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# A configuration-space truncation scheme for the Heisenberg spin-1 model

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**Abstract.** A Monte Carlo sampling technique based on $2 \times 2$ rotations of the Heisenberg spin-1 Hamiltonian containing both anisotropic and next-nearest-neighbour (NNN) terms has been attempted. Closed rings of six, eight, 10 and 12 spin-1 sites have been studied and the ground and the first excited states have been obtained. The validity of the procedure has also been tested using the spin correlation function for the ground state.

## 1. Introduction

In recent years there have been extensive configuration interaction (CI) studies of medium-sized systems using model Hamiltonians. These studies generally involve diagonalization of large sparse matrices which can be chosen to be symmetric. Typical examples are the Hubbard $t$–$J$ model with first neighbour transfer terms [1–6] for electron systems and the anisotropic Heisenberg Hamiltonian with first- and second-neighbour transfer terms [7–10] for spin-1 systems. If we ignore both spin and point-group symmetry, the dimensionality of the configuration state function (CSF) increases rapidly with increasing number of particles. Though the Hamiltonian matrices are relatively easy to generate if we assume orthonormal site orbitals or spins, the diagonalization leads to difficulties even for a few lowest-lying states.

A way out of the above problem would be to use the Monte Carlo diagonalisation (MCD) procedures of sampling the CSF space [13–16]. In recent notes De Raedt and von der Linden [15, 16] suggested a sampling technique based on succesive $2 \times 2$ plane rotations to generate a good ground state. This method was found to be quite good and avoided some of the problems inherent in MCD techniques. The procedure is based on essentially starting with a reference state having the lowest-valued diagonal element (called the 1-1 element) and choosing as its partner a state which yields maximal reduction in the 1-1 element. The plane rotation which yields this reduction is noted and the Hamiltonian is modified using it. The next CSF in the link to the ground state is now the one which yields maximal reduction in the modified 1-1 element. This procedure continues until all off-diagonal elements in the reference row are below a certain preassigned level. The resulting 1-1 element is then a good approximation to the ground state. The procedure is straightforward to implement and can be readily programmed. One of the most time-consuming steps in this procedure is the need to generate the Hamiltonian matrix to locate the CSF which leads to maximum reduction in the 1-1 element.

In view of the above, we attempted to modify the approach to some extent to have fewer determinations of the Hamiltonian matrix elements. Instead of picking up the CSF which leads to a maximal reduction in the 1-1 element, we select any CSF which yields

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reduction of the 1-1 element below a preassigned value. A limited number of sweeps is done over CSF space to select a set of states contributing significantly to the ground state. The Davidson or Rettrup [17, 18] algorithm is then used over this selected subspace to find the few lowest states.

This procedure has been used in the present work to study the antiferromagnetic Heisenberg Hamiltonian with anistropic interaction and next-nearest-neighbour (NNN) interaction for the spin-1 system. The first two eigenenergies and the spin correlation functions have been calculated. It has been found that a severely truncated space chosen as in the present approach yields a reasonably good result. The procedure is outlined in section 2 and the results of studies on a number of systems are presented in section 3.

## 2. The procedure

Consider an orthonormal set of CSFs, $\{\psi_i \mid i = 1, \ldots, n\}$ spanning the Hilbert space of a many-body Hamiltonian. The matrix representation of the Hamiltonian over such a basis is symmetric and may be assumed to be real. If $n$ is sufficiently large, the diagonalization of the matrix could be a formidable problem even if only a few of the lowest states are to be obtained. Monte Carlo methods can be employed if the matrix is relatively sparse. One such method was recently proposed by De Raedt and von der Linden [15, 16] and successfully implemented in the diagonalization of the first neighbour Hubbard Hamiltonian for spin-$\frac{1}{2}$ systems. The results they reported were quite good. The only disadvantage in their method was the need to repeatedly generate the Hamiltonian matrix elements during sampling of the CSF space to chose the optimum path leading to a good ground state. So we consider a modification of the approach in the present paper which considerably minimizes the number of matrix element evaluations. Before outlining our modification, we summarize briefly the technique of De Raedt and von der Linden [15, 16]. Let

