Quantum Correlation Functions of 1-Dimensional Paramagnets

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ABSTRACT

We calculate hydrodynamic mode longitudinal and transverse spin correlation functions for polarized quantum one-dimensional lattices containing two, four, and eight spins using a Heisenberg nearest neighbor interaction. We also analyze the spectra of these systems.

INTRODUCTION

Recently, Cowan and Mullin[1] have used a moments method to study spin transport in polarized paramagnetic (high temperature) quantum crystals. Their analytic calculations of the diffusion coefficients have been qualitatively confirmed with numerical calculations of correlation functions on 1-d lattices with *classical* Heisenberg spin dynamics by Tang and Waugh[2] and Ragan et al.[3]. However, it is not clear whether the classical simulations are strictly comparable to the analytic quantum results. It is the goal of this paper to calculate the *quantum* correlation functions directly so that they can be compared to the classical results. Such calculations have been carried out for low temperature systems [4]. A severe limitation of the approach, however, is that the quantum calculation can only be carried out for small N systems.

Consider a one-dimensional lattice containing N spins. We can write the state vectors as a product of single spin states:

$$|\psi_n\rangle = \prod_{j=1}^{N} |S_j^z\rangle, \tag{1}$$

where $|\psi_n\rangle$ is one of the 2^N possible state vectors, and $|S_j^z\rangle$ equals $|\uparrow\rangle$ or $|\downarrow\rangle$. We can also represent these state vectors in binary notation[1], which is useful when generating the Hamiltonian and spin matrices.

Now, the Hamiltonian contains the Heisenberg exchange interaction and the interaction with the magnetic field.

$$\hat{H} = \hat{H}_{ex} + \hat{H}_b = -J\sum_{j,k} \hat{S}_j \cdot \hat{S}_k + b\sum_j \hat{S}_j^z$$

The solution to the Schrödinger equation is

$$\psi(t) = \psi(0)e^{-\frac{i}{\hbar}(\hat{H}_{ex}+\hat{H}_b)t}$$

We would like to simplify our calculations by transforming our solution to the Larmor frame. This will eliminate $\hat{H}_b$ from the solution, and the dynamics of the system will only depend on the exchange Hamiltonian. Our rotation operator is $\hat{R}(t) = e^{\frac{i}{\hbar}\hat{H}_b t}$ so we have,

$$\psi'(t) = \hat{R}(t)\psi(t) = e^{\frac{i}{\hbar}\hat{H}_b t}\psi(0)e^{-\frac{i}{\hbar}(\hat{H}_{ex}+\hat{H}_b)t} = \psi(0)e^{-\frac{i}{\hbar}\hat{H}_{ex} t}$$

[1] See the Appendix for an explaination.

We must now determine the exchange Hamiltonian matrix, $\hat{H}_{ex} = -\frac{J}{2}\sum_{j,k}\hat{S}_j \cdot \hat{S}_k$. (From here on we will drop the subscript.) To construct the Hamiltonian, we will rewrite the interaction in terms of the Pauli exchange operator[2].

$$\hat{S}_j \cdot \hat{S}_k = (2\hat{P}_{jk} - 1)$$

$$\hat{H} = -\frac{J}{2}\sum_{j,k}\hat{S}_j \cdot \hat{S}_k = -J\sum_{j,k}(\hat{P}_{jk} - \frac{1}{2})$$

The exchange operator, $\hat{P}_{jk}$ simply exchanges the spins of the for the j^{th} and k^{th} spins. We can illustrate this on the previous example for $|\psi_5\rangle = |\downarrow\uparrow\downarrow\uparrow\rangle$: if $\hat{P}_{23}$ is acting on $|\psi_5\rangle$, we have

$$\hat{P}_{23}|\downarrow\uparrow\downarrow\uparrow\rangle = |\downarrow\downarrow\uparrow\uparrow\rangle = |0011\rangle = |\psi_3\rangle$$

For the ground state, all spins are up. In addition, the ground state is a stationary state. In order to make the ground state have zero energy, we will add $J/2$ to each term in the Hamiltonian. We have

$$\hat{H} = -J\sum_{j,k}(\hat{P}_{jk} - 1). \tag{2}$$

Let's see how the Hamiltonian acts on our previous example, $|\psi_5\rangle = |\downarrow\uparrow\downarrow\uparrow\rangle$.

