Deconfinement phase transition in a two-dimensional model of interacting $2 \times 2$ plaquettes

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A two-dimensional model of interacting plaquettes is studied by means of the real space renormalization group approach. Interactions between the plaquettes are mediated solely by spin excitations on the plaquettes. Depending on the plaquette-plaquette coupling $J$, we find two regimes:

1. “confinement” $J_c < J \leq 1$, where the singlet ground state forms an infinite (“confined”) cluster in the thermodynamical limit. Here the singlet-triplet gap vanishes, which is the signature for long range spin-spin correlators.

2. “deconfinement” $0 \leq J < J_c$, where the singlet ground state “deconfines” - i.e. factorizes - into finite $n$-clusters of size $2^n \times 2^n$, with $n \leq n_c(J)$. Here the singlet-triplet gap is finite. The critical value turns out to be $J_c = 0.4822\ldots$

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I. INTRODUCTION

We will discuss in this paper the 2$D$ Hamiltonian

$$H = H_0 + J \cdot H_J$$

(1.1)

where $H_0$ is given by isolated plaquettes occupied with spin-1/2 states and $H_J$ describes nearest neighbour interactions of these plaquettes as shown in Fig. 1. For $J = 1$, the model (1.1) reduces to the well known 2$D$ antiferromagnetic Heisenberg model. The modified Hamiltonian (1.1) has been proposed in studies of structural instabilities of two-dimensional systems.

The singlet-triplet gap (“spin gap”) has been studied by various methods:

1. Nonlinear $\sigma$ model as a low energy effective theory [1, 2]

2. modified spin wave theory [3, 4]

3. cluster expansion up to fourth order starting from $J = 0$, i.e. isolated plaquettes [2]

In the spin-1/2 case, the model (1.1) is expected [7] to have a quantum phase transition at a critical value $J_c^1$, which is signalled by a vanishing singlet-triplet gap for $J > J_c^1$. The results of these works are:

1. no phase transition for the spin 1/2 case in the nonlinear $\sigma$ model [8] for any $J \leq 1$.

2. $J_c = 0.118$ for the modified spin wave theory [versus $J_c = 0.112$ in linear spin wave theory [6]].

3. $J_c = 0.54$ for the cluster expansion.

$^1$ The critical value $J_c$ is related to the parameter $\gamma_c$ introduced in [8] by $J_c = (1 - \gamma_c)/(1 + \gamma_c)$

A value $J_c = 0.555$ was obtained by means of Ising series expansions [7].

$J_c$ has been determined by means of the CORE method (contractor renormalization expansion) first by Capponi et al. [3] and recently by Albuquerque et al. [10]. These results are somewhat lower $J_c = 0.548$.

Recent Monte Carlo simulations [11,12] yield values close to $J_c = 0.549$.

The nonlinear $\sigma$ model approach yields different results for different cut-off schemes. In [Kawakami et al. (8)] no phase transition was found for $S = 1/2$, whereas in [Takano et al. (13)] a critical $J_c (0.2 \leq J_c \leq 0.25)$ was obtained.

The phase transition of the magnetic system has been discussed in its correspondence to a superfluid-insulator transition of the boson model [14].

The authors of ref. (10) start from singlet ($S = 0$) and triplet ($S = 1$) plaquette states. Excited states $|S, m\rangle$, $S = 0, 1, 2$, $m = -S, \ldots, S$ are absolutely necessary to generate interactions, since singlets alone cannot interact due to total spin conservation.

