{4} + \frac{3755433743 x^8}{2} - \frac{1977566959 x^6}{2} + \frac{149166828 x^4}{4} - \frac{196830 x^2}{2} \\
\delta^M_{c13} &= \frac{446772107 x^{12}}{4} - \frac{2044508149 x^{10}}{2} + \frac{10343721579 x^8}{2} \\
&\quad -27001597819 x^6 + 1073575434 x^4 - 649539 x^2 \\
\delta^M_{c14} &= \frac{182477940639 x^{12}}{8} - \frac{2097642068485 x^{10}}{4} + \frac{2447876418449 x^8}{2} \\
&\quad -34365837438 x^6 + 7524115139 x^4 - 2125764 x^2 \\
\delta^M_{c15} &= -\frac{6855641551 x^{14}}{4} + \frac{4764540794257 x^{12}}{2} - \frac{170554817150787 x^{10}}{8} \\
&\quad +25875363869594 x^8 - 4143420881204 x^6 + 51653871357 x^4 - 6908733 x^2 \tag{23}
\end{align*}
\]

and using the excited state coefficients from Ref. [8] we have the shift in the excited state cumulants

\[
\begin{align*}
\delta^G_{c1} &= 2 \\
\delta^G_{c2} &= 2 x^2 \\
\delta^G_{c3} &= 0 \\
\delta^G_{c4} &= -8 x^4 - 12 x^2 \\
\delta^G_{c5} &= -46 x^4 - 60 x^2 \\
\delta^G_{c6} &= 209 x^6 + 115 x^4 - 228 x^2 \\
\delta^G_{c7} &= 3962 x^6 + 4798 x^4 - 780 x^2 \\
\delta^G_{c8} &= -\frac{40123 x^8}{4} + \frac{132689 x^6}{4} + 59703 x^4 - 2532 x^2 \\
\delta^G_{c9} &= -\frac{795907 x^8}{2} - \frac{204405 x^6}{2} + 558754 x^4 - 7980 x^2 \\
\delta^G_{c10} &= \frac{3252469 x^{10}}{4} - \frac{33276617 x^8}{4} - 9011003 x^6 + 4548463 x^4 - 24708 x^2 \\
\delta^G_{c11} &= \frac{109203791 x^{10}}{2} - \frac{193681633 x^8}{2} - \frac{394547565 x^6}{2} \\
&\quad +34055630 x^4 - 75660 x^2 \\
\delta^G_{c12} &= -88838574 x^{12} + 754813809 x^{10} + 5952720589 x^8 + 3261131208 x^6 \\
&\quad -4001975480 x^4 + 83156352 x^2 - 4096 \tag{24}
\end{align*}
\]

The expansion for the Lanczos coefficients are given exactly [17], [18] up to their truncation order by
\[ \alpha(z) = -1/2 \]
\[ + 3 z \]
\[ - \frac{11 z^2}{2} \]
\[ + \left( \frac{89}{18} \frac{68}{9 x^2} \right) z^3 \]
\[ + \left( \frac{167}{72} + 397 \frac{298}{9 x^2} \right) z^4 \]
\[ + \left( \frac{45967}{1200} + 14257 \frac{58376}{225 x^4} + 9784 \frac{9784}{45 x^6} \right) z^5 \]
\[ + \left( \frac{2668781}{10800} + 19041737 \frac{704387}{21600 x^2} + 5758538 \frac{5758538}{2025 x^6} + 144088 \frac{144088}{81 x^8} \right) z^6 \]
\[ + \left( \frac{40546957}{52920} + 10673263429 \frac{2863042529}{12700800 x^4} + 352800 x^4 \right) \frac{234213799}{99225} x^6 + 14449160 \frac{14449160}{441 x^8} - 1356032 \frac{1356032}{81 x^{10}} \right) z^7 \]