$$\begin{aligned}\hat{H}|\psi_5\rangle \quad = \quad & -J(\hat{P}_{12} + \hat{P}_{23} + \hat{P}_{34} + \hat{P}_{41} - 4)|\downarrow\uparrow\downarrow\uparrow\rangle = \\ & -J(|\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\uparrow\downarrow\downarrow\rangle - 4|\downarrow\uparrow\downarrow\uparrow\rangle) = \\ & -J(|1001\rangle + |0011\rangle + |0110\rangle + |1100\rangle - 4|0101\rangle) = \\ & -J(|\psi_9\rangle + |\psi_3\rangle + |\psi_6\rangle + |\psi_{12}\rangle - 4|\psi_5\rangle)\end{aligned}$$

We can now generate the Hamiltonian:

$$\hat{H}_{jk} = J[4\delta_{jk} - \delta_{j\alpha} - \sum_{l=1}^{N-1}\delta_{j\beta}], \tag{3}$$

where

$$\alpha = j + (2^{N-1} - 1)[(j-1) \bmod 2 - (\lfloor\frac{j-1}{2^{N-1}}\rfloor) \bmod 2],$$

and

$$\beta = j + 2^{l-1}[(\lfloor\frac{j-1}{2^{l-1}}\rfloor) \bmod 2 - (\lfloor\frac{j-1}{2^{l}}\rfloor) \bmod 2].$$

Once the Hamiltonian is determined, we need to find the eigenvalues, E_n to determine the propagator,

$$\hat{U}_{jk}^{(energy)} = \delta_{jk}e^{iE_n t}. \tag{4}$$

The eigenvalues are the energies of each of the state vectors when written in the energy basis. Hence, the propagator is written in the energy basis, whereas the state vectors in Eq. (1) are written in a different basis, which we will call the standard basis. We can transform the propagtor to the standard basis by constructing a transformation matrix with the normalized eigenvectors, $|e_n\rangle$, of the Hamiltonian. The transformation matrix is

$$\hat{T} = [|e_1\rangle||e_2\rangle|...|e_N\rangle]. \tag{5}$$

[2]For a detailed description of this procedure, see Feynman [5]

Transforming the propagator into the standard basis, we have

$$\hat{U} = \hat{T}^{-1}\hat{U}^{(energy)}\hat{T}. \tag{6}$$

The next step is to determine the spin operator matrices, $\hat{S}_j^x$, $\hat{S}_j^y$, and $\hat{S}_j^z$ that act on the j^{th} spin of a particular state vector. These matrices can be determined by using the angular momentum commutation relationships.

$$\hat{S}^x_{(j)lm} = \frac{\hbar}{2}\delta_{l\gamma}, \tag{7}$$

$$\hat{S}^y_{(j)lm} = i\frac{\hbar}{2}\gamma\delta_{l\gamma}, \tag{8}$$

$$\hat{S}^z_{(j)lm} = \frac{\hbar}{2}\gamma\delta_{lm} \tag{9}$$

where

$$\gamma = l - 2^{m-1}(2\lfloor\frac{l-1}{2^{m-1}}\rfloor \bmod 2 - 1),$$

To calculate the correlation function, we will need to construct the q-mode parallel and transverse spin operators. These are

$$\hat{s}_q^z = \sum_j \hat{S}_j^z \cos\frac{2\pi qj}{N}, \tag{10}$$

$$\hat{s}_q^+ = \sum_j (\hat{S}_j^x + i\hat{S}_j^y)e^{-\frac{2\pi iqj}{N}}. \tag{11}$$

$$\hat{s}_q^- = \sum_j (\hat{S}_j^x - i\hat{S}_j^y)e^{-\frac{2\pi iqj}{N}}. \tag{12}$$

It is also necessary to construct the density matrix, which determines the statistical weighting of each spin due to polarization. The density matrix is

$$\hat{\rho}_{jk} = \delta_{jk}e^{\frac{b}{\sqrt{3}}(\sum_l -(-1)^{|S_l^z\rangle})} = \delta_{jk}e^{\frac{b}{\sqrt{3}}(\sum_l 2\lfloor\frac{j-1}{2^{k-1}}\rfloor \bmod 2 - 1)} \tag{13}$$

Here, $|S_l^z\rangle$ is written in binary notation, and the magnitude of b corresponds to the strength of the magnetic field.