In a recent paper [15], we have studied how interactions on the 4 plaquette compound - depicted in Fig. 1 - are created by single plaquette excitations. The con-

![Figure 1: 4-plaquette system with $2^n \times 2^n = 4 \times 4$ sites - here $n = 2$; the single plaquette on the right shows the enumeration of plaquette sites.](image-url)
servation of total spin at each interaction point is implement-
by means of the Wigner-Eckart Theorem for the
transition matrix elements
\[
\langle S'_l, m'_l | S_q(x) | S_l, m_l \rangle = v_q \left( \begin{array}{cc} S'_l & S_l \\ m'_l & m_l \end{array} \right) M(S'_l, x, S_l).
\] (1.2)

They can be expressed in terms of a Clebsch-Gordan co-
efficient and one reduced matrix element \(M(S'_l, x, S_l)\). The
latter only depends on the initial and final plaquette spin \(S_l, S'_l\) and the triplet operator \(S_q(x)\) at site \(x\). The
phase \(v_q (v_+ = -1, v_0 = v_- = 1)\) results from the trans-
formation properties of the spin operator \(S_q(x)\) under the
group \(SU(2)\). The interaction between neighbouring
plaquettes can be traced back to the product of reduced
matrix elements at sites \(x\) and \(y\) (Fig. 2)

![Diagram](image)

FIG. 2: Interaction of neighbouring plaquettes.

\[
\overline{M}(S'_l, S_l; S'_r, S_r) = \sum_{(x,y)} M(S'_l, x, S_l) M(S'_r, y, S_r)
\] (1.3)

Quintuplet excitations \((S = 2)\) have not been consid-
ered in ref. 10. We want to stress here that triplet-
quintuplet transitions are large - comparable with singlet-
triplet transitions. It is shown in 15 that the gaps
(singlet-triplet and triplet-quintuplet) decrease in the
renormalization process. We will see in this paper that
the inclusion of quintuplet excitations will move the crit-
ival value \(J\) substantially to a lower value.

The paper is organized as follows:
In Section II we summarize the details of the real space
renormalization group approach in 2D models.
In Section III we evaluate the renormalization group
flow for various couplings and gaps.
In Section IV we discuss the deconfinement of the
ground state wavefunction for \(J < J_c\).
In Section V we present a finite size analysis of the
singlet-triplet gap in both regimes: \(J_c < J < 1\) (con-
fined), \(0 < J < J_c\) (deconfined).
Section VI is devoted to the staggered magnetization.

II. REAL SPACE RENORMALIZATION GROUP
IN 2D MODELS.

In 13 we first studied the interaction matrices \(\Delta_S^{(2)}\)
of the four plaquette system (Fig. 1) in the sectors with
total spin \(S\). The elements of the interaction matrices
are fixed on one hand by the Clebsch-Gordan coefficients,
which arise in the construction of eigenstates with total
spin \(S\) (on the 4-plaquette system) and the evaluation
of the Wigner-Eckart Theorem 12 for the transition
matrix elements. On the other hand \(\Delta_S^{(2)}\) only depends
on the following couplings
\[
\gamma = \frac{1}{a} M(21; 10) \] (2.1)
\[
\beta = \frac{1}{a} M(11; 11) \] (2.2)
\[
\varepsilon = \frac{1}{a} M(22; 11) \] (2.3)

and gaps
\[
\rho = \frac{E_1 - E_0}{a} \] (2.4)
\[
\kappa = \frac{E_2 + E_0 - 2E_1}{a} \] (2.5)

We have factored out from the couplings (2.1)-(2.3) the
“fundamental” interaction
\[
a = M(1, 0; 1, 0) \] (2.6)

which is induced by the singlet-triplet transitions on the
plaquette.

In Appendix A of ref. 15 one can find the explicit form
of the interaction matrices \(\Delta_S\) (for \(J = 1\)) \(S = 0, 1, 2\)
under the premise that on the four plaquettes only ro-
tational symmetric configurations with singlets, triplets
and at most one quintuplet contribute. In this case the
dimensions \(d_S\) of the interaction matrices \(\Delta_S\) turn out to be
\[
(d_0, d_1, d_2) = (7, 9, 14). \] (2.7)

The factor \(J\) in (2.1) is taken into account in the in-
teraction matrices \(\Delta_S^{(n)}\) on an \(n = 2\) cluster \((2^n \times 2^n)\)
from the ground states on an \(n = 1\) cluster, we turned to the question,
whether it is possible in general to construct the inter-
action matrix \(\Delta_S^{(n+1)}\), \(S = 0, 1, 2\) from the correspond-
ing quantities of a \(n \times n\) cluster. This is indeed possible
under the assumption that the low energy states on the
\((n + 1)\)-cluster can be built up again solely from sin-
glet, triplet, quintuplet ground states on \(n\)-clusters. The
\(n\)-dependence only appears in a renormalization of the
couplings (2.1)-(2.3) and energy differences (2.5).

