Renormalization of the Ising model in a transverse field

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The renormalization scheme recently proposed by White is applied to the Ising model in a transverse field. It is found that this scheme is a significant improvement over standard techniques as far as the computation of the ground state is concerned. It is shown that the errors in the ground state energy are the largest in the neighborhood of the phase transition. Thus, this method has no special virtue in predicting the location of the phase transition and its associated critical exponents.

I. INTRODUCTION

It is widely believed that the critical behavior of quantum systems at finite temperature does not differ in an essential way from that of corresponding classical systems. The phase transitions at zero temperature may demonstrate however a typical quantum character through the quantum fluctuations in the ground state. The determination of the nature of the ground state and its energy is a central point of the quantum many body problems and few methods exist which can handle strongly interacting systems. One of the techniques is the truncation method, introduced by Drell *et. al.*[1] for lattice systems and used by many authors to study spin and fermionic systems.[2,3] A comparison of the various approaches is made by Stella *et al.*[4]

This method employs an iterative and approximate construction of the low-lying states of the system. The lattice is divided into blocks of which the Hamiltonian is exactly diagonalized. By selecting a number of low-lying eigenstates of the block and projecting the full Hamiltonian on these eigenstates, an effective or renormalized Hamiltonian is constructed for the blocks as new units. By repeating the operation the ground state is formed in a hierarchical way and its energy calculated iteratively by accumulating the energies of the blocks. Since the method constructs an approximate wave function for the whole system, the ground state energy so found is necessarily bounded from below by the exact one. The accuracy of the method is determined by the number of states retained in the calculation.

It is intuitively clear that the determination is particularly subtle in the neighborhood of a continous phase transition where generally large fluctuations are expected. The advantage of the renormalization scheme is that it can handle such fluctuations in principle. It remains to be seen whether a specific scheme does do it indeed adequately.

The quality of the procedure has been usually judged on its accuracy in the analysis of a phase transition. A system to which the method has been applied particularly succesfully is the Ising model in a transverse field (ITF).[2,3] However, Inglói[5] has recently argued that the success for the ITF is accidental and that in general the truncation method mixes bulk and surface properties in an unacceptable way. Moreover, if we consider the accuracy of the energy, the situation is definitely poorer. For the ITF we find an energy larger than the exact one by up to 7%. Although modifications have been proposed[6], the results for other systems (especially fermionic ones) are usually even more discouraging. It is also important that energies do not seem to be improved by any reasonable increase in the number of states kept. For example Bray and Chui[7] have calculated the energies of the lowest few levels in the Hubbard $d = 1$ model and their results were off by 5–10 % for a 16-site chain in spite of the fact that around 1000 states were kept. It strongly suggests that the true reason for the problems lies elsewhere.

In a series of recent papers White[8] has criticized the standard technique and proposed a scheme that indeed for the Heisenberg spin chain gives amazingly accurate answers for the energy. He argues that the shortcoming of the standard truncation method is due to the boundary conditions imposed on the block states by ignoring the interactions with the surrounding. The idea is to embed the block in a superblock of which the lowest state is determined. Then from this state the density matrix for the block is constructed. The eigenvalues of the density matrix determine the importance of the corresponding states for the truncation.

As a test of this method we apply it in this paper to the ITF, because this model shows a continous phase transition and it is a sensitive probe in situations with large fluctuations. The main results concern the $d = 1$ case where a comparison with the exact result is possible and where also the ideal superblock (the infinite system) can be handled. In Sec. II we collect the relevant information of the exact solution. In Sec. III we give the results for various truncations in $d = 1$, and in Sec. IV we extend the calculation to the $d = 2$ ITF. In Sec. V we comment on the problem of optimization of a renormalization scheme with a given number of states kept and show that neither of the proposed methods is optimal. The paper ends with a conclusion on the trends of the results.

II. THE EXACT SOLUTION OF THE $d = 1$ ITF

In one dimension the ITF is represented by the Hamiltonian

$$\mathcal{H} = -J \sum_i S_i^x S_{i+1}^x - h \sum_i S_i^z, \tag{1}$$

where the operators S_i^x and S_i^z defined on sites of a chain are spin 1/2 operators represented by Pauli matrices. It has been exactly solved by Pfeuty[9] and up to now this represents one of the most relevant exact solutions for quantum phase transitions. To facilitate the following consideration, we recall the main facts.

