The excitation spectrum of the two-chain Heisenberg ladder with antiferromagnetic interactions is studied. Our approach is based on the description of the excitations as triplets above a strong-coupling singlet ground state. The quasiparticle spectrum is calculated by treating the excitations as a dilute Bose gas with infinite on-site repulsion. Additional singlet ($S=0$) and triplet ($S=1$) excitations are found as quasiparticle bound states. Thus it is demonstrated that the spectrum consists of one elementary triplet, one composite triplet, and one composite singlet.

In addition, the hard core constraint $t^i_{αi}t^j_{βj} = 0$ has to be enforced on every site [1]. This exclusion of double occupancy reflects the quantization of spin and ensures the uniqueness of the mapping from (1) to (3). At the quadratic level the Hamiltonian (3) can be diagonalized by a combination of Fourier and Bogoliubov transformations $t_{αk} = u_k t_{αk} + v_k t_{⊥k}$. This gives the excitation spectrum: $\omega_k^2 = A_k^2 - B_k^2$, where $A_k = J_⊥ + J \cos k$ and $B_k = J \cos k$.

In order to address the problem of bound states of two triplets a reliable description of the one-particle spectrum is needed. We find, in agreement with previous work [11], that the effect of the quartic terms in (3) on the triplet spectrum is small and therefore we proceed by treating these terms in mean field theory. This is equivalent to taking into account only one-loop diagrams (first order in $J$). These diagrams lead to the renormalization:

$$A_k = J_⊥ + J(1 + 2f_1) \cos k, \quad B_k = J(1 - 2g_1) \cos k,$$

where $f_1 = <t^i_{αi}t^i_{αi+1}> = N^{-1} \sum_q v_q^2 \cos q$ and $g_1 = <t^i_{αi}t^j_{βi}> = N^{-1} \sum_q u_q v_q \cos q$.

The dominant contribution to the spectrum renormalization is related to the hard core condition. Previous treatments have used mean-field approximations [11] and are essentially uncontrolled, especially for a quasi-1D system. To deal with the constraint we will use the diagrammatic approach developed by us in Ref. [13]. An infinite on-site repulsion is introduced in this approach in order to forbid double occupancy:

$$H_U = \frac{U}{2} \sum_{i,α,β} t^i_{αi}t^j_{βi}t^i_{βi}t^j_{αi}, \quad U \to \infty$$

Since the interaction is infinite, the exact scattering amplitude $\Gamma_{αβ,γδ}(K) = \Gamma(K)δ_{αγ}δ_{βδ}$. $K \equiv (k, \omega)$, for the triplets has to be found. This quantity satisfies the Bethe-Salpeter equation, shown in Fig.1(a) and depends
on the total energy and momentum of the incoming particles \( K = K_1 + K_2 \). The interaction (5) is local and non-retarded which allows for an analytic solution of the equation for \( \Gamma \):

\[
\Gamma^{-1}(K) = i \int \frac{d^2Q}{(2\pi)^2} G(Q) G(K - Q) = - \frac{1}{N} \sum_q \frac{u^2 u^2_{-q}}{\omega - \omega_q - \omega_{k-q}} + \left\{ \begin{array}{l} u \to v \\
 \omega \to -\omega \end{array} \right\}
\]

(6)

Here \( G(Q) \) is the normal Green’s function (GF) \( G(k,t) = -i < T(t_{ka}(t)t_{ka}(0)) > \) and the Bogoliubov coefficients \( u^2_k, v^2_k = \pm 1/2 + A_k/2\omega_k \). The basic approximation made in the derivation of \( \Gamma(K) \) is the neglect of all anomalous scattering vertices, which are present in the theory due to the existence of anomalous GF’s, \( G_\alpha(k,t) = -i < T(t_{\alpha ka}(t)t_{\alpha ka}(0)) > \). Our crucial observation \([12]\) is that all anomalous contributions are suppressed by a small parameter which is present in the theory - the density of triplet excitations \( n = \sum_\alpha < t_{\alpha ka}(t) t^\dagger_{\alpha ka}(0) > = 3N^{-1} \sum_q v^2_q \). We find that \( n \approx 0.1 \) (\( J_\perp/J = 2 \)), \( n \approx 0.25 \) (\( J_\perp/J = 1 \)) and it generally increases as \( J_\perp \) decreases. Since summation of ladders with anomalous GF’s brings additional powers of \( v \) into \( \Gamma \), their contribution is small compared to the dominant one of Eq.(6). For consistency we also neglect the second term in Eq.(6). Thus the triplet excitations can be viewed as a strongly-interacting dilute Bose gas and Eq.(6) as the first term in an expansion in powers of the gas parameter \( n \) \([12]\).

