Hardcore Magnons in the S = 1/2 Heisenberg Model on the Square Lattice

K.P. Schmidt

1 Institute of Theoretical Physics, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

G.S. Uhrig

2 Theoretische Physik, FR 7.1, Geb. E2.6, Universität des Saarlandes, D-66123 Saarbrücken, Germany

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We propose a versatile approach to treat commonly arising constraints. It is illustrated for interacting magnons of the Heisenberg antiferromagnet on a square lattice. For systems of L × L sites a non-perturbative continuous unitary transformation (CUT) is used to derive an effective Hamiltonian conserving the number of magnons. They are bosonic particles with a hardcore constraint which is captured by a local, repulsive interaction U. The limits U → ∞ and L → ∞ are achieved by extrapolation. The residual spin gap Δ1 is smaller than 0.01J reflecting the gapless nature of the magnons. The one-magnon dispersion displays all known characteristics.

Strongly correlated systems in low dimensions display a large variety of fascinating properties like high-Tc superconductivity, quantum antiferromagnetism, quantum ferromagnetism or charge ordering. Theoretically, these phenomena are investigated in simplified models like the Hubbard model, the Heisenberg model and the t-J model. These models are derived from ab-initio calculations, from more elaborate models, for instance three-band Hubbard models, or they are motivated by phenomenological considerations.

In the t-J model transitions to double occupancies are forbidden. This represents a hardcore constraint. An analogous constraint arises if the magnons in an ordered Heisenberg model of spin S are treated as bosons. At most 2S magnons may be present at each site. A reliable treatment of such constraints is still a great challenge to condensed matter theory. Straightforward approaches like mean-field approximations fail because of the large (infinite) energy scale of the hardcore repulsion.

In the present work we describe an innovative approach to treat hardcore constraints and other strong interactions. This approach is exemplified by the antiferromagnetic Heisenberg model on the square lattice. The ground state of this model displays long-range Néel order with magnetic Heisenberg model on the square lattice. The ground state of this model displays long-range Néel order with magnetic Heisenberg model on the square lattice.

The Heisenberg model on the square lattice reads

\[ H = J \sum_{\langle i,j \rangle} S_i S_j \]  

(1)

where \( J > 0 \) denotes the antiferromagnetic exchange constant, \( S_i \) is the vector operator of a spin \( S = 1/2 \) on site \( i \), and \( \langle i,j \rangle \) stands for the summation over nearest neighbors. We take the Néel state with ↓-spins on the A-lattice and ↑-spins on the B-lattice as reference state. This reference state will be mapped to the ground state by a continuous unitary transformation (CUT). The elementary excitations are local spin flips which flip the ↓-spin up on the A-lattice or the ↑-spin up on the B-lattice. Let \( a_\uparrow (a_\downarrow) \) be the corresponding usual bosonic creation (annihilation) operators. These magnon excitations are hardcore particles, i.e., there can be at most one magnon per site. We impose this constraint by a local repulsive magnon-magnon interaction\(^16\).

\[ H^U = U \sum_i a_\uparrow a_\downarrow a_\uparrow a_\downarrow \ . \]

(2)

The hardcore constraint is recovered for \( U \to \infty \).

In terms of the magnons, the Hamiltonian \(^1\) reads

\[ H^{\text{init}} = \sum_q \left[ \omega_q a_\uparrow a_\downarrow + B_q \left( a_\uparrow a_\downarrow + h.c. \right) \right] + \sum_{k,k',q} V_{k,k',q} a_\uparrow a_\downarrow a_\uparrow a_\downarrow \]

(3)

up to a constant. All energies are given in units of \( J \). The one-particle couplings are \( \omega_q = 2 \), \( B_q = \frac{1}{2} (\cos(q_x) + \cos(q_y)) \), and the two-particle couplings are \( V_{k,k',q} = U/N - 1/(2N) [\cos(k_x' + q_x - k_x) + \cos(k_y' + q_y - k_y) + \cos(k_x') + \cos(k_y')] \).
q_y - k_y) + \cos(q_x) + \cos(q_y)] = U/(2N) + f(k, k', q). The Hamiltonian remains invariant under translations by one lattice constant a (set to unity) in spite of the Néel state as reference state because a spin rotation by 180° has been performed on one sublattice. The two-particle couplings are manifestly symmetric under the exchange $k \leftrightarrow k'$ and $q \leftrightarrow k' + q - k$. Numerically, we deal with a finite sample of linear size $L$ with $N = L \times L$ sites and periodic boundary conditions.