$$H_{ij} = \langle i|\mathbf{H}|j\rangle \tag{1}$$

be the elements of the Hamiltonian matrix over the CSFs. Let $\psi_{i_1}$, $\psi_{i_2}$ be two CSFs for which $H_{i_1i_1}$, $H_{i_2i_2}$ have the lowest and next lowest values ($H_{i_1i_1} \leqslant H_{i_2i_2}$) and $H_{i_1i_2} \neq 0$ amongst the set $\{H_{ij}|j = 1, \ldots, n\}$. Imposing the plane rotation matrix

$$R^{(1)}_{i_1i_1} = \cos\theta_1 \qquad R^{(1)}_{i_1i_2} = -R^{(1)}_{i_2i_1} = -\sin\theta_1 \qquad R^{(1)}_{i_2i_2} = \cos\theta_1 \qquad R^{(1)}_{i_ki_l} = \delta_{i_ki_l} \tag{2}$$

on the Hamiltonian as

$$\mathbf{H}^1 = R^{(1)}\mathbf{H}R^{(1)^{-1}} \tag{3}$$

the $H^{(1)}_{i_1i_2}$ element is equated to zero yielding a determination of $\theta_1$ through

$$\tan 2\theta_1 = \frac{2H_{i_1i_2}}{H_{i_1i_1} - H_{i_2i_2}}. \tag{4}$$

This enables $H^{(1)}_{i_1i_1}$ to be determined. A search is carried out over all possible $i_2$ such that the lowest value of this element ($H^{(1)}_{i_1i_1}$) results. Using this $\theta_1$ , $H^{(1)}_{i_1i_1}$ etc are determined. The procedure is repeated with the addition of $\psi_{i_3}$ ($i_3 \neq i_1, i_2$) and so on, till the full configuration space is exhausted. It is this search which is time consuming .

The basic elements occurring at the level of addition of $\psi_{i_k}$ in De Raedt and von der Linden [15, 16] procedure are

$$\tan 2\theta_k = \frac{2H_{i_1 i_{k+1}}^{(k-1)}}{H_{i_1 i_1}^{(k-1)} - H_{i_{k+1} i_{k+1}}^{(k-1)}} \tag{5}$$

$$H_{i_1 i_1}^{(k)} = H_{i_1 i_1}^{(k-1)} C_k^2 + 2H_{i_1 i_{k+1}}^{(k-1)} C_k S_k + H_{i_{k+1} i_{k+1}}^{(k-1)} S_k^2 \tag{6}$$

$$H_{i_1 i_{k+1}}^{(k)} = \left(H_{i_{k+1} i_{k+1}}^{(k-1)} - H_{i_1 i_1}^{(k-1)}\right) C_k S_k + H_{i_1 i_{k+1}}^{(k-1)} \left(C_k^2 - S_k^2\right) \tag{7}$$

$$H_{i_1 i_{k+2}}^{(k)} = H_{i_1 i_{k+2}}^{(k-1)} C_k + H_{i_{k+1} i_{k+2}}^{(k-1)} S_k \tag{8}$$

$$H_{i_{k+2} i_{k+2}}^{(k)} = H_{i_{k+2} i_{k+2}}^{(0)} \tag{9}$$

with

$$C_k = \cos\theta_k \qquad S_k = \sin\theta_k \qquad H_{ij}^0 = H_{ij}. \tag{10}$$

Starting with $k = 1$ the quantities in (5–10) are computed in the procedure due to De Raedt and von der Linden [15, 16] till all $n$ CSFs are exhausted. The criterion for picking up a CSF, $\psi_{i_k}$, is decided depending on a minimum prescribed limit for

$$\Delta = H_{i_1 i_1}^{(k)} - H_{i_1 i_1}^{(k-1)}. \tag{11}$$

In order to determine which $\psi_{k+1}$ at the $k$th level leads to a maximum lowering of $\Delta$ of (11) we need to compute all the three quantities on the right-hand side of (5) plus $H_{i_1 i_1}^{(k)}$, for all the residual $(n - k)$ CSFs.

In order to avoid this multiple evaluation of $H_{ij}$ we proceed as follows. Having chosen the starting pair $\psi_{i_1}$, $\psi_{i_2}$ we proceed to cover all the remaining $(n - 2)$ CSFs sequentially. At every stage, $k$, we determine $\theta_k$ and hence $|\Delta|$. We now vary $\theta_k$ over a small range of values and note the value for which $|\Delta|$ is maximum. If this maximum is less than a preassigned value we skip this and go to the next one. After all $n$ CSFs have been sampled, we repeat the procedure for a few more (at most 10) sweeps and collect all the CSFs contributing significantly to the ground state. In all sparse matrices, this procedure has been found to pick up about 30% of the full CSF space. Since the path chosen is not, now, optimal, the ground state energy is not very good, so we use the Rettrup or Davidson [17, 18] algorithm for sparse matrices over the subspace to obtain the ground state and a few low-lying excited states.