The self-energy, corresponding to the scattering amplitude \( \Gamma \) is given by the diagrams in Fig.1(b):

\[
\Sigma(k,\omega) = \frac{4}{N} \sum_q v^2_q \Gamma(k + q, \omega - \omega_q). \quad (7)
\]

In order to find the renormalized spectrum, one has to solve the coupled Dyson’s equations for the normal and anomalous GF’s. After separating the result for the normal GF into a quasiparticle contribution and incoherent background, we find \([12]\):

\[
G(k,\omega) = \frac{Z_k U^2_k}{\omega - \Omega_k + i\delta} - \frac{Z_k V^2_k}{\omega + \Omega_k - i\delta} + G_{\text{inc}}. \quad (8)
\]

The renormalized triplet spectrum and the renormalization constant are:

\[
\Omega_k = Z_k \sqrt{|A_k + \Sigma(k,0)|^2 - B^2_k}, \quad \Omega^{-1}_k = 1 - \left( \frac{\partial\Sigma}{\partial\omega} \right)_{\omega=0}. \quad (9)
\]

The renormalized Bogoliubov coefficients in (8) are:

\[
U^2_k, V^2_k = \pm \frac{1}{2} + \frac{Z_k[A_k + \Sigma(k,0)]}{2\Omega_k}. \quad (10)
\]

Equations (8,9,10) have to be solved self-consistently for \( \Sigma(k,0) \) and \( Z_k \). From Eq.(8) it also follows that one has to replace \( u_k \to \sqrt{Z_k} U_k, v_k \to \sqrt{Z_k} V_k \) in (4), (8) and (9) (see also Eq.(14) below).

Let us demonstrate how this approach works in the strong-coupling limit \( J_\perp \gg J \). To first order in \( J/J_\perp \), \( A_k = J_\perp + J \cos k \) and \( B_k = J \cos k \). This leads to \( \omega_k \approx A_k = J_\perp + J \cos k, u_k \approx 1, v_k \approx -(J/2J_\perp) \cos k \) and \( f_0 = 1, g_0 = -J/AJ_\perp \). Substitution into (4), (8) and (9) gives

\[
\Gamma(k,\omega) = 2J_\perp - \omega, \quad (11)
\]

\[
\Sigma(k,\omega) = (J/J_\perp)^2(3J_\perp - \omega)/2.
\]

Then from Eq.(8) we find the quasiparticle residue \( Z = 1 - (1/2)(J/J_\perp)^2 \) and the dispersion

\[
\frac{\Omega_k}{J} = \frac{J_\perp}{J} + \cos k + \frac{J}{4J_\perp} - \frac{J}{4J_\perp} \cos 2k. \quad (12)
\]

The result (12) agrees with that obtained by direct \( J/J_\perp \) expansion \([3]\) to this order. For arbitrary \( J_\perp \) a self-consistent numerical solution of Eqs.(8,9,10) is required. The triplet excitation spectrum obtained from this solution for \( J_\perp/J = 2 \) is shown in Fig.3. For comparison the dispersion obtained by 8-th order dimer series expansion \([3]\) is also plotted. The agreement between the two curves is excellent which reflects the smallness of the triplet density \( n \approx 0.1 \). However for smaller values of the inter-chain coupling, e.g. \( J_\perp = J \) the disagreement between our and the numerical results is as large as 20% at \( k = 0 \) which reflects a transition into a regime, dominated by very strong quantum fluctuations. Since a more refined analysis is required in this regime from now on we will concentrate on the case \( J_\perp/J = 2 \).

The quartic interaction in the Hamiltonian \([3]\) leads to attraction between two triplet excitations. We will show that the attraction is strong enough to form a singlet \((S=0)\) and a triplet \((S=1)\) bound state. Let us consider the scattering of two triplets: \( q_1 \alpha + q_2 \beta \to q_3 \gamma + q q_0 \) and introduce the total \((Q)\) and relative \((q)\) momentum of the pair \( q_1 = Q/2 + q, q_2 = Q/2 - q, q_3 = Q/2 + p, \) and \( q_4 = Q/2 - p \). The bare (Born) scattering amplitude is (see Fig.2(a)):

\[
M_{\alpha\beta,\gamma\delta} = J (\delta_{\alpha\gamma} \delta_{\beta\delta} - \delta_{\alpha\delta} \delta_{\beta\gamma}) \cos(q+p) + J (\delta_{\alpha\delta} \delta_{\beta\gamma} - \delta_{\alpha\gamma} \delta_{\beta\delta}) \cos(q-p) + U (\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}). \quad (13)
\]