A CUT\textsuperscript{18,19} is used to derive an effective Hamiltonian $H^{\text{eff}}$ which conserves the number of magnons\textsuperscript{20,21}. This is done by solving the flow equation

$$\partial_\ell H(\ell) = [\eta(\ell), H(\ell)]$$

(4)

where $\ell$ is a continuous auxiliary variable and $\eta(\ell)$ the infinitesimal anti-Hermitian generator. The initial condition is $H(\ell = 0) = H^{\text{init}}$. In the present work, the CUT is realized in a self-similar, renormalizing fashion in momentum space. The commutators for all expressions are computed using the standard bosonic algebra in a self-similar, renormalizing fashion in momentum space. At maximum quartic terms in the bosonic operators are kept. Higher terms involving six bosons are neglected after normal-ordering with respect to the bosonic vacuum. So the Hamiltonian remains in the self-similar form of a Hamiltonian of pairwise interacting bosons

$$H(\ell) = \sum_q \left[ \omega_q a_q^\dagger a_q + B_q^{(\ell)} \left( a_q^\dagger a_{-q}^\dagger + \text{h.c.} \right) \right]$$

(5)

$$+ \sum_{k,k',q} V_{k,k',q} a^\dagger_{k-\Delta} a^\dagger_{k+\Delta} q a_{-q} a_{k'}$$

$$+ \sum_{k,k,k_1,k_2,k_3} \Delta^{(\ell)}_{k_1,k_2,k_3} \left( a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3} a_{k_1+k_2+k_3} + \text{h.c.} \right).$$

The anti-Hermitian generator $\eta(\ell)$ is chosen to be

$$\eta(\ell) = \sum_q B_q^{(\ell)} \left( a_q^\dagger a_{-q}^\dagger + \text{h.c.} \right)$$

(6)

$$+ \sum_{k,k,k_1,k_2,k_3} \Delta^{(\ell)}_{k_1,k_2,k_3} \left( a^\dagger_{k_1} a^\dagger_{k_2} a^\dagger_{k_3} a_{k_1+k_2+k_3} + \text{h.c.} \right).$$

The effective Hamiltonian $H^{\text{eff}} := H(\ell = \infty)$ is characterized by $\omega^{\text{eff}} := \omega^{(\ell = \infty)}$ and by $V_{k,k',q} := V_{k,k',q}^{(\ell = \infty)}$; the other terms have to vanish.

Comparing the coefficients of the same terms on the left and on the right hand side of Eq. (4) yields the (high dimensional) set of differential equations to be solved, which is done numerically. We treat systems of up to $14 \times 14$ sites. The transformation can safely be carried out as long as the non-diagonal part of the Hamiltonian is decreasing monotonically\textsuperscript{22}. As a measure of the non-diagonal part we define the residual off-diagonality

$$\text{ROD}^2 := \frac{\sum_q \left( B_q^{(\ell)} \right)^2 + \sum_{k_1,k_2,k_3} \left( \Delta^{(\ell)}_{k_1,k_2,k_3} \right)^2}{\sum_q \left( B_q^{(\ell = 0)} \right)^2}.$$  

(7)

Unfortunately, the numerical treatment of the flow equations reveals a significant increase of the ROD: no $H^{\text{eff}}$ can be obtained. In looking for the reason for this failure we must keep in mind that the ROD decreases as long as it is dominated by terms in which the change of the number of elementary excitations is correlated to the change of the energy as measured by the diagonal part of the Hamiltonian\textsuperscript{21,23,24}. In our system this means that an increase in the number of magnons has to imply an increase of the diagonal energy. If states with an incremented number of excitations are lower in energy the CUT breaks down. So a negative gap implies the failure of the CUT, see e.g. Ref. \textsuperscript{22}. This happens also in the system at hand. There is a bound state of two magnons with such a high binding energy that its excitation energy is negative.

Why does this happen? The spin rotation symmetry requires that there has to be a tightly bound state. Dealing with finite clusters there is no true symmetry breaking so that the ground state is a singlet and the elementary excitation is a gapped triplet with three degenerate states $S^z = \{ -1,0,1 \}$. The description in terms of magnons, i.e. spin flips up or down, canonically provides two of them, namely at $S^z \in \{ -1,1 \}$. The triplet with $S^z = 0$ has to be found in the sector with at least two magnons, one spin flip up and one down. The energy of this state is equal to the energy of an elementary magnon, i.e. the $S^z = 0$ triplet must be a bound state of two magnons. This argument unambiguously shows that a magnon description of quantum antiferromagnets in or close to the paramagnetic phase implies a very strong interaction between these magnons.