We define the parallel and transverse correlation functions, respectively, as[6]

$$G^z(t) = \frac{\langle\hat{s}_q^z(t)\cdot\hat{s}_q^z(0)\rangle}{\langle\hat{s}_q^z(0)\cdot\hat{s}_q^z(0)\rangle}, \tag{14}$$

$$G^+(t) = \frac{\langle\hat{s}_q^+(t)\cdot\hat{s}_q^-(0)\rangle}{\langle\hat{s}_q^+(0)\cdot\hat{s}_q^-(0)\rangle}. \tag{15}$$

By applying the propagator to Eq. (10) and (11), the q-mode spin operators are made time dependent. Since we are interested in the hydrodynamic mode, $q = 1$.

$$G^z(t) = \frac{\langle\hat{s}_1^z(t)\cdot\hat{s}_1^z(0)\rangle}{\langle\hat{s}_1^z(0)\cdot\hat{s}_1^z(0)\rangle} = \frac{\langle\hat{\rho}\,\hat{U}^\dagger\hat{s}_1^z\,\hat{U}\hat{s}_1^z\rangle}{\langle\hat{\rho}\,\hat{s}_1^z\,\hat{s}_1^z\rangle} = \frac{\mathbf{Tr}[\hat{\rho}\,\hat{U}^\dagger\hat{s}_1^z\,\hat{U}\hat{s}_1^z]}{\mathbf{Tr}[\hat{\rho}\,\hat{s}_1^z\,\hat{s}_1^z]}. \tag{16}$$

$$G^+(t) = \frac{\langle\hat{s}_1^+(t)\cdot\hat{s}_1^-(0)\rangle}{\langle\hat{s}_1^+(0)\cdot\hat{s}_1^-(0)\rangle} = \frac{\langle\hat{\rho}\,\hat{U}^\dagger\hat{s}_1^+\,\hat{U}\hat{s}_1^-\rangle}{\langle\hat{\rho}\,\hat{s}_1^+\,\hat{s}_1^-\rangle} = \frac{\mathbf{Tr}[\hat{\rho}\,\hat{U}^\dagger\hat{s}_1^+\,\hat{U}\hat{s}_1^-]}{\mathbf{Tr}[\hat{\rho}\,\hat{s}_1^+\,\hat{s}_1^-]}. \tag{17}$$

It is possible to observe the spectrum for a given lattice by taking the Fourier Transform of the correlation function:

$$G_q^z(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} G_q^z(t)e^{i\omega t}dt \tag{18}$$

CORRELATION FUNCTION OF THE QUANTUM DIMER AS AN ILLUSTRATION

For a two spin system, the state vectors in the standard basis are

$$|\psi_0\rangle = |\downarrow\downarrow\rangle, |\psi_1\rangle = |\downarrow\uparrow\rangle, |\psi_2\rangle = |\uparrow\downarrow\rangle, |\psi_3\rangle = |\uparrow\uparrow\rangle. \tag{19}$$

We use Eq. (3) to calculate the Hamiltonian matrix (for simplicity, we will make the constant $J = 1$):

$$\hat{H} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & -2 & 0 \\ 0 & -2 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

By finding the eigenvalues and normalized eigenvectors, we can construct the transformation and the propagator matrices using Eqs. (4) and (5).

$$\hat{U}^{(energy)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-4it} \end{pmatrix}.$$

$$\hat{T} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}.$$

The next step is to transform the propagator into the standard basis(Eq. (6)). We have

$$\hat{U} = \hat{T}^{-1}\hat{U}^{(energy)}\hat{T} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2}+\frac{1}{2}e^{-4it} & \frac{1}{2}-\frac{1}{2}e^{-4it} & 0 \\ 0 & \frac{1}{2}-\frac{1}{2}e^{-4it} & \frac{1}{2}+\frac{1}{2}e^{-4it} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Eqs. (7), (8), and (9) give us the spin operators.

$$\hat{S}_1^x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \hat{S}_2^x = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\hat{S}_1^y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \hat{S}_2^y = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix},$$

$$\hat{S}_1^z = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \hat{S}_2^z = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

We use Eq. (13) to construct the density matrix.

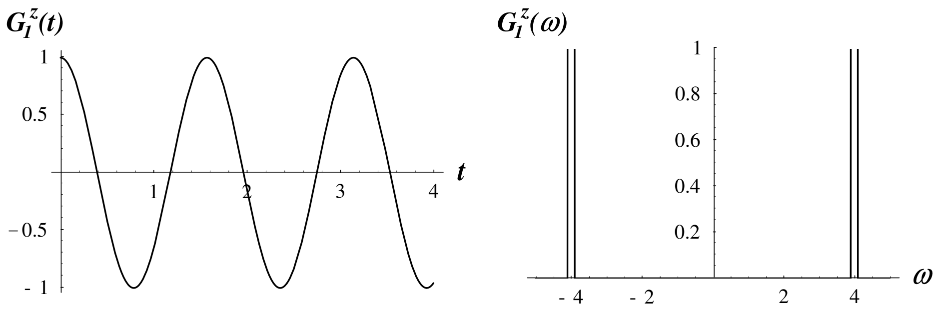

FIGURE 1: Plot of $G_1^z(t)$ and spectra for a 2-spin lattice in an unpolarized and highly polarized system.