Here, we refer to 15 [eqns. (6.1)-(6.4); (6.5),(6.6)] for the used formulas of the renormalization of the
couplings and recursion formulas for the scaled energy
differences. Note, that \(J\) does not appear in the first group
of equations, whereas the remaining two (scaled energy
differences) are linear in \(J\).

Each step \(n \rightarrow n + 1\) in the renormalization procedure
demands the diagonalization of the interaction matrices
\[ \Delta_g^{(n+1)}, S = 0, 1, 2: \]
\[ \Delta_0^{(n+1)}|\sigma^{(n+1)}⟩ = \sigma^{(n+1)}|\sigma^{(n+1)}⟩ \]  
\[ \Delta_1^{(n+1)}|\tau^{(n+1)}⟩ = \tau^{(n+1)}|\tau^{(n+1)}⟩ \]  
\[ \Delta_2^{(n+1)}|ξ^{(n+1)}⟩ = ξ^{(n+1)}|ξ^{(n+1)}⟩ \]

The eigenstates \(|\sigma^{(n+1)}⟩, |\tau^{(n+1)}⟩, |ξ^{(n+1)}⟩\) with the largest eigenvalues \(\sigma^{(n+1)}, \tau^{(n+1)}, ξ^{(n+1)}\) enter in the quantities

\[ I^{(n+1)}(a, b), G^{(n+1)}(a, b) \quad (a, b) = (1, 0), (2, 1) \]
\[ F_{ξ}^{(n+1)}(a, a), F_{ξ}^{(n+1)}(a, a) \quad (a, a) = (1, 1), (2, 2) \]

according to the bilinear forms:

\[ I^{(n+1)}(a, b) = \sum_{k,i} \tau^{(n+1)}_k I_{k,i}(a, b)σ^{(n+1)}_i \]  
\[ G^{(n+1)}(a, b) = \sum_{l,k} \tau^{(n+1)}_l G_{l,k}(a, b)τ^{(n+1)}_k \]
\[ F_{ξ}^{(n+1)}(a, a) = \sum_{k} \left( τ^{(n+1)}_k \right)^2 F_{ξ,k}(a, a) \]
\[ F_{ξ}^{(n+1)}(a, a) = \sum_{l} \left( ξ^{(n+1)}_l \right)^2 F_{ξ,l}(a, a) . \]

The contraction \(I_{j,i}(1, 0)\), etc. are independent of \(n\) and listed in Appendix B of paper [13].

III. NUMERICAL EVALUATION OF THE RENORMALIZATION GROUP FLOW.

We now turn to the numerical evaluation of the recursion formula of the couplings [eqns. (6.1) – (6.4) in [13]] and gaps [eqns. (6.5),(6.6) in [13]] in order to study the \(n\)-dependence (i.e. finite size \(2^{n+1} × 2^{n+1}\)) and \(J\)-dependence. We start with the singlet-triplet gap \(\rho^{(n+1)}\), which yields the signature for long range order: From Fig. 3 we see, that there are two different regimes:

a) \(J_c ≤ J ≤ 1\)

Here the singlet-triplet gap approaches zero with increasing system size. For \(J = 1\) we are close to zero already on small systems for \(n_0 = 3\). For decreasing \(J\), \(n_0(J)\) increases and seems to diverge for \(J → J_c\).

b) Below this critical value (\(J < J_c\)) the singlet-triplet gap \(\rho^{(n+1)}\) does not converge to zero anymore. Note also that there is a change in the curvature of \(\rho^{(n+1)}\) with \(n\), which is for large \(n\) convex if \(J_c < J\) but concave if \(J_c > J\). This allows for a very precise determination of \(J_c = 0.4822\.)