For a zero field the system goes to the doubly degenerate Ising-like ground state. For a strong field, the system reduces to a set of noninteracting sites, which leads to a singlet ground state. It shows that the ITF should exhibit a transition for a finite ratio h/J. To demonstrate this exactly, we first make the transformation

$$S_i^x = b_i^\dagger + b_i, \quad S_i^z = 2b_i^\dagger b_i - 1, \tag{2}$$

which produces a so-called *hard-core* boson representation (at a site b_i behaves as a fermion).

$$\mathcal{H} = Nh - J \sum_i (b_i^\dagger + b_i)(b_{i+1}^\dagger + b_{i+1}) - 2h \sum_i b_i^\dagger b_i, \tag{3}$$

where N is a number of sites. Next, using the Wigner-Jordan transformation[10]

$$b_i = \exp\left[-i\pi \sum_l^{i-1} c_l^\dagger c_l\right] c_i, \quad b_i^\dagger = c_i^\dagger \exp\left[i\pi \sum_l^{i-1} c_l^\dagger c_l\right], \tag{4}$$

we go over to a quadratic form in the Fermi operators c_i. Neclecting for $N \to \infty$ the boundary term we obtain

$$\mathcal{H} = Nh - J \sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i) - 2h \sum_i c_i^\dagger c_i. \tag{5}$$

It is worth remembering that such a transformation is possible due to the fact, that we have a one-dimensional system with only nearst-neighbor interactions. To diagonalize the Hamiltonian we carry out the Bogoliubov canonical transformation with k numbering the elementary plane waves:

$$c_j = \sum_k [A_k \eta_k e^{ikr_j} - iB_k \eta_k^\dagger e^{-ikr_j}], \tag{6}$$

with

$$|A_k|^2 = \frac{1}{2N}\left(1 - \frac{x + \cos k}{\lambda(k)}\right), \quad |B_k|^2 = \frac{1}{2N}\left(1 + \frac{x + \cos k}{\lambda(k)}\right), \tag{7}$$

where $\lambda(k) = \sqrt{1 + 2x\cos k + x^2}$ and $x = h/J$. In this way we have obtained a system of noninteracting fermions:

$$\mathcal{H} = E_0 + 2J \sum_k \lambda(k) \eta_k^\dagger \eta_k, \tag{8}$$

with the ground state defined as $\eta_k|\mathbf{0}\rangle = 0$. The ground-state free energy has the form

$$\epsilon_0 \equiv -E_0/NJ = \frac{2(1+x)}{\pi} \mathcal{E}\left(\frac{4x}{(1+x)^2}\right), \tag{9}$$

where the symbol $\mathcal{E}$ means the elliptic integral of second order.[11] Pfeuty has shown that the phase transition appears for $x = 1$.

III. THE $d = 1$ ITF

Let us assume that we know the state of the entire lattice, for example, the ground state $|\psi_0\rangle$. In practice, it will be a state of a superblock. If we want to generate a set of states for a part of the lattice, which are especially appropriate to represent its properties for the whole lattice, we can use the density matrix.[12] Suppose that $|i\rangle$ is a complete set of states of a block and $|j\rangle$ are the states of the rest of the lattice. Then we can write $|\psi_0\rangle = \sum_{i,j} \psi_{ij} |i\rangle |j\rangle$, where for simplicity we assume that the coefficients ψ_{ij} are real. The density matrix is defined as

$$\rho_{mn} \equiv \sum_j \psi_{mj} \psi_{nj}. \tag{10}$$

As White has argued, the eigenvectors of ρ_{mn} with the largest eigenvalues are the optimal states to keep in the truncation method.

For the $d = 1$ ITF, let us first consider the case with keeping two states. The advantage is that the Hamiltonian can be again written as a spin Hamiltonian at each iteration (see Ref. 3 and also our discussion in Sec. V). It is obvious that building a suitable superblock we should add spins symmetrically with regard to the block. However, if we choose periodic boundary conditions for the superblock, this will not be important. We have also checked that the results for open boundary condition (with symmetrical positions) are qualitatively the same as for the periodic one and converge to the same values when the size of superblock goes to infinity. In the Appendix we calculate the form for the density matrix based on the exact solution, considering the whole lattice as superblock.

For each superblock we have found a finite value of x_c, where the system undergoes a phase transition. As we can see in Table I, the suggestion by White does not yield an accurate critical point ($x_c = 1$). We always obtain a value worse than in the standard approach, although the increase of the superblock improves it slightly.

Next we present the energies in Table II. As the point of reference we have chosen the values for the exact energy, putting down only the differences for the other

TABLE I. The values of the critical point for different superblocks with two states.

