Quantum disorder due to singlet formation: The Plaquette lattice

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I study the order/disorder transition due to singlet formation in a quantum spin system by means of exact diagonalization. The system is built by spin 1/2 on a two-dimensional square lattice with two different kinds of antiferromagnetic Heisenberg interactions. The interaction $J_p$ connects 4 nearest neighbor spins on a plaquette. The interaction $J_n$ connects the plaquettes with each other. If $J_p = J_n$ the system reduces to the simple square lattice case. If one of the interactions becomes sufficiently larger then the other the purely quantum effect of singlet formation drives the system into a disordered phase with only short range correlations in the plaquettes and a spin gap. I study the transition point by evaluating the spin gap and spin–spin correlations. I compare the results with previously calculated data from a non–linear $\sigma$ model approach, spin wave theory and series expansion calculations. I confirm a critical value of $J_n \approx 0.6$ for the quantum phase transition point.

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I. INTRODUCTION

Low dimensional quantum antiferromagnets have attracted a great deal of attention during the last decade, both theoretically and experimentally. Such magnets show a wide variety of magnetic low–temperature behavior, like magnetic long range order or spin disorder with or without a spin gap. Especially the question how magnetic long range order is influenced by different parameters like frustration, temperature, spin quantum number or lattice topology has been addressed.

A wide variety of different numerical methods like quantum Monte Carlo, renormalization group calculations, series expansion or spin wave theory has been developed and used for carrying out research in this field. All these methods have their advantages but also some disadvantages. Monte Carlo calculations suffer severe from the sign problem in frustrated systems. Series expansions and spin wave calculations may break down at phase transition points. The most promising renormalization group theory, the density matrix renormalization group is still limited to one–dimensional problems.

In this respect the exact diagonalization of finite lattices is still a very powerful method because the calculated data is a priori exact for the finite lattice under consideration. The exponentially fast growing Hilbert space necessary for the calculations limits the enumeration for spin half system to a total of N=36 spins yet. Still this task is computationally very demanding and one of the computational challenges of the new century will be the ongoing task to push this limit as far as possible by using all the available resources at hand. Exact diagonalization will always be one of the forerunners of using all the promised computer power coming up in the future and nevertheless it will be not enough to go too far away.

Despite the mentioned limitations to rather small finite lattices it has been shown that with particular care one can draw important conclusions about the ordering behavior of different low–dimensional quantum spin systems, e.g. the frustrated ferrimagnet in 1d, the kagomé lattice in 2d, or the Heisenberg antiferromagnet on the body–centered cubic lattice in 3d.

In this paper I will examine a particular interesting quantum spin system which shows a purely quantum phase transition by singlet formation. There is an experimental study of a new compound $Na_5RbCu_4(AsO_4)_4Cl_2$ under way which suggest that this system might be described by the model I consider here. I also note that a similar model has been studied previously with a non–linear $\sigma$-model approach and spin wave theory, plaquette expansion and Ising series expansion. At the end I will compare the results of all this methods with each other.

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II. THE MODEL

I consider the Heisenberg antiferromagnet on a two–dimensional square lattice with two different kinds of antiferromagnetic spin exchange parameters $J_p > 0$ and $J_n > 0$.

$$H = J_p \sum_{\text{inter}} \hat{s}_i \hat{s}_j + J_n \sum_{\text{intra}} \hat{s}_i \hat{s}_j$$  \hspace{1cm} (1)

The summation $\sum_{\text{inter}}$ with $J_p$ takes place between 4 nearest neighbor spins on a particular plaquette. The $\sum_{\text{intra}}$ with $J_n$ takes place between nearest neighbors on different plaquettes (cf. Fig.1). The quantum spin $\hat{s}_i$ equals $\frac{1}{2}$. For simplicity I put $J_p=1$ for the rest of the paper and take $J_n$ as the changing parameter.

FIG. 1: The Plaquette lattice with N=16 spins and periodic boundaries. Bold lines denote $J_p$ bonds, thin lines denote $J_n$ bonds.

I note that the Hamiltonian is symmetric if one exchanges $J_n$ and $J_p$ and therefore I consider the range of $J_n \in [0, 1]$ only. For $J_n = 1$ this system represents the simple square lattice.

III. RESULTS

A. The classical ground state

The ground state of the classical model where the spins $\hat{s}_i$ can be considered as classical vectors $\vec{s}_i$ is actually very simple. Because there is no frustration in the system it will remain in the Néel–state for all values of $J_n > 0$. This classical ground state is illustrated in the left part of Fig.2. Only if $J_n = 0$ the ground state becomes highly degenerated and then the Néel–state is only one of the possible ground states due to the free rotation of the spins in one plaquette respectively to any other plaquette. This behavior is depicted in the right part of Fig.2.

Of course the question is now, what will happen if quantum fluctuations come into play? I will discuss this in the next paragraph by considering the spin gap and spin–spin correlation data for the quantum system on finite lattices with N=16,20,32 and 36 spins and periodic boundary conditions.

Since the Heisenberg Hamiltonian commutes with the square of total spin $\hat{S}^2$, $\hat{S} = \sum_i \hat{s}_i$, each eigen state of $\hat{H}$ belongs to a certain subspace of the Hilbert space with fixed quantum number $S$ of the total spin ($\hat{S}^2 = \hat{S}(\hat{S} + 1)$). To calculate the ground state and the first excited state of $\hat{H}$ for finite lattices I use the Lanczos technique.