$$\hat{\rho} = \begin{pmatrix} e^{-\frac{2b}{\sqrt{3}}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{\frac{2b}{\sqrt{3}}} \end{pmatrix}.$$

The parallel and transverse spin matrices are the final components necessary before we can calculate the correlation functions. Using Eqs. (14) and (15) we have

$$\hat{s}_1^z = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \hat{s}_1^+ = \begin{pmatrix} 0 & -2 & 2 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \hat{s}_1^- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & -2 & 0 \end{pmatrix},$$

From here, it is straight forward to calculate the correlation functions:

$$G_1^z(t) = \frac{\mathbf{Tr}[\hat{\rho}\,\hat{U}^\dagger \hat{s}_1^z\,\hat{U}\hat{s}_1^z]}{\mathbf{Tr}[\hat{\rho}\,\hat{s}_1^z\,\hat{s}_1^z]} = \cos 4t,$$

$$G_1^+(t) = \frac{\mathbf{Tr}[\hat{\rho}\,\hat{U}^\dagger \hat{s}_1^+\,\hat{U}\hat{s}_1^-]}{\mathbf{Tr}[\hat{\rho}\,\hat{s}_1^+\,\hat{s}_1^-]} = \frac{e^{\frac{2b}{\sqrt{3}}+4it} + e^{-4it}}{1 + e^{\frac{2b}{\sqrt{3}}}},$$

and the spectra:

$$G_1^z(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \cos 4t e^{i\omega t} dt = \sqrt{\frac{\pi}{2}}(\delta(\omega - 4) + \delta(\omega + 4)),$$

$$G_1^+(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{\frac{2b}{\sqrt{3}}+4it} + e^{-4it}}{1 + e^{\frac{2b}{\sqrt{3}}}} e^{i\omega t} dt = \frac{\sqrt{2\pi}(\delta(\omega - 4) + e^{\frac{2b}{\sqrt{3}}}\delta(\omega + 4))}{1 + e^{\frac{2b}{\sqrt{3}}}}.$$

REFERENCES

[1] B. Cowan, W.J. Mullin and E. Nelson, *J. Low Temp. Phys.* **77**, 181 (1989); B. Cowan, W.J. Mullin and S. Tehrani-Nasab, *Physica* **194-196**, 921 (1994); S. Kingsley, B. Cowan, W.J. Mullin and S. Tehrani-Nasab, *Czech. J. Phys* **46**, 493 (1996);B. Cowan, W.J. Mullin, S. Tehrani-Nasab, and G.H. Kirk, unpublished.

[2] C. Tang and J.S. Waugh, *Physical Review B* **45**, 748 (1992).

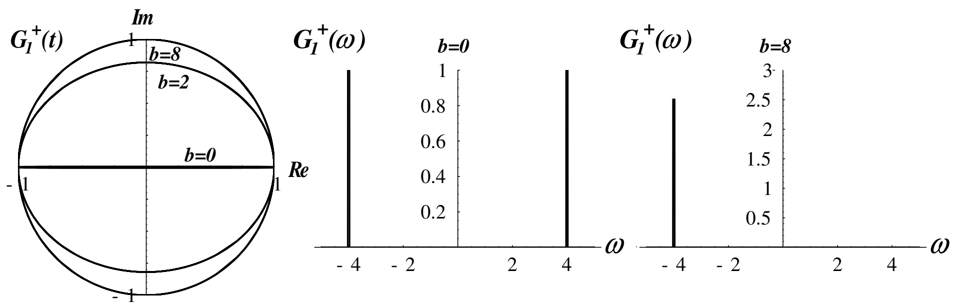

FIGURE 2: Parametric plot of $Re[G_1^z(t)]$ and $Im[G_1^z(t)]$ as t goes from 0 to 20 seconds and spectra for various degrees of polarization for a 2-spin lattice varying degrees of polarization.