Let us next turn to the coupling ratio \(a^{(n+1)} \over 2a^{(n)}\) [(6.1) in [13]]. As function of \(n\) this quantity has a maximum, which travels to larger values of \(n\), if \(J\) is lowered (Fig. 4).

For \(J_c ≤ J ≤ 1\) all curves approach a common limit for large \(n:\)

\[ \frac{a^{(n+1)}}{2a^{(n)}} = 0.52 . \]  

For \(J ≤ J_c\) we observe a monotonic decrease to a limiting value, different from (3.2):

\[ \frac{a^{(n+1)}}{2a^{(n)}} = 0.25 . \]

The \(n\)-dependence of the coupling \(γ^{(n+1)}\) [(6.2) in [13]] is shown in Fig. 3.

For \(J_c ≤ J ≤ 1\) all curves approach a common limit

\[ γ^{(n+1)} → 1.0849 . \]
for large \( n \), whereas we observe a monotonic increase with \( n \) for \( J < J_c \) and a common limit
\[
\gamma^{(n+1)} \to 1.3411. \tag{3.5}
\]

We only want to mention that the “diagonal” couplings \([6.3] \text{ and } [6.4] \text{ in } [15] \), which do not change the plaquette spins, die out after a few steps.

**IV. DECONFINEMENT OF THE GROUND STATE WAVEFUNCTION.**

It was pointed out in Section II, that the renormalization group procedure demands in each step \( n \to n+1 \) the diagonalization \([2.8]-[2.10] \) of the interaction matrices. We only keep those eigenvectors \( |\sigma^{(n+1)}\rangle \) with largest eigenvalue \( (\sigma_1^{(n+1)}) \).

We want to discuss now the physical meaning of the eigenvector components:
\[
\sigma_1^{(n+1)} = \langle i, 0; n+1 | \sigma^{(n+1)} \rangle \quad i = 1, \ldots, 7 \tag{4.1}
\]
in the orthonormal basis \( |i, 0; n+1\rangle \) in the singlet sector defined in Table II of ref. [15]. E.g. \( (\sigma_1^{(n+1)})^2 \) has to be interpreted as the probability to find in the singlet ground state the four plaquette configuration
\[
|1, 0\rangle = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{4.2}
\]
with four noninteracting singlets. If
\[
(\sigma_1^{(n+1)})^2 \to 1, \tag{4.3}
\]
the singlet ground state \( |\sigma^{(n+1)}\rangle \) “deconfines” to the configuration \( |1, 0\rangle \) with four noninteracting singlets.

In Fig. 5 we show \( (\sigma_1^{(n+1)})^2 \) as function of \( n \) - i.e. the system size \( (2^{n+1} \times 2^{n+1}) \).

**V. FINITE-SIZE ANALYSIS OF THE SINGLET-TRIPLET GAP.**

In the confined regime \( J_c \leq J \leq 1 \) the singlet-triplet gap
\[
E_1^{(n)} - E_0^{(n)} \sim 4^{-n\nu_1} \tag{5.1}
\]
vanishes with an exponent
\[
\nu_1 = -\frac{\log(1 + x)}{\log 4} \tag{5.2}
\]
which can be determined from the first derivative

\[ x = \frac{d(\tau - \sigma)}{d\rho} = \frac{\partial(\tau - \sigma)}{\partial \rho} + \frac{\partial(\tau - \sigma)}{\partial \kappa} \cdot \frac{\partial \kappa}{\partial \rho} \]  