Superblock	St. app.	3	4	7	8	∞
x_c	1.275	1.469	1.402	1.349	1.342	1.328

TABLE II. The energies for different superblocks with two states.

Energy	ϵ_0		$\Delta\epsilon_0 \times 10^{-6}$		
x	Exact	St. app.	3	7	∞
0	1	0	0	0	0
0.1	1.002502	2407	4	2	2
0.2	1.010025	8647	35	14	14
0.3	1.022630	16681	162	69	69
0.4	1.040417	24795	468	227	225
0.5	1.063544	32016	1049	598	585
0.6	1.092239	37837	2012	1378	1311
0.7	1.126829	42055	3522	2909	2667
0.8	1.167810	44815	5876	5732	5113
0.9	1.216001	46657	9666	10556	9559
1.0	1.273240	49218	16475	18776	19172
1.1	1.342864	55667	29355	32983	37120
1.2	1.419619	60613	42730	46813	49533
1.3	1.500823	61320	53527	56027	57620
1.4	1.585188	59427	59942	57409	57747
1.5	1.671926	57091	60428	55861	56040
1.6	1.760508	54694	58148	53870	53982
1.7	1.850559	52336	55611	51783	51856
1.8	1.941804	50156	53109	49729	49779
1.9	2.034035	48081	50733	47759	47794
2.0	2.127089	46140	48510	45892	45917
3.0	3.083929	32533	33535	32496	32498
5.0	5.050126	20296	20482	20291	20291
10.0	10.025016	10432	10455	10431	10431

TABLE IV. The energies for the superblocks with four and eight states.

$x/\Delta\epsilon_0 \times 10^{-6}$	St. app. (four states)	White's app. (four states)	White's app. (eight states)
0	0	0	0
0.1	1002	2	1
0.2	3779	6	1
0.3	7970	31	3
0.4	13234	98	3
0.5	19269	254	4
0.6	25773	569	13
0.7	32402	1151	29
0.8	38700	2153	22
0.9	43782	3663	67
1.0	42110	1804	356
1.1	38901	719	437
1.2	36379	391	222
1.3	34171	239	124
1.4	32208	157	74
1.5	30450	108	50
1.6	28869	76	29
1.7	27439	56	21
1.8	26141	42	14
1.9	24959	32	11
2.0	23877	25	11
3.0	16631	4	1
5.0	10332	1	$< 10^{-6}$
10.0	5304	$< 10^{-6}$	$< 10^{-6}$

cases. As we can see White's approach yields definitively better energies than the standard one. From a practical point of view, it is worth stressing that already the three-site superblock gives results close to the exact ones. On the other hand, from Tables I and II, we can also draw the conclusion that relatively far from the point of a phase transition, we always obtain a great improvement in the energy, as suggested by White. The bigger the superblock, the better its ground state approximates the ground state of a entire lattice and the better are the results. An opposite tendency exists around the critical value presumably due to the increase of the quantum fluctuations. In this point the number of states, important for the phase transition, increases rapidly. A larger superblock does not improve the energy, as we can see in Table II. However, we stress that this deficiency appears only in the neighborhood of the critical point.

To complete our calculations we present the values of the critical exponent ν, which describes the divergence of the correlation length around a critical point. Table III shows that also the critical exponent is somewhat better than for the standard approach. However, we notice that the tendency of the results is not monotonous for increasing superblock size. This is likely to be connected with a general deficiency of the method around the critical point.

White has found that the accuracy of the representation of the ground state increases roughly exponentially with the number of states kept. Table IV presents results (differences of the energy with respect to the exact values) with four and eight states retained, where the superblocks contain two or three additional sites as compared with a block. We also put the values of the energy with four states kept for the standard approach. Whereas the results for a standard approach demonstrate a weak progress, the superblock results become more rapidly accurate for a larger number of states. Comparing Tables II and IV we find that the smallest superblock (three sites) with two states kept gives better values for $x \leq 1.1$ than the standard approach case with four states. On the other hand always the worst accuracy is close to the critical point. It influences the localization of the critical points, as shown in Table V. The results for the standard approach are taken from Ref. 2.

TABLE III. The critical exponent ν for different superblocks with two states.

Superblock	Exact	St. app.	3	7	∞
ν	1	1.47	1.374	1.316	1.369

TABLE V. The localization of the critical point for four and eight states.