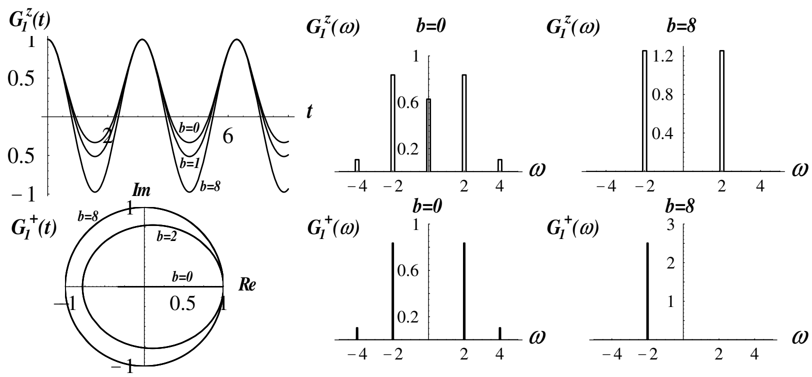

FIGURE 3: Plot of $G_1^z(t)$ and parametric plot of $Re[G_1^+(t)]$ and $Im[G_1^+(t)]$ and spectra for various degrees of polarization for a 4-spin lattice.

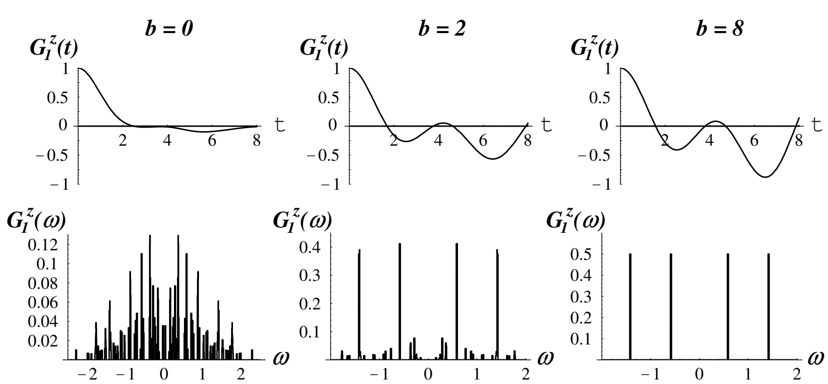

FIGURE 4: Plot of $G_1^z(t)$ and spectra for an 8-spin lattice with various degrees of polarization.

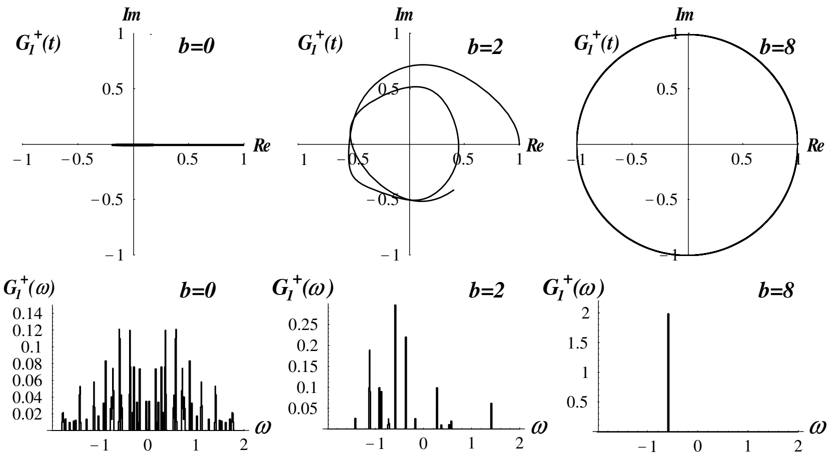

FIGURE 5: Parametric plot of $Re[G_1^+(t)]$ and $Im[G_1^+(t)]$ as t goes from 0 to 20 seconds and spectra for various degrees of polarization for an 8-spin lattice varying degrees of polarization.

[3] R. Ragan, K. Grunwald, and C. Glenz, *J. Low Temperature Phys.* **126**, 45 (2002).

[4] F.D.M. Haldane and M.R. Zirnbauer, *Phys. Rev. Lett.*, **71**, 4055 (1993).

[5] R. Feynman, *The Feynman Lectures on Physics* (Addison-Wesley 1965).

[6] D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions* (Addison-Wesley 1990).

APPENDIX

We can also represent the state vectors in Eq. (1) in binary notation in the following manner. For the j^{th} position, we will write $|1\rangle$ if $|S_j^z\rangle = |\uparrow\rangle$ and $|0\rangle$ if $|S_j^z\rangle = |\downarrow\rangle$. The subscript n in Eqn. (1) is determined by the following relation:

$$n = \sum_{j=1}^{N} \delta_{1|S_j^z\rangle} 2^{N-j}.$$

For example, suppose we are dealing with a 4-spin system and one of the state vectors is $|\downarrow\uparrow\downarrow\uparrow\rangle$. Using the system above, we would write this as $|0101\rangle$. Therefore, we would write this vector as $|\psi_5\rangle$.