## 3. Applications and results

We have implemented the above scheme for two spin-1 systems, both being antiferromagnetic Heisenberg rings, one with the anisotropic term and the other with the next-nearest-neighbour (NNN) term. The spin-1 systems are of current interest since Haldane [7] conjectured the difference between the behaviour of spin-$\frac{1}{2}$ and spin-1 systems. The Heisenberg Hamiltonian with the anisotropic term

$$H_1 = \sum_i \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + (\lambda - 1) S_i^z \cdot S_{i+1}^z\right) \tag{12}$$

has been studied quite extensively. It is well established that an extended phase, which includes the isotropic point, with a gap in the spectrum and no magnetization exists for

**Table 1.** Ground- and first-excited-state eigenvalues for spin-1 rings of 6, 8, 10 and 12 sites in the $S = 0$ state at the Heisenberg point: $\lambda = 1.0$ and $\alpha = 0.0$.

| | Dimensionality | | Ground-state eigenvalue | | | First-excited-state eigenvalue | | |
|---|---|---|---|---|---|---|---|---|
| $N$ | Full | Truncated | Exact | Truncated | % error | Exact | Trunctated | % error |
| 6 | 141 | 141 | − 8.617 | − 8.617 | 0.00 | − 7.897 | − 7.897 | 0.00 |
| 8 | 1 107 | 884 | −11.337 | −11.330 | 0.06 | −10.743 | −10.742 | 0.01 |
| 10 | 8953 | 6085 | −14.094 | −14.090 | 0.03 | −13.569 | −13.568 | 0.01 |
| 12 | 73789 | 20586 | −16.870 | −16.800 | 0.41 | −16.385 | −16.369 | 0.10 |

**Table 2.** Spin correlation function $\rho_{zz} = \langle S_i^z S_j^z \rangle$ for spin-1 rings of 6, 8, 10 and 12 sites in $S = 0$ at the Heisenberg point: $\lambda = 1.0$ and $\alpha = 0.0$.

| | Dimensionality | | $zz$-correlation function $\rho_{zz}$ | | |
|---|---|---|---|---|---|
| $N$ | Full | Truncated | Exact | Truncated | % error |
| 6 | 141 | 141 | −0.286 | −0.286 | 0.00 |
| 8 | 1 107 | 884 | 0.216 | 0.219 | -1.39 |
| 10 | 8953 | 6085 | −0.182 | −0.183 | −0.55 |
| 12 | 73 789 | 20586 | 0.145 | 0.173 | −19.31 |

**Table 3.** Variation of the ground- and the first-excited-state eigenvalues with the variation of $\lambda$ for the anisotropic Hamiltonian with nearest neighbour (NN) interactions: $N = 12$, $S = 0$, full-space dimensionality = 73 789, truncated-space dimensionality = 20 586. $\lambda$ is the anisotropic parameter.

| | Ground-state eigenvalue | | | First-excited-state eigenvalue | | |
|---|---|---|---|---|---|---|
| $\lambda$ | Exact | Truncated | % error | Exact | Truncated | % error |
| 0.2 | −13.935 | −13.554 | 2.73 | −12.995 | −12.033 | 7.40 |
| 0.4 | −14.477 | −14.174 | 2.09 | −13.437 | −12.629 | 6.01 |
| 0.6 | −15.116 | −14.893 | 1.48 | −13.953 | −13.703 | 1.79 |
| 0.8 | −15.889 | −15.747 | 0.89 | −14.972 | −14.939 | 0.22 |
| 1.0 | −16.870 | −16.800 | 0.41 | −16.385 | −16.369 | 0.10 |
| 1.2 | −18.190 | −18.168 | 0.12 | −18.020 | −18.013 | 0.04 |
| 1.4 | −19.897 | −19.892 | 0.03 | −19.852 | −19.849 | 0.02 |
| 1.6 | −21.845 | −21.843 | 0.01 | −21.833 | −21.832 | 0.00 |
| 1.8 | −23.918 | −23.918 | 0.00 | −23.915 | −23.915 | 0.00 |
| 2.0 | −26.068 | −26.068 | 0.00 | −26.067 | −26.067 | 0.00 |

$\lambda \leqslant 1.18$ while for $\lambda > 1.18$ there exists a gapless phase with staggered magnetization. For the Heisenberg Hamiltonian with NNN interaction

$$H_2 = \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \alpha \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) \tag{13}$$

it has been found that there is a gap in the spectrum. With these Hamiltonians we calculate the eigenenergies and correlation functions and demonstrate that the energies of the few lowest states and the wavefunction of the ground state are reasonably good.