and

\[ \beta^2(z) = + \frac{x^2 z}{2} \]
\[ - \frac{5 x^2 z^2}{4} \]
\[ + \left( \frac{5}{2} + \frac{7 x^2}{6} \right) z^3 \]
\[ + \left( \frac{29}{6} + 137 \frac{26}{72} \frac{3 x^2}{3 x^2} \right) z^4 \]
\[ + \left( \frac{422}{45} + \frac{565 x^2}{288} - \frac{1613}{30 x^2} - \frac{254}{5 x^4} \right) z^5 \]
\[ + \left( \frac{2961379}{21600} - \frac{361171 x^2}{57600} - \frac{160703}{2160 x^2} - \frac{388447}{675 x^4} + \frac{3496}{9 x^6} \right) z^6 \]
\[ + \left( \frac{1465471213}{3628800} - \frac{18027853 x^2}{362880} - \frac{3540413}{2100 x^2} \right) \frac{31161547}{113400} x^4 - \frac{91790458}{14175 x^6} + \frac{94360}{27 x^8} \right) z^7 \]

The expansion for the change in the Lanczos coefficients corresponding to the staggered magnetisation is given by

\[ \delta^{SM} \alpha(z) = 1/2 \]
\[ - 2 z \]
\[ + \left( \frac{19}{9} + \frac{10}{3 x^2} \right) z^3 \]
\[ + \left( \frac{23}{2} + \frac{376}{9 x^2} + \frac{46}{x^4} \right) z^4 \]
\[ + \left( \frac{32653}{900} + \frac{43007}{900 x^2} + \frac{20827}{75 x^4} + \frac{40064}{75 x^6} \right) z^5 \]
\[ + \left( \frac{1852433}{64800} - \frac{37342427}{32400 x^2} - \frac{6621893}{2700 x^4} + \frac{991187}{2025 x^6} + \frac{286984}{45 x^8} \right) z^6 \]
\[ + \left( \frac{55919677}{127008} - \frac{21521839999}{2116800 x^2} - \frac{2231398105}{63504 x^4} - \frac{10777758037}{198450 x^6} \right) \frac{899068624}{33075 x^8} + \frac{75159136}{945 x^{10}} \right) z^7 \]

and

\[ \delta^{SM} \beta^2(z) = \left( \frac{64}{9} - \frac{68}{9 x^2} \right) z^4 \]
The expansion for the shift in the Lanczos coefficients describing the triplet energy gap is given by

\[ \delta^G \alpha(z) = +2 - 12z \]

\[ + \left( +34 - \frac{24}{x^2} \right) z^2 \]

\[ + \left( -\frac{388}{3} + \frac{4118}{9x^2} - \frac{448}{3x^4} \right) z^3 \]

\[ + \left( \frac{52681}{72} - \frac{77915}{24x^2} + \frac{44726}{9x^4} - \frac{3920}{3x^6} \right) z^4 \]

(29)

and

\[ \delta^G \beta^2(z) = +2x^2z \]

\[ + \left( -3x^2 + 6 \right) z^2 \]

\[ + \left( \frac{71x^2}{3} - \frac{239}{3} + \frac{32}{x^2} \right) z^3 \]

\[ + \left( -\frac{1943x^2}{72} + \frac{3929}{8} - \frac{5413}{6x^2} + \frac{784}{3x^4} \right) z^4 \]

\[ + \left( \frac{143947x^2}{720} - \frac{164471}{48} + \frac{710417}{72x^2} - \frac{481214}{45x^4} + \frac{7840}{3x^6} \right) z^5 \]

(30)