(5.3)

of the largest eigenvalues \( \sigma, \tau \) of the interaction matrices \( \Delta \) in the singlet \((S = 0)\) and triplet \((S = 1)\) sector:

\[
\frac{\partial(\tau - \sigma)}{\partial \rho} = \langle \tau \rangle \frac{\partial \Delta_{1}}{\partial \rho} \langle \tau \rangle - \langle \sigma \rangle \frac{\partial \Delta_{0}}{\partial \rho} \langle \sigma \rangle
\]

\[
= -4(\tau_{1}^{2} - \sigma_{1}^{2}) - 2(\tau_{2}^{2} + \tau_{3}^{2} + \tau_{4}^{2} + \tau_{5}^{2})
+ 2(\sigma_{2}^{2} + \sigma_{7}^{2})
\]  

(5.4)

\[
\frac{\partial(\tau - \sigma)}{\partial \kappa} = \langle \tau \rangle \frac{\partial \Delta_{1}}{\partial \kappa} \langle \tau \rangle - \langle \sigma \rangle \frac{\partial \Delta_{0}}{\partial \kappa} \langle \sigma \rangle
\]

\[
= 1 - \tau_{1}^{2} - \tau_{2}^{2} - \tau_{3}^{2} - \tau_{4}^{2} - \tau_{5}^{2} - \tau_{6}^{2} - \tau_{7}^{2} - \sigma_{2}^{2} - \sigma_{7}^{2}
\]  

(5.5)

The \( n \)- and \( J \)-dependence of \( \frac{\partial(\tau - \sigma)}{\partial \rho} \) - which is the dominant part of (5.3) - is presented in Fig. 8. In the common limit

\[ x^{(n+1)}(J) \rightarrow -\frac{3}{4} \]  

(5.6)

which leads to a universal exponent \( \nu_1(J) = 1 \).

In the deconfined regime \( 0 < J < J_c \) we find a nonvanishing singlet-triplet gap:

\[ E_1^{(n)} - E_0^{(n)} = E_1^{(\infty)} - E_0^{(\infty)} + f^{(n)} \]  

(5.8)

with a finite-size correction

\[ f^{(n+1)} - f^{(n)} = J \cdot a^{(n)}(\tau^{(n+1)} - \sigma^{(n+1)}) \]  

(5.9)

which follows from the difference \( \tau^{(n+1)} - \sigma^{(n+1)} \) of the largest eigenvalues \( \tau^{(n+1)}, \sigma^{(n+1)} \) in the triplet and singlet sector and the fundamental coupling \( a^{(n)} \) (2.6), which can be extracted from Fig. 10. The large \( n \) limit of the difference

\[ \tau^{(n+1)} - \sigma^{(n+1)} \rightarrow 2 \]  

(5.10)

turns out to be 2 for all \( 0 < J < J_c \) whereas the coupling

\[ a^{(n+1)}(J) = a(J) \cdot 2^{-n} \]  

(5.11)

decreases with the system size \( N = 4^n \) as \( \frac{1}{\sqrt{N}} \) for all \( 0 \leq J < J_c \). \( a(J) \) is shown in Fig. 9.

Finally we want to present our results from the recursion formula [(8.3) in ref. 15]
for the staggered magnetization on an \((n + 1)\)-cluster. Note, that the renormalization procedure only enters via the components \(\sigma_i^{(n+1)}, i = 1, \ldots, 7\) on an \((n + 1)\)-cluster and the coupling \(\gamma(n)\).

The \(7 \times 7\) matrix \(\Gamma_{ij}(\gamma(n))\) is presented in Appendix C of [15]. In Fig. 10 we present the ratio \(R^{(n+1)}\) as function of \(n\) and \(J\) for the case \((d_0 = 7, d_1 = 9, d_2 = 14)\) for large \(n\),

\[
R^{(n+1)} = \frac{\langle \sigma_i^{(n+1)} \sigma_i^{(n+1)} \rangle}{\langle \sigma_i^{(n)} \sigma_i^{(n)} \rangle} = \sum_{i',i=1}^{7} \sigma_i^{(n+1)} \sigma_{i'}^{(n+1)} \Gamma_{i',i}(\gamma(n)) \quad (6.1)
\]

all the curves approach a common limit
\[
R^{(n)} \to 0.7401 \ldots \quad \text{for } J_c \leq J \leq 1 \quad (6.2)
\]
\[
R^{(n)} \to 0.25 \quad \text{for } 0 \leq J \leq J_c
\]