The fact that we neglected higher interactions spoils the delicate balance of magnon motion and magnon-magnon interaction. The numerics revealed that the attractive magnon-magnon interaction is overestimated leading to a too strongly bound $S^z = 0$ state. To remedy this problem we reduce the interaction by hand (see below) so that the spin symmetry, namely the degeneracy between the one-magnon states at $\Delta_1 := \omega^{\text{eff}}_{q=0} = 0$ and the two-magnon bound state at $\Delta_2 := \omega^{2\text{mag}}_{K=(0,0)}$ is restored, i.e. $\Delta_1 = \Delta_2$. Here $\omega^{2\text{mag}}_K$ is the energy of the two-magnon bound state at total momentum $K$ which can be determined by standard numerics once $H^{\text{eff}}$ has been found. For $K = (0,0)$, we solve the secular equation $H^{\text{eff}} \sum_q A_q^\dagger[q] - q = \Delta_2 \sum_q A_q[q] - q$ where $|q|$ stands for a single magnon at momentum $q$. The $S = 1$ state with $S^z = 0$ displays the symmetry $A_q^\dagger[(\pi,\pi)] = -A_q$. The attractive interaction is diminished by reducing initial nearest-neighbor attraction by the reduction factor $0 < \lambda \leq 1$

$$V_{k,k',q} \rightarrow V_{k,k',q}^{\lambda} = U/(2N) + \lambda f(k, k', q).$$

(8)

The case $\lambda = 0$ corresponds to the total omission of the attractive magnon-magnon interaction keeping only the repulsive hardcore interaction. The actual initial Hamiltonian $H^{\text{init}}$ is recovered for $\lambda = 1$. The value of $\lambda$ is
fixed to $\lambda_c$ where $\Delta_2 = \Delta_1$ holds. The above analysis of the failure of the direct CUT turns out to be valid. As long as $\lambda \lesssim \lambda_c$ the ROD decreases monotonically for large $\ell$ and the flow equations converge.

The effective Hamiltonians $H_{\text{eff}}(L, U)$ were obtained for systems up to $L = 14$ and $U = 500$. The flow equations were integrated until the ROD fell below $10^{-4}$. The large value of the interaction $U$ necessitates a careful numerical treatment of the flow equations for small values of the flow $\ell \leq 1/U$ leading to a slowing down of the program. Thus parallelization is mandatory to be able to deal with large systems.

Fig. 1 depicts a generic example how the bound state energy $\Delta_2$ depends on the reduction factor $\lambda$. At $\lambda_c \approx 0.82592$ a clear intersection is discernible; the corresponding gap value is $\Delta_1(L=8) = \Delta_2(L=8) = 0.25008$. The fact that $\Delta_2 < 2\Delta_1$ (dashed-dotted curve in Fig. 1) shows that a true binding phenomenon is observed for appreciable interaction $\lambda \gtrsim 0.76$. For small values of $\lambda$ the repulsive interaction parametrized by $U$ dominates and the system shows a large gap of the order $J$.

The same procedure has been performed for many values of $L$ and $U$. All reduction factors $\lambda_c$ range from 0.81 to 0.83. Extrapolating them in $1/U$ and in $1/L$ leads to $\lambda_c(L = \infty, U = \infty) = 0.825$. The deviation of $\lambda_c(L = \infty, U = \infty)$ from unity, i.e. $\approx 17\%$, is a first estimate for the size of the truncation error. In Fig. 2 the corresponding gaps $\Delta_1(L, U)$ are shown. Linear extrapolation in $1/U$ yields the values at $U = \infty$. We found that a subsequent extrapolation in $1/L$ does not work. But an extrapolation in $1/\sqrt{L}$ works obviously very well. Except for $L = 4$, all data points lie nicely on straight lines. This makes us confident to proceed on the basis of the $1/\sqrt{L}$ extrapolation although we do not know of an a priori reason for this unusual scaling. We presume that it results from using the Néel state as starting point for the treatment of finite clusters.

It is reassuring that the residual gap $\Delta(L = \infty, U = \infty)$ is as small as 0.006. We take this fact as evidence that we could restore the spin symmetry by the procedure of reducing the initial attractive interaction in Eq. 8.