[1] D. Horn and M. Weinstein Phys. Rev. D30, (1984) 1256.
[2] J. Cioslowski Phys. Rev. Lett. 58, (1987) 83; Phys. Rev. A36, (1987) 374.
[3] R.F. Bishop and H. Kümml Phys. Today 40, (1987) 52.
[4] R.F. Bishop Theor. Chim. Acta 80, (1991) 95.
[5] L.C.L. Hollenberg, Phys. Rev. D47 (1993) 1640.
[6] N.S. Witte and L.C.L. Hollenberg, Z. Physik B 95 (1994) 531.
[7] L.C.L. Hollenberg and N.S. Witte, to appear in Phys. Rev. B.
[8] W.H. Zheng, J. Oitmaa and C.J. Hamer Phys. Rev. B52, (1995) 10278.
[9] L.C.L. Hollenberg, Phys. Lett. A 182 (1993) 238.
[10] M.J. Tomlinson and L.C.L. Hollenberg, Phys. Rev. B50 (1994) 1275.
[11] N.S. Witte and L.C.L. Hollenberg, submitted to J. Phys.: Condens. Matt.
[12] L.C.L. Hollenberg, M.P. Wilson and N.S. Witte, Phys. Lett. B 361 81.
[13] M. Beuchat, Honours Report, University of Melbourne (1993).
[14] L.C.L. Hollenberg and M.J. Tomlinson, Aust. J. Phys. 47 (1994) 137.
[15] N.S. Witte, J. MacIntosh and L.C.L. Hollenberg, in preparation.
[16] H.X. He, C.J. Hamer and J. Oitmaa J. Phys. A 23, (1990) 1775.
[17] G. Grigolini, G. Grosso, G. Pastori Parravicini, and M. Sparpaglione, Phys. Rev. B27 (1983) 7342.
[18] P. Giannoni, G. Grosso, and G. Pastori Parravicini G. Phys. Stat. Sol. (b) 128 (1985) 643.
[19] C.J. Hamer, W.H. Zheng, and P. Arndt, Phys. Rev. B46 (1992) 6276.
[20] W.H. Zheng, J. Oitmaa, and C.J. Hamer Phys. Rev. B43 (1991) 8321.
[21] F. Harris *Phys. Rev.* **B47** (1993) 7903.

[22] R.F. Bishop, R.G. Hale, and Y. Xian *Phys. Rev. Lett.* **73** (1994) 3157.
TABLE I. The ground state energy $\epsilon_0$ and estimated error for the 2D XXZ Model calculated using the plaquette expansion as a function of the anisotropy parameter $x$ and the order of truncation $r$. Those energies where one has the case of a real minima are unmarked, whereas those energies which are given by the real part evaluated at a complex minima are marked by a asterix.

| $\epsilon_0$ | $r = 2$ | 3 | 4 | 5 | 6 | 7 |
|--------------|--------|---|---|---|---|---|
| $x = 0.2$    | -0.50663(3) | -0.506661(2) | -0.5066639(5) | -0.5066646(2) | -0.50666494(8) | -0.50666508(4) |
| 0.5          | -0.540(1)   | -0.5415(1)   | -0.54159(2)   | -0.541617(6)  | -0.541627(3)   | -0.541631(1)   |
| 0.8          | -0.599(5)   | -0.605(1)    | -0.6068(2)    | -0.606975(6)  | -0.60697(2)    | -0.60693(2)    |
| 0.9          | -0.622(8)   | -0.633(2)    | -0.6363(3) *  | -0.63667(7) * | -0.6365(2) *   | -0.6360(1)     |
| 0.95         | -0.64(1)    | -0.648(4)    | -0.6526(2) *  | -0.65280(3) * | -0.653(1) *    | -0.6521(4)     |
| 0.98         | -0.64(1)    | -0.658(4)    | -0.6627(1) *  | -0.66276(2) * | -0.663(1) *    | -0.6622(5)     |
| 0.99         | -0.65(1)    | -0.661(5)    | -0.66604(9) * | -0.66613(4) * | -0.666(1) *    | -0.6657(6)     |
| 1.0          | -0.65(1)    | -0.664(5)    | -0.66945(7) * | -0.66952(7) * | -0.670(1) *    | -0.6691(6)     |
| $M$ | $r = 2$ | 3  | 4  | 5  | 6  | 7  |
|-----|--------|----|----|----|----|----|
| $x = 0.2$ | 0.49563(7) | 0.495543(8) | 0.4955293(8) | 0.4955281(4) | 0.4955275(2) | 0.4955275(2) |
| 0.5 | 0.475(2) | 0.4717(4) | 0.47112(8) | 0.47100(2) | 0.470960(9) | 0.470946(4) |
| 0.8 | 0.44(1) | 0.424(6) | 0.416(1) | 0.4143(4) | 0.4152(6) | 0.4162(4) |
| 0.9 | 0.43(2) | 0.40(2) | 0.373(5) * | 0.3794(4) * | 0.377(3) * | 0.383(3) |
| 0.95 | 0.43(2) | 0.39(3) | 0.367(4) * | 0.371(2) * | 0.37(1) * | 0.366(6) |
| 0.98 | 0.42(3) | 0.38(2) | 0.364(3) * | 0.367(3) * | 0.359(1) * | 0.358(5) |
| 0.99 | 0.42(3) | 0.37(2) | 0.363(3) * | 0.365(3) * | 0.35676(7) * | 0.355(5) |
| 1.0 | 0.42(3) | 0.37(2) | 0.362(3) * | 0.364(4) * | 0.355(4) * | 0.353(5) |
TABLE III. The excited state gap $\mathcal{G}$ and estimated error for the 2D XXZ Model calculated using the plaquette expansion as a function of the anisotropy parameter $x$ and the order of truncation $r$. Again those energies where one has the case of a real minima are unmarked, whereas those energies which are given by the real part evaluated at a complex minima are marked by a asterix.