VII. DISCUSSION AND PERSPECTIVES.

We have studied in the \(2D\) model with interacting plaquettes various observables like the scaled singlet-triplet gap \(\rho^{(n+1)}\) (Fig. 3) as function of \(n\) (i.e. system size \(2^{n+1} \times 2^{n+1}\)) and the coupling parameter \(J\) in (4.4). We find spectacular differences in the confinement \((J_c < J \leq 1)\) and deconfinement \((J < J_c)\) regime, which allows - for a given truncation scheme - for an extremely precise determination of the critical coupling \(J_c\) in all these quantities. This means, that the interaction matrices \(\Delta^{(n+1)}\), \(S = 0, 1, 2\) \((2.8)-(2.10)\) and thereby the renormalization group equations \((6.2)-(6.6)\) in (15) depend on \(J\) in an extremely sensitive way. The reason is a feedback between the scaled energy differences \(\rho^{(n)}, \kappa^{(n)}\) - which enter in the diagonals of \(\Delta^{(n+1)}\) - and the largest eigenvalues \(\sigma^{(n+1)}, \tau^{(n+1)}, \xi^{(n+1)}\) \((2.8)-(2.10)\).

This feedback also leads to a dramatic change in the eigenstates \(|\sigma^{(n+1)}\rangle, |\tau^{(n+1)}\rangle, |\xi^{(n+1)}\rangle\). E.g. the square of the first component \(|\sigma_1^{(n+1)}\rangle\) for \(i = 1\) \(\left(\sigma_1^{(n+1)}\right)^2\) in the singlet eigenvector \(|\sigma^{(n+1)}\rangle\) changes completely if we go from the confined \((J_c \leq J \leq 1)\) to the deconfined \((J < J_c)\) regime. In the deconfined regime \(\left(\sigma_1^{(n+1)}\right)^2\) is almost one, which means, that the ground state factorizes into 4 noninteracting singlets. In the confined phase \(\left(\sigma_1^{(n+1)}\right)^2\) is very small. Therefore, the remaining components \(\sigma_i^{(n+1)}, i = 2, \ldots, 7\) contribute significantly to the eigenstate \(|\sigma^{(n+1)}\rangle\).

These contributions are characterized by excitations of the cluster spins on the four plaquette system. Excitations of cluster spins are necessary to induce cluster-cluster interactions. The vanishing of the singlet-triplet gap - as it is observed in the confinement regime \(J_c \leq J \leq 1\) - is a consequence of the cluster-cluster interactions induced by cluster excitations (triplet and quintuplet). We have checked the dependence on the truncation of the interaction matrix by suppressing in Tables II, III, IV (of ref. [15]) all states with one quintuplet plaquette. The dimensions of the interaction matrices reduce to

\[
(d_0, d_1, d_2) = (5, 3, 4) \quad (7.1)
\]

which of course worsens the renormalization group approach. This is signalled by a somewhat larger singlet-triplet gap. As a consequence the deconfined regime \((J \leq J_c)\) is enlarged.

If we look at the deconfinement parameter \(\left(\sigma_1^{(n+1)}\right)^2\), Fig. 11 for the case \((7.1)\), we observe a shift to a larger value of \(J_c\):

\[
J_c(5, 3, 4) = 0.5615 \ldots \quad J_c(7, 9, 14) = 0.4822 \ldots \quad (7.2)
\]
This value is close to the result of ref. (10) obtained without quintuplet excitations. Therefore, the difference in the two values (7.2) reflects the effect of rotational symmetric excited states on the 4 plaquette cluster with one quintuplet. We expect that further excited states with $n_Q = 2, 3, 4$ quintuplets will lead to changes in the values $J_c$ as well. The Monte Carlo simulations of Janke et al. (12) suggest, that the RG results should converge non-monotonously towards 0.549.

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