Method/ numb. st. kept	4	8
St. app.	0.936	0.995
White's app.	0.918	0.971

IV. THE $d = 2$ ITF

Now we extend our calculation to the two-dimensional ITF. The ideas and formalism as developed and applied to the one-dimensional case are the same. The calculations have been carried out for the triangular lattice with a three-site block. A six-site superblock was made of one block and three additional sites, which were situated symmetrically with respect to the edges.

As is well known,[13] at $T = 0$ the $d = 2$ ITF also exhibits a phase transition accompanied by a change of the ground state properties. The value of x_c is expected to depend strongly on the nature of the lattice, but the following approximation is reasonable:[14] $x_c \sim (z - 1)$, where z is the number of neighbors. Hence, for our case we have to expect the localization of the critical point close to 5. To examine the influence of boundary conditions, we considered open as well as periodic boundary conditions. Table VI presents also the values of the critical exponent ν. In the standard case our results for x_c and ν differ from those given by Hirsch and Mazenko,[15] although the formulas used are equivalent.

In view of the similarity of the trends in Table VI and the corresponding Table I and according to the approximation[14] we believe that again the density matrix approach gives worse results for the critical point than the standard one. Next, because any statistical mechanics system on a lattice in d dimensions can be considered as isomorphic to a quantum-mechanical[16] Hamiltonian system on a lattice in $d - 1$ dimensions, we can compare the value ν with the high-temperature expansion result for the $d = 3$ Ising model, where $\nu \simeq 0.625$.[17] We see a slight improvement of the critical exponent for White's approach but the results are poor. At the same time we confirm that the influence of boundary conditions is weak, and so we can reduce our calculations to the periodic case.

To supplement our remarks we present now results for the energy in Table VII. With lack of an exact solution the highest values are the best. They are closer to the exact solution which is an upper limit for them (including the minus sign in ϵ_0). We notice a great advantage of White's approach in the low x region. Moreover, the standard approach results have there a nonphysical minimum. From the perturbation expansion, we know that for $x \to 0$ the exact solution is $\epsilon_0 \simeq 3 + \frac{x^2}{12}$. So we see that White's approach does not give an optimal behavior, because the energy behaves as $\epsilon_0 \simeq 3 + \frac{x^2}{16}$. For x above the critical point the standard approach is slightly better than White's. In limit $x \to \infty$, where the exact expansion is $\epsilon_0 \simeq x + \frac{3}{4x}$, the both curves converge in the same incorrect way $\epsilon_0 \approx x + \frac{2}{7x}$. It is likely that these discrepancies (comparing with $d = 1$ case) will disappear when we take into account more states.

TABLE VI. The position of the critical point and the critical exponent ν for the six-site superblock ($d = 2$ ITF).

Case	St. app.	6 open	6 periodic
x_c	5.247	5.509	5.621
ν	1.547	1.482	1.432

TABLE VII. The energies for the $d = 2$ ITF.

x / ϵ_0	St. app.	White's app.
0	3	3
0.5	2.932473	3.015525
1.0	2.787654	3.059998
1.5	2.747374	3.124207
2.0	2.825550	3.206145
2.5	3.025046	3.340864
3.0	3.321545	3.549838
3.5	3.696838	3.835671
4.0	4.127254	4.195869
4.5	4.592847	4.616909
5.0	5.076715	5.080579
5.5	5.567187	5.566992
6.0	6.059976	6.059760
6.5	6.554235	6.554057
7.0	7.049532	7.049392
7.5	7.545600	7.545488
8.0	8.042259	8.042171
8.5	8.539382	8.539309
9.0	9.036877	9.036818
9.5	9.534675	9.534627
10.0	10.032724	10.032683
50.0	50.005986	50.005986
100.0	100.002963	100.002963

V. OPTIMIZATION OF THE TRUNCATION METHOD

As we mentioned in the Introduction the truncation method is based on an approximate wave function for the whole system. Thus the energy it yields is bound from below by the exact value as is also shown by the various approximations collected in Tables II and IV. So it is a natural question to ask whether one of these approximations is the best procedure conceivable for a given number of states kept in the truncation. We answer this question for the simplest case of keeping two states.