| $x$ | $r = 2$ | 3     | 4     | 5     |
|-----|--------|-------|-------|-------|
| 0.2 | 1.943(4) | 1.938(1) | 1.936(5) | 1.936 |
| 0.5 | 1.67(4)  | 1.617(7) | 1.607(2) | 1.603 |
| 0.8 | 1.2(1)   | 1.03(5)  | 0.962(9) | 0.953 |
| 0.9 | 1.1(2)   | 0.8(2)   | 0.56(5) * | 0.61 * |
| 0.95| 1.0(2)   | 0.6(2)   | 0.47(3) * | 0.51 * |
| 0.98| 1.0(2)   | 0.5(2)   | 0.42(3) * | 0.45 * |
| 0.99| 1.0(3)   | 0.5(1)   | 0.40(2) * | 0.42 * |
| 1.0 | 1.0(3)   | 0.5(1)   | 0.39(2) * | 0.40 * |
TABLE IV. Comparison of the most accurate plaquette expansion values for the ground state energy $\epsilon_0$ with those of the $t$-expansion, the connected moments expansion, spin-wave theory and series expansions, taken for various anisotropy parameters $x$.

| $x$  | $\epsilon_0$ plaquette expansion | $t$-expansion$^a$ | $t$-expansion$^b$ | CMX$^c$ | 3rd Order$^d$ series$^e$ coupled$^f$ |
|------|----------------------------------|-------------------|-------------------|--------|------------------------|-----------------|
| 0.2  | $-0.5066651(1)$                 | $-0.5066653$      | $-0.50666529$     | $-0.50657179$ | $-0.5066653$         |
| 0.5  | $-0.541631(1)$                  | $-0.541636(3)$    | $-0.54163641$     | $-0.5413803$  | $-0.5416371$         |
| 0.8  | $-0.60693(2)$                   | $-0.6067604$      | $-0.60677223$     | $-0.607376$  | $-0.60902(2)$        |
| 0.9  | $-0.6360(2)$                    | $-0.6353801$      | $-0.63537633$     | $-0.636654$  | $-0.635844(4)$       |
| 0.95 | $-0.6521(2)$                    | $-0.6510589$      | $-0.65101764$     | $-0.652718$  | $-0.65189(1)$        |
| 0.98 | $-0.6622(2)$                    | $-0.6609228$      | $-0.66083842$     | $-0.66287$   | $-0.66211(2)$        |
| 0.99 | $-0.6656(3)$                    | $-0.6651(6)$      | $-0.66418527$     | $-0.66637$   | $-0.66563(6)$        |
| 1.0  | $-0.6691(3)$                    | $-0.668(1)$       | $-0.6676946$      | $-0.669993$  | $-0.6693(1)$         | $-0.6691(3)$    |