B. The spin gap $\Delta$

First I will analyze the spin gap $\Delta$

$$\Delta = E_{\min}(S_{\min} + 1) - E_{\min}(S_{\min}).$$  \hspace{1cm} (2)
For bipartite antiferromagnets like the one studied here one can show that the ground state belongs to the $S = 0$ subspace and the first excitation is a triplet with $S = 1$. Considering our model one can immediately note, that for $J_n = 0$ all the plaquettes will be in a singlet state with the total spin of the plaquette being zero. The first excitation will then be a state were one plaquette is in its triplet state and a simple analytical calculation then shows: $\Delta = 1$.

As stated for $J_n = 1$ one obtains the simple square lattice case where a Néel–like magnetic long range order without a spin gap is well established [10]. For some value of $J_n$, between 0 and 1 I will observe the opening of a spin gap at the phase transition point.

In Fig. 3 I show the data from exact diagonalization calculations for lattices with up to 36 spins and an extrapolation to the thermodynamic limit.

I use a finite size extrapolation $\Delta \propto N^{-1}$ for the entire range of calculated data but will keep in mind that this is a reasonable good approximation for $J_n \geq 0.6$ only (apparent in the small errorbars) but much less appropriate for $J_n \leq 0.5$ (visible in larger errorbars). I used two data sets with N=16-32 and N=16-36. They give very similar result for $J_n \geq 0.6$, but deviate apparently for $0.3 < J_n < 0.5$. But even so one can clearly distinguish the two phases, one with a finite spin gap and one without and hence I draw two dotted fit lines for $J_n \leq 0.5$ and one dashed fit line for $J_n \geq 0.6$.

The extrapolated data shows a small finite value for $\Delta$ at $J_n = 1$ but this is due to the rough approximation only. I assume a finite spin gap opens up above any value greater than the vertical dashed line (cf. Fig. 3) in the thermodynamic limit. The crossing of the two dotted fit lines with the dashed one can then be approximated as a value for the phase transition point: $J_n^{\text{crit}} \approx 0.65 \pm 0.05$. 

FIG. 2: The classical ground state spin configuration of the Plaquette lattice. Left: The Néel–state for $J_n > 0$, right: $J_n = 0$ with a free rotation of the local axis in each plaquette.

FIG. 3: The spin gap $\Delta$ versus $J_n$. The crosses, squares and circles represent the calculated data for N=16,20, 32 and 36 sites. The triangles with the errorbars are the extrapolated data with two input sets: N=16-32 and N=16-36. For the dashed and dotted lines see text.
C. The spin–spin correlation

In order to further evaluate the phase transition point I study the spin–spin correlation data plotted in Fig. 4. Here I show the spin–spin correlation between two spins connected by a $J_n$ bond $\langle \hat{s}_i \hat{s}_j \rangle_{\text{intra}}$ and between two spins connected by a $J_p$ bond $\langle \hat{s}_i \hat{s}_j \rangle_{\text{inter}}$.

The intra–plaquette correlation starts from 0 as expected for non–coupled plaquettes and ends at a certain finite value for $J_n = 1$. The inter–plaquette correlation starts from $-1/2$ (this value can be calculated analytically) and ends at the same value as $\langle \hat{s}_i \hat{s}_j \rangle_{\text{intra}}$ due to the symmetry at this point.

Both curves show an inflection point at around $J_n \approx 0.5$ which can be assumed to be connected to the phase transition. Therefore I carry out a numerical differentiation $\partial \langle \hat{s}_i \hat{s}_j \rangle_{\text{intra}} / \partial J_n$ in order to study this inflection point in more detail in the left part of Fig. 5. By numerical differentiation this inflection point is transformed into a minimum $\delta_{\text{min}}$ which is then shown versus the system size in the right part of Fig. 5.

In the left part of Fig. 5 one can see that with increasing system size the minimum shifts towards greater $J_n$ and also gets deeper. One may argue that in the thermodynamic limit one will observe a delta peak right at the quantum phase transition point. In the right part of Fig. 5 I plot the peak position $\delta_{\text{min}}$ versus the inverse system size $1/N$ and extrapolate a value $J_n^{\text{crit}} \approx 0.55 \pm 0.05$. This result is close to the value from the spin gap data.

IV. CONCLUSION

In this paper I presented an exact diagonalization study of an antiferromagnetic Heisenberg quantum spin systems with $s=1/2$ with two kinds of interactions, the Plaquette lattice. I calculated the spin gap and the spin–spin correlation...
for finite lattices and obtained a quantum phase transition at $J_{\text{crit}} \approx 0.6 \pm 0.1$. This is a purely quantum phase transition due to singlet formation which has no classical counterpart. Our result compares well with 4th order plaquette expansion result of $J_{\text{crit}} \approx 0.54$ \cite{8} or the Ising series expansion result $J_{\text{crit}} \approx 0.55$ \cite{9}. Our result shows clearly that the spin wave result $J_{\text{crit}} \approx 0.112$ \cite{7} can be ruled out. The non-linear $\sigma$ model approach \cite{6} does completely fail to predict any transition to an ordered phase without a spin gap.

Whether this phase transition is first or second order is still to be answered, the spin–spin correlation data with a developing delta peak points more to a first order transition. But clearly a more detailed study is necessary to clarify this and corresponding work is under way.

Anyway, this study has shown that the exact diagonalization of finite lattices can be successfully used for complex many–body problems and that the results may help to verify and extend the validity of other methods.

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