The Hamiltonian of the system has a simple invariance with respect to a simultaneous change in sign of S_i^x and S_i^y while keeping S_i^z invariant (such that the commutation relations are not affected) since $\mathcal{H}$ is even in S_i^x. The operator S_i^x flips a spin i and thus there exist two subspaces, which differ by one spin flip, and $\mathcal{H}$ has no matrix elements between the two subspaces. For a two-site block the states in the two subspaces can be written as

$$|\Uparrow\rangle = \frac{1}{\sqrt{1+q^2}}(|\uparrow\uparrow\rangle + q|\downarrow\downarrow\rangle),$$
$$|\Downarrow\rangle = \frac{1}{\sqrt{1+p^2}}(|\uparrow\downarrow\rangle + p|\downarrow\uparrow\rangle). \tag{11}$$

The two states building up the $|\Downarrow\rangle$ state are equivalent through particle exchange, and so we may set $p = 1$ and

we are left with one free parameter q. Indeed all approximations keeping two states can be characterized by a function $q(x)$. For example we have for the standard approach and the three-site superblock

$$q_{\text{St. app.}}(x) = (\sqrt{1+4x^2} - 2x),$$
$$q_3(x) = \frac{1 - 2x + 2\sqrt{1-x+x^2}}{3}. \tag{12}$$

So the problem boils down to finding the optimal $q(x)$. In terms of the states (11) the renormalization is so simple that we may write down the explicit formulas for arbitrary $q(x)$. The renormalization of x' reads

$$x' = 2x\left(\frac{1-q}{1+q}\right) - \left(\frac{1-q}{1+q}\right)^2, \tag{13}$$

and the recursive relation for the ground state energy $\epsilon_0 = -E_0/NJ$ becomes

$$\epsilon_0(x) = \frac{1}{2}\left(x\frac{1-q^2}{1+q^2} + \frac{(1+q)^2}{2(1+q^2)}\right) + \frac{(1+q)^2}{4(1+q^2)}\epsilon_0(x'). \tag{14}$$

In the neighborhood of the fixed point $x = 0$ and $x = \infty$ the analysis of (13) is easy

$$q_{\text{opt}}(x) \simeq 1 - x, \quad \epsilon_{\text{opt}}(x) \simeq 1 + \frac{x^2}{4}, \quad \text{for } x \to 0, \tag{15}$$

$$q_{\text{opt}}(x) \simeq \frac{1}{4x}, \quad \epsilon_{\text{opt}}(x) \simeq x + \frac{1}{7x}, \quad \text{for } x \to \infty. \tag{16}$$

From (12) one sees that $q_3(x)$ indeed has the optimal behavior for $x \to 0$ and $x \to \infty$ and that the standard approach fails for $x \to 0$ but that it is optimal for $x \to \infty$. We note that $\epsilon_{\text{opt}}(x)$ as obtained from (14) disagrees already in the second term with the exact expansion $\epsilon_0(x) \simeq x + \frac{1}{4x}$.

We have not determined the optimal curve $q_{\text{opt}}(x)$ but restricted ourselves to an analysis arround the unstable fixed point which follows from variations of ϵ with respect to q. We find $q_{\text{opt}}(x_c) = 0.2065$ and the associate $x_c = 1.3717$. However, one cannot find an expansion of $q(x)$ around this fixed point which signals the fact that the optimal energy is generated by two branches of $q_{\text{opt}}(x)$, starting from $x = 0$ and $x = \infty$ as given by (15) and (16), which do not meet at the same intermediate point. The energies of the branches cross at a first order transition, a situation not uncommon for variational procedures.[18] This proves that neither of the renormalization schemes which have a continuous $q(x)$ is optimal as far as the energy is concerned.

VI. CONCLUSION

The origin of the shortcoming of the standard method is due to the fact that eigenstates of an isolated block are chosen to be the states kept. In this way all connections to neighboring blocks are neclected during the diagonalization. We have tested White's proposal for a model with a phase transition in the ground state (the $d = 1$ ITF) and have confirmed his statement about a greater accuracy of the energy. The accuracy increases rapidly when we keep more states in each renormalization step. The density matrix approach therefore may be expected to be useful for other models with a phase transition in spite of the errors around the position of the phase transition. In this region the quantum fluctuations are the strongest and one is not able to keep a sufficient number of states anyway. For this reason White's method has no special virtue in predicting the location of the phase transition and its associated critical exponents.

The methods involving a projection to a reduced number of states give an approximation to the energy which is bounded from below by the exact ground state energy. Thus a variational principle exists which may be exploited to improve a particular method. Optimalization of renormalization transformations with free parameters is however a cumbersome affair with unwanted side effects such as a first order transition. Therefore it does not seem profitable to spend much effort on optimization rather than inclusion of more states.