The CSFs spanning the Hilbert space $V_3{\otimes}^N$ are the tensor mononials,

$$V_3{\otimes}^N = \{(\phi_{j_1}^1 \phi_{j_2}^2 \ldots \phi_{j_N}^N) \mid j_k \in (1, 2, 3)\} \tag{14}$$

where $\phi_i$ are spin states of spin-1 particles. The matrices obtained are quite sparse.

**Table 4.** Variation of the ground- and the first-excited-state eigenvalues with the variation of $\alpha$ for the isotropic Hamiltonian with nearest- and next-nearest-neighbour (NN and NNN) interactions: $N = 12$, $S = 0$, full-space dimensionality = 73 789, truncated-space dimensionality = 20 586. $\alpha$ is the next-nearest-neighbour (NNN) parameter.

| | Ground-state eigenvalue | | | First-excited-state eigenvalue | | |
|---|---|---|---|---|---|---|
| $\alpha$ | Exact | Truncated | % error | Exact | Truncated | % error |
| 0.1 | −15.971 | −15.943 | 0.18 | −15.441 | −15.432 | 0.06 |
| 0.2 | −15.159 | −15.154 | 0.03 | −14.557 | −14.550 | 0.05 |
| 0.3 | −14.472 | −14.465 | 0.05 | −13.759 | −13.748 | 0.08 |
| 0.4 | −13.953 | −13.929 | 0.17 | −13.132 | −13.075 | 0.43 |
| 0.5 | −13.692 | −13.634 | 0.42 | −12.910 | −12.807 | 0.80 |
| 0.6 | −13.916 | −13.687 | 1.65 | −13.385 | −13.089 | 2.21 |
| 0.7 | −14.555 | −14.058 | 3.41 | −14.074 | −13.559 | 3.66 |
| 0.8 | −15.368 | −14.608 | 4.95 | −14.875 | −14.141 | 4.93 |
| 0.9 | −16.473 | −15.251 | 7.42 | −16.153 | −14.793 | 8.42 |
| 1.0 | −17.986 | −15.955 | 11.29 | −17.567 | −15.621 | 11.08 |

**Table 5.** Variation of the spin correlation function $\rho_{zz}$ with $\lambda$ for the anisotropic Hamiltonian with nearest-neighbour (NN) interactions: $N = 12$, $S = 0$, full-space dimensionality = 73 789, truncated-space dimensionality = 20 586. $\lambda$ is the anisotropic parameter.

| | zz-correlation function $\rho_{zz}$ | | |
|---|---|---|---|
| $\lambda$ | Exact | Truncated | % error |
| 0.2 | −0.006 | 0.000 | 100.00 |
| 0.4 | −0.004 | 0.002 | 150.00 |
| 0.6 | 0.003 | 0.012 | -300.00 |
| 0.8 | 0.033 | 0.049 | − 48.48 |
| 1.0 | 0.145 | 0.173 | − 19.31 |
| 1.2 | 0.415 | 0.434 | − 4.58 |
| 1.4 | 0.655 | 0.659 | − 0.61 |
| 1.6 | 0.772 | 0.773 | − 0.13 |
| 1.8 | 0.833 | 0.834 | − 0.12 |
| 2.0 | 0.871 | 0.871 | 0.00 |

**Table 6.** Variation of the spin-correlation function $\rho_{zz}$ with $\alpha$ for the isotropic Hamiltonian with nearest- and next-nearest-neighbour (NN and NNN) interactions: N= 12, $S = 0$ , full-space dimensionality = 73 789, truncated-space dimensionality = 20 586. $\alpha$ is the next-nearest-neighbour parameter.