$^a$Reference [8]  
$^b$Reference [8]  
$^c$Reference [8]  
$^d$Reference [19]  
$^e$Reference [20]  
$^f$Reference [21], [22]

TABLE V. Comparison of the most accurate plaquette expansion values for the staggered magnetisation $\mathcal{M}$ with those of the $t$-expansion, the connected moments expansion, spin-wave theory and series expansions, taken for various anisotropy parameters $x$.

| $x$  | $\mathcal{M}$ plaquette expansion | $t$-expansion$^a$ | CMX$^b$ | 3rd Order$^c$ series$^d$ coupled$^e$ |
|------|-----------------------------------|-------------------|--------|------------------------|----------------|
| 0.2  | $0.4955275(2)$                    | $0.495527(1)$     | $0.4955269$ | $0.49573699$ | $0.4955265$ |
| 0.5  | $0.470946(4)$                     | $0.4710(4)$       | $0.47097192$ | $0.47172243$ | $0.4709287$ |
| 0.8  | $0.4162(4)$                       | $0.4173(6)$       | $0.41727472$ | $0.416390$  | $0.416896(5)$ |
| 0.9  | $0.383(3)$                        | $0.386(4)$        | $0.39065099$ | $0.383864$  | $0.38553(2)$ |
| 0.95 | $0.365(3)$                        | $0.36(1)$         | $0.37519399$ | $0.3607157$ | $0.36266(6)$ |
| 0.98 | $0.357(3)$                        | $0.35(2)$         | $0.36517718$ | $0.340646$  | $0.3422(2)$ |
| 0.99 | $0.355(4)$                        | $0.34(2)$         | $0.36170935$ | $0.33068$   | $0.3319(4)$ |
| 1.0  | $0.353(5)$                        | $0.33(3)$         | $0.35817561$ | $0.3069$    | $0.307(1)$         | $0.35$          | $0.340(5)$ |

$^a$Reference [8]  
$^b$Reference [8]  
$^c$Reference [19]  
$^d$Reference [20]  
$^e$Reference [21], [22]
TABLE VI. Comparison of the most accurate plaquette expansion values for the excited state gap $\mathcal{G}$ with those of the $t$-expansion, the connected moments expansion, spin-wave theory and series expansions, taken for various anisotropy parameters $x$.

| $x$ | plaquette expansion | $t$-expansion* | CMX$^b$ | 3rd Order$^c$ | series$^d$ |
|-----|---------------------|----------------|--------|--------------|------------|
|     |                     | D Padé         |        | spin-wave    | expansion  |
| 0.2 | 1.9357(6)           | 1.9338(2)      | 1.93383753 | 1.942248     | 1.933815   |
| 0.5 | 1.603(3)            | 1.594(10)      | 1.59431537 | 1.629782     | 1.59736(4) |
| 0.8 | 0.953(9)            | 0.96(2)        | 0.99272985 | 0.98798172   | 0.970(3)   |
| 0.9 | 0.61(4)*            | 0.65(5)        | 0.74009985 | 0.65721412   | 0.66(1)    |
| 0.95| 0.50(3)*            | 0.52(10)       | 0.60488156 | 0.44092456   | 0.45(3)    |
| 0.98| 0.44(3)*            | 0.45(15)       | 0.52114736 | 0.26588297   | 0.26(6)    |
| 0.99| 0.42(5)*            | 0.4(2)         | 0.49280432 | 0.18381204   | 0.17(8)    |
| 1.0 | 0.40(5)*            | 0.3(3)         | 0.46424870 | 0.0          | 0.0(1)     |

*Reference [8]
$^b$Reference [8]
$^c$Reference [19]
$^d$Reference [20]