The proposed methods perform better in $d = 1$ than in $d > 1$. Already for $d = 2$ we see that, with a few number of states retained, the various procedures do not reach the perturbation results for low x or large x. The inclusion of more states is necessary for accurate results but the density matrix method is severely limited by computational problems connected with the size of the superblock.

Inclusion of more states presents also a serious problem for the renormalization analysis of a phase transition. As long as one is interested in energies one does not have to bother about the meaning of the matrices generated in the iteration process. From a renormalization viewpoint one would like to interpret each step in the process as a transition to a renormalized Hamiltonian. For two states retained one can simply adhere to a spin representation as we outlined in Sec. V. For more states one should analyze the steps in terms of basic operators associated with the more complicated degrees of freedom represented by the blocks. It is not difficult to locate a critical point x_c on the basis of the nature of the asymptotic block Hamiltonian.[2] It either corresponds to a doubly degenerate ground state (x small) or to a single ground state (x large) with x_c as a dividing point. But even for the case of four states kept, we could not interprete the iteration steps for $x = x_c$ as a flow to an instable fixed point. This may be due to an intrinsic shortcoming of truncation methods. In all cases some eigenstates are kept while others are disregarded. It may happen that an included state becomes degenerate with a disregarded state. As function of x a crossing of levels may occur at some high iteration step and consequently a branching to different asymptotic behavior. We have noticed this phenomenon in a few cases which prevented us from determining critical exponents from the eigenvalues of the linearized flow matrix.

The overall conclusion is that the employment of a den-

sity matrix of some superblock for the projection technique gives a substantial improvement of the ground state energy. The projection technique needs however further refinement in the neighborhood of a phase transition for a determination of the critical properties.

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APPENDIX

When we are going to consider the infinite superblock due to the exact solution, it is more convenient to use the Fermi operators c_i and occupation numbers operators n_i instead of formula (10). We present it for the case of two states. We have four states for a two-site block labeled by $(\uparrow\uparrow)$, $(\uparrow\downarrow)$, $(\downarrow\uparrow)$, $(\downarrow\downarrow)$ or 1, 2, 3, and 4. Because of the Hermiticity and parity symmetry of the Hamiltonian only five different elements of the density matrix ρ_{mn} are nonzero; $|\mathbf{0}\rangle$ is a true ground state of the $d = 1$ ITF:

$$\rho_{11} \equiv \langle \mathbf{0}|n_1 n_2|\mathbf{0}\rangle, \quad \rho_{44} \equiv \langle \mathbf{0}|(1-n_1)(1-n_2)|\mathbf{0}\rangle,$$

$$\rho_{41} = \rho_{14} \equiv \langle \mathbf{0}|c_1^\dagger c_2^\dagger|\mathbf{0}\rangle, \quad \rho_{32} = \rho_{23} \equiv \langle \mathbf{0}|c_1^\dagger c_2|\mathbf{0}\rangle,$$

$$\rho_{22} = \rho_{33} \equiv \langle \mathbf{0}|(1-n_1)n_2|\mathbf{0}\rangle, \quad \rho_{m,n} \equiv 0 \text{ otherwise.} \tag{A1}$$

These elements can be expressed as combinations of the elliptic integrals of first and second order, $\mathcal{K}$, $\mathcal{E}$ with $m = \frac{4x}{(1+x)^2}$,

$$L_1 = \frac{1}{2} + \frac{x-1}{2\pi x}\mathcal{K}(m) + \frac{1+x}{2\pi x}\mathcal{E}(m),$$

$$L_2 = -L_3 = \frac{x^2(1+3x^2) - (1+x^2)^2}{6\pi x^2(1+x)}\mathcal{K}(m) + \frac{(1+x)(1-2x^2)}{6\pi x^2}\mathcal{E}(m),$$

$$L_4 = \frac{1}{6\pi x^2}\left(\frac{4x^2 - (1+x^2)^2}{1+x}\mathcal{K}(m) + (1+x)(1+x^2)\mathcal{E}(m)\right).$$

Then we obtain

$$\rho_{11} = L_1^2 + L_2 L_3 + L_4^2, \quad \rho_{44} = (1-L_1)^2 + L_2 L_3 + L_4^2,$$

$$\rho_{14} = L_4, \quad \rho_{33} = L_1 - L_1^2 - L_2 L_3 - L_4^2, \quad \rho_{23} = L_3. \tag{A2}$$

It is also worth noticing that formulas (A1) could be extended to systems without an exact solution. In this case one may use, as $|\mathbf{0}\rangle$, the state coming from approximate theories such as, e.g., the mean field theory.

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