The \( J \) and the \( U \) terms arise from the quartic interaction in (3) and the constraint \([3]\) respectively. We also have to take into account that the triplet excitation differs from the bare one due to the Bogoliubov transformation and the quasiparticle residue. Therefore we have to make the substitution:

\[
M_{\alpha\beta,\gamma\delta} \to \sqrt{Z_{q_1} U_{q_1}} \sqrt{Z_{q_2} U_{q_2}} \sqrt{Z_{q_3} U_{q_3}} \sqrt{Z_{q_4} U_{q_4}} M_{\alpha\beta,\gamma\delta}. \quad (14)
\]
The bound state satisfies the Bethe-Salpeter equation for the poles of the exact scattering amplitude $M$. This equation is presented graphically in Fig.2(b) and has the form \[[14]:

\[ E_Q - \Omega_{Q/2+q} - \Omega_{Q/2-q} \] \psi(q) = \frac{1}{2} \int \frac{dp}{2\pi} M(Q, q, p) \psi(p). \tag{15} \]

Here $M(Q, q, p)$ is the scattering amplitude in the appropriate channel (see Eqs.(16,19) below), $E_Q$ is the energy of the bound state and $\psi(q)$ is the two-particle wave function. Let us introduce the minimum energy of two excitations with given total momentum (lower edge of the two-particle continuum) $E_Q^\ominus = \min_q \{ \Omega_{Q/2+q} + \Omega_{Q/2-q} \}$. If a bound state exists then its energy is lower than the continuum $E_Q < E_Q^\ominus$. The binding energy is defined as $\epsilon_Q = E_Q^\ominus - E_Q > 0$.

In the singlet ($S=0$) channel the scattering amplitude is:

\[ M^{(0)} = \frac{1}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} M_{\alpha\beta,\gamma\delta} = -4J \cos q \cos p + 2U. \tag{16} \]

First we consider the strong-coupling limit $J_\perp \gg J$. In this limit $Z_q = U_q = 1$ and $\Omega_q = J_\perp + J \cos q$. The edge of the continuum is $E_Q^\ominus = 2J_\perp - 2J \cos Q/2$ and therefore the Bethe-Salpeter equation [14] is reduced to the simple form

\[ \left[ \epsilon_Q^{(0)} + 2JC_Q(1 + \cos q) \right] \psi(q) = 2J \cos q \int \frac{dp}{2\pi} \cos p \psi(p) - U \int \frac{dp}{2\pi} \psi(p). \tag{17} \]

We have introduced here the notation $C_Q = |\cos Q/2|$. The solution of (17) is:

\[ \psi^{(0)}(q) = \sqrt{2(1 - C_Q^2)} \frac{\cos q + C_Q}{\epsilon_Q^{(0)} / J + 2C_Q(1 - \cos q)} \epsilon_Q^{(0)} = J(1 - C_Q)^2. \tag{18} \]

We stress that the infinite on-site repulsion enforces the condition $\int dp \psi(p) = 0$ which means that the bound state is d-wave like. Thus we see that in the strong-coupling limit a singlet bound state always exists. At $J_\perp = 2J$ Eq.(15) with the substitutions (16,14) has to be solved numerically and the result is presented in Fig.3. We find that for $k \lesssim 2\pi/5$ the binding energy is practically zero in this case.

In the triplet ($S=1$) channel the scattering amplitude is:

\[ M^{(1)} = \frac{1}{2} \epsilon_{\mu\alpha\beta} \epsilon_{\nu\gamma\delta} M_{\alpha\beta,\gamma\delta} = -2J \sin q \sin p. \tag{19} \]

In this formula there is no summation over the index $\mu$ which gives the spin of the bound state. By solving the Bethe-Salpeter equation in the limit $J_\perp \gg J$ we obtain for the wave-function and the binding energy:

\[ \psi^{(1)}(q) = \sqrt{\frac{1/2 - 2C_Q^2}{\epsilon_Q^{(1)} / J + 2C_Q(1 + \cos q)}} \frac{\sin q}{\epsilon_Q^{(1)} = 2J(1 - C_Q^2)^2, \ C_Q < 1/2.} \tag{20} \]

For $C_Q > 1/2$ we find $\epsilon_Q^{(1)} = 0$ which means that the triplet bound state only exists for momenta $k > Q_c = 2\pi/3$ (in the strong-coupling limit). At $J_\perp = 2J$ the numerical solution of Eq.(15), plotted in Fig.3, shows that the bound state exists down to $k \approx \pi/2$. We find that the coupling in the triplet channel is weaker than the one in the singlet channel.