| | zz-correlation function $\rho_{zz}$ | | |
|---|---|---|---|
| $\alpha$ | Exact | Truncated | % error |
| 0.1 | 0.105 | 0.113 | − 7.62 |
| 0.2 | 0.054 | 0.054 | 0.00 |
| 0.3 | 0.003 | 0.002 | 33.33 |
| 0.4 | −0.022 | −0.022 | 0.00 |
| 0.5 | 0.024 | 0.019 | 20.83 |
| 0.6 | 0.148 | 0.116 | 21.62 |
| 0.7 | 0.192 | 0.175 | 8.85 |
| 0.8 | 0.179 | 0.190 | − 6.15 |
| 0.9 | −0.073 | 0.186 | 354.79 |
| 1.0 | −0.197 | 0.173 | 187.82 |

The results are summarized in the following tables. For the anisotropic Hamiltonian, these calculations were done for $N = 6, 8, 10, 12$ and for $\lambda \in [0, 2]$. Calculations for the NNN Hamiltonian were done for $\alpha \in [0, 1]$. For all $N$, we have done the sampling at $\lambda = 1$ and $\alpha = 0$, that is at the Heisenberg point, and used the same truncated subspace to find the ground state and the excited state for the entire parameter domain. Table 1 lists the energies and percentage deviations for the Heisenberg Hamiltonian for different $N$ at $\lambda = 1$ and $\alpha = 0$. We observe that the ratio of the dimension of truncated space to the full dimension decreases with increasing $N$. For $N = 12$ only 28% of the total space is selected. In spite of such severe truncation the percentage errors in the energies do not increase very much. Table 2 shows the ground-state correlation functions at the Heisenberg point $\lambda = 1$ and $\alpha = 0$. The $zz$-correlation function $\rho_{zz}$ is defined as

$$\rho_{zz} = \langle S_i^z S_j^z \rangle. \tag{15}$$

These functions are very much sensitive to the quality of the wavefunction. Moreover, we notice that for $N = 12$ the truncated space correlation function value is about 80% of the full-space correlation function value. Table 3 and 4 show energies of the anisotropic and NNN Hamiltonians at different values of the respective parameters. For the anisotropic Hamiltonian the error is higher for small $\lambda$, since the sampling of CSFs was done at $\lambda = 1$. Similarly for the NNN Hamiltonian the error increases with increasing $\alpha$ because the sampling was done at $\alpha = 0$. In tables 5 and 6 we give the spin correlation functions for the anisotropic Hamiltonian (12) and the NNN Hamiltonian (13) respectively. In the case of the anisotropic Hamiltonian the the correlation functions improves down the table, a behaviour similar to that shown by the energy. In the case of the NNN Hamiltonian the correlation function more or less worsens as $\alpha$ increases, which is once again similar to the behaviour shown by the energy.

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## References

[1] Hubbard J 1963 *Proc. R. Soc.* A **276** 238; 1964 *Proc. R. Soc.* A **277** 237; 1964 *Proc. R. Soc.* A **281** 401
[2] Soos Z G and Ramasesha S 1984 *Phys. Rev.* B **29** 5410
[3] Shiba H and Pincus P 1972 *Phys. Rev.* B **5** 1966
Shiba H 1972 *Prog. Theor. Phys.* **48** 2171
[4] Mazumdar S and Soos Z G 1979 *Synth. Met.* **1** 77
[5] Ramasesha S and Soos Z G 1984 *Int. J. Quantum. Chem.***25** *1003*
[6] Callaway J, Chen D P, Kanhere D G and Qiming Li 1990 *Phys. Rev.* B **42** 465 (1990)
[7] Haldane F D M 1983 *Phys. Lett.* **93A** 464; 1983 *Phys. Rev. Lett.* **50** 1153
[8] Botet R and Jullien R 1983 *Phys. Rev.* B **27** 613
[9] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799
[10] Hatsugai Y and Kohmoto M 1991 *Phys. Rev.* B **44** 11 789
[11] Hirsch J E 1985 *Phys. Rev.* B **31** 4403
[12] Hirsch J E 1987 *Phys. Rev.* B **35** 1851
[13] Zhang Y and Callaway J 1989 *Phys. Rev.* B **39** 9397
[14] Hirsch J E, Scalapino D J, Sugar R L and Blankenbecler R 1982 *Phys. Rev.* B **26** 5033
[15] De Raedt H and von der Linden W 1992 *Phys. Rev.* B **45** 8787
[16] De Raedt H and von der Linden W 1992 *Int. J. Mod. Phys. C* **3** 97
[17] Davidson E R 1975 *J. Comput. Phys.* **17** 87
[18] Rettrup S 1982 *J. Comput. Phys.* **45** 100