![FIG. 1: Example of the one-magnon gap $\Delta_1$ (circles) and the two-magnon bound state energy $\Delta_2$ (squares) as function of the factor $\lambda$ in Eq. 8. The solid lines are splines; the inset zooms at the intersection $\Delta_1 = \Delta_2$.](image1)

![FIG. 2: The one-magnon gap $\Delta_1(L, U)$ as function of $1/\sqrt{L}$. The value at $U = \infty$ stem from extrapolation in $1/U$. Solid lines are linear inter-/extrapolations.](image2)

![FIG. 3: Upper panel: quantum correction factor $Z_c$ of the spin wave velocity is extrapolated in $1/U$ and $1/L$; for comparisons, see main text. Lower panel: inter-/extrapolation of the dispersion at two points of high symmetry. The points represent results extrapolated linearly in $1/U$ to $U = \infty$.](image3)

Next, we study the spin wave velocity $c$. It is characterized by the correction factor $Z_c$ which quantifies the renormalization relative to the result of spin wave theory $c = 2\sqrt{Z_c}^{1.3.5}$. Since finite lattices are studied the determination of a group velocity at vanishing momentum
is not possible. Thus we exploit the well-known shape of the dispersion, and derive the velocity from
\[ c = \max_{q \in BZ} \frac{\omega_q^{\text{eff}}}{|q|} \]  
(9)
where we use implicitly that the spin gap \( \Delta_1 \) vanishes. The upper panel in Fig. 7 depicts the results and their extrapolations. Since the bosonic dispersion \( \omega_q^{\text{eff}} \) appears generically as square root \( \sqrt{\Delta_q^2 + f(q)} \) with a smooth function \( f(q) \) with \( f(0,0) = 0 \) it is consistent to extrapolate finite values \( \omega_q^{\text{eff}} \) in \( 1/L \) when the vanishing gap \( \Delta_1 \) scales like \( 1/\sqrt{L} \). We obtain \( Z_s(L = \infty, U = \infty) = 1.14 \) which is about 3% away from the best values \( Z_s^{\text{eff}} = 1.17947 \) (third order spin wave theory) and \( Z_e^{\text{eff}} = 1.178(1) \) (high order series expansion). In view of the error estimate of 17% on the basis of \( 1 - \lambda_c \), the deviation in the low energy part of the spectrum is small and the result shows that the CUT approach is a valid way to tackle hardcore constraints.

At high energies it is known that the difference between \( \omega_{(\pi/2,\pi/2)}^{\text{eff}} \) and \( \omega_{(0,0)}^{\text{eff}} \) is difficult to find. The third order spin wave results hardly display any dispersion between \( q = (\pi/2,\pi/2) \) and \( q = (0,\pi) \). But series expansion and quantum Monte Carlo calculations clearly show an appreciable difference between the dispersion at \( q = (\pi/2,\pi/2) \) and \( q = (0,\pi) \). One finds at \( q = (\pi/2,\pi/2) \) a saddle point with \( \omega_{(\pi/2,\pi/2)}^{\text{eff}} \approx 2.17 \) and at \( q = (0,\pi) \) the maximum with \( \omega_{(0,\pi)}^{\text{eff}} \approx 2.39 \). In the lower panel of Fig. 7 the corresponding results in our approach are displayed. The appropriate extrapolations finally yield \( \omega_{(\pi/2,\pi/2)}^{\text{eff}} \approx 1.84 \) and \( \omega_{(0,\pi)}^{\text{eff}} \approx 2.23 \). Hence, the former value deviates by about 15% and the latter one by about 7%. These deviations do not surprise in view of the first estimate of 17% on the basis of \( 1 - \lambda_c \). We conclude that the omission of terms beyond the two-magnon interaction implies a truncation error of about 17%. This is an encouraging result because it is surely possible to include at least the dominant parts of the higher magnon terms for further improvement.

Further support for the approach chosen comes from the fact that \( \omega_{(\pi/2,\pi/2)}^{\text{eff}} \) is significantly lower than \( \omega_{(0,\pi)}^{\text{eff}} \) which agrees qualitatively with the results by series expansion and quantum Monte Carlo. The quantitative difference, however, is overestimated by about a factor 2 which is attributed to the truncation of higher magnon terms. But the results show that the approach proposed captures the essential physics also at higher physics in contrast to diagrammatic spin wave theory.

In summary, we propose non-perturbative continuous unitary transformations to treat the interactions arising from constraints. This is successfully illustrated for magnons in the Heisenberg quantum antiferromagnet on the square lattice. All qualitative aspects of the dispersion are retrieved when the symmetry between elementary magnons and bound pairs of magnons is restored. This finding demonstrates that magnons in an antiferromagnet constitute a strongly correlated system. Quantitatively, the results agree with previous findings within 17%. Presently, the CUT approach is less accurate than the highly developed series expansions. But its accuracy can certainly be enhanced and it is a versatile tool which can be used for the constraints in a multitude of models, including also doped systems, because it is formulated in the standard form of second quantization.

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