The size of the bound state is determined by the spatial extent of the bound state wave function:

\[ R_{\text{rms}} = \sqrt{\langle r^2 \rangle} = \left\{ \int \left( \frac{\partial \psi(q)}{\partial q} \right)^2 dq \frac{1}{2\pi} \right\}^{1/2} \tag{21} \]

In the strong-coupling limit we find, by substituting Eqs.(18,20),

\[ R_{\text{rms}} = \left\{ \frac{(1 + C_Q^2)^{1/2}(1 - C_Q)^{-1}}{(1 + 4C_Q^2)^{1/2}(1 - 4C_Q^2)^{-1}} \right\}^{1/2}, \ S = 0 \]

(22)

in units of the lattice spacing. As expected the size of the bound state increases with decreasing binding energy and near the threshold $R_{\text{rms}} \sim (\epsilon)^{-1/2}, \epsilon \to 0$, as can be seen from Eqs.(18,20,22). The self-consistent solution for $J_\perp = 2J$ is shown on Fig.4. Except for momenta, very close to the threshold, the bound states in both channels have typical sizes of a few lattice spacings.

Finally, there is no bound state in the tensor ($S = 2$) channel. This can be seen from the expression for the scattering amplitude in this case $M^{(2)} = 2J \cos q \cos p + 2U$ which corresponds to repulsion.

In conclusion, we have studied two-particle bound states in the two-leg antiferromagnetic Heisenberg ladder and have shown that a singlet bound state is always present, while a triplet one exists only in a limited range of momenta. In order to find the one-particle spectrum we have used a new diagrammatic method to take into account the hard-core constraint by treating the excitations as a dilute Bose gas. Our approach is very general and applicable to any spin model for which the excitations can be described as triplets above a strong-coupling singlet ground state. We can claim that bound states are present practically in any system with dimerization. By using the techniques described in this Letter we have also proven the existence of bound states in the two-layer Heisenberg model. Our general picture for the structure of the excitation spectrum fits very well into the recently suggested strong analogy between quantum chromodynamics and quantum antiferromagnetism [14]. One can consider the elementary on-site spin 1/2 as a quark and...
the set of triplet and singlet excitations as vector and scalar mesons. From this analogy one can expect that there are even more complex excitations, such as many-particle bound states, in quantum spin models of this type [14].

We would like to thank M. Kuchiev, J. Oitmaa and Z. Weihong for stimulating discussions and J. Oitmaa for critical reading of the manuscript. This work was supported by the Australian Research Council.

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FIG. 1. (a) Equation for the scattering amplitude $\Gamma$. (b) Diagrams for the self-energy, corresponding to $\Gamma$.

FIG. 2. (a) The bare (Born) scattering amplitude $M$. (b) The Bethe-Salpeter equation for the poles of the exact scattering amplitude $\tilde{M}$.

FIG. 3. The excitation spectrum of the ladder for $J_\perp = 2J$. The solid lines are the elementary triplet spectrum (lower curve at $k = \pi$) and the lower edge of the two-triplet continuum (upper curve). The dots are numerical results obtained by dimer series expansions [5]. The dashed and the dot-dashed lines represent respectively the triplet and singlet bound states.

FIG. 4. The size $R_{rms}$ of the bound states. The vertical dashed lines represent the points where the binding energy vanishes.
\[ \begin{align*} 
&K_1 \alpha \quad K_3 \gamma \\
&\Gamma \quad = \quad U \\
&K_2 \beta \quad K_4 \delta
\end{align*} \]
\[
\begin{align*}
\alpha & \quad \gamma \\
\beta & \quad \delta
\end{align*}
\]

\[
M = \frac{Q}{2} + q \quad \frac{Q}{2} + p
\]

\[
\tilde{M} = \frac{Q}{2} - q \quad \frac{Q}{2} - p
\]

(a)

(b)

\[
U + J
\]

FIG.2.
FIG. 3.

two–particle continuum

$\Omega_{k}/J$ vs. $k$ for $S=0$ and $S=1$. 

---

*Note:* The figure illustrates the behavior of the function $\Omega_{k}/J$ as a function of $k$ for different spin states ($S=0$ and $S=1$). The curves show the two-particle continuum in the context of a physical system, typically encountered in condensed matter physics or quantum mechanics.
