We calculate the excitation spectra for the one-d Heisenberg-Ising antiferromagnets by expansions around the Ising limit. For $S = 1/2$, the calculated expansion coefficients for the spinon-spectra agree term by term with the solution of Johnson and McCoy. For $S = 1$, the solitons become gapless before the Heisenberg limit is reached, signalling a transition to the Haldane phase. By applying a staggered field we calculate the one-magnon spectra for the $S = 1$ Heisenberg chain. For $S = 3/2$ the quantum renormalization of the spin-wave spectra is calculated to be approximately 1.16.

The study of spin-chains has produced many exciting ideas in many-body physics. The combination of exact solutions, field theories and numerical studies have led to a rather comprehensive understanding of the physical properties of these systems [1]. One of the most remarkable physics to come out of one-dimensional antiferromagnets is the difference between the excitation spectra of integer and half-integer spin-chains. The $S = 1/2$ chain is integrable and a lot is rigorously known about its excitation spectra. de Cloiseaux and Pearson [2] were the first to obtain expressions for the spectrum of the Heisenberg model. Later Johnson and McCoy [3] obtained expressions for the low lying excitations of the Heisenberg-Ising model.

Fadeev and Takhtajan [4] argued that the elementary excitations for the spin-half case are spinons and have the quantum numbers of a neutral fermion. Using semiclassical arguments, Haldane [5] showed that the topological excitations for integer spin-chains had integer spin and those for half-integer spin-chains had half-integer spin. He further argued that for integer spin these solitons become gapless before the Heisenberg limit is reached. Condensation of these solitons leads to a novel ground state, with a gap in the magnon excitation spectra. For half integer spins the spectra remains similar to the spin-half case, becoming gapless and linear at the Heisenberg point. By now there are numerous numerical [6] confirmations of these remarkable facts.

In this paper we show that the spectra for the topological excitations such as spinons and solitons as well as the small spin-deviation excitations or magnons can be calculated systematically by a straightforward Raleigh-Schrodinger perturbation theory. This is simply a consequence of the fact that in one-dimensional a domain-wall between two ground states is a localized object and has a well defined dispersion. While the perturbation expansion gives essentially the complete answer for systems with significant Ising anisotropy, it is also very accurate for Heisenberg systems. For $S = 1/2$, our calculated coefficients for the spinon spectra agree term by term with a direct expansion of the closed form results of Johnson and McCoy [3]. We also calculate the soliton excitation spectra for the $S = 1$ chain and find that it becomes gapless before the Heisenberg model is reached. As shown by Haldane [5] these solitons play the same role as the domain-walls in the 1 + 1-dimensional classical Ising model, where vanishing free-energy cost for the domain-walls leads to a second order phase transitions.

In addition to the topological excitations we also calculate the spectrum for magnons which are the quanta for small spin-deviations around a given state. For $S = 1/2$ chain, a magnon is not a sharply defined state even in the Ising limit as its energy is degenerate with that of two spinons. Thus it can break apart into two spinons. For $S \geq 1$, magnons are well defined elementary excitations near the Ising limit. For $S = 1$, we add a staggered field term to the Hamiltonian, with a coefficient which goes to zero at the Heisenberg point. The presence of this term avoids the condensation of solitons with non-zero Ising anisotropy, and allows us to calculate the magnon excitation spectra in the Heisenberg limit. Even simple addition of available terms in the series leads to a spectrum which agrees with previous numerical estimates to within a few percent.

For $S = 3/2$ we are not aware of any previous numerical calculation of the spin-wave excitation spectra. Our calculations provide extremely accurate estimates of the spectra for systems with significant Ising anisotropy. We find that the series also show good convergence upto the Heisenberg limit especially away from the gapless point near $q = 0$, where they are consistent with a linear spectra but converge more slowly. We estimate the quantum renormalization of the spin-wave spectrum from the maximum spin-wave energy as was done in recent experiments on CsVCl$_3$ [7]. We obtain this renormalization to be approximately 1.16. This is larger than the order $1/S$ spin-wave estimate of 1.12 [8] but still smaller than the central estimates of the experiments which give 1.26 [9]. However, the experimental uncertainties are ±0.2 due to large uncertainties in the value of $J$.

In the Ising limit all these excitations are localized, and those localized at different points in space are degenerate. The magnons consist of a single spin-deviation in a Neel state, whereas a soliton or a spinon is a domain wall.
between two degenerate ground states. A simple way
to think of the topological excitations is in terms of the
ground state of a large odd-site ring. In the Ising limit,
an $N$-site ring has at least $N$ degenerate ground states,
corresponding to the different locations where the neigh-
boring spins are not antiparallel. This broken bond can
be thought of as the domain-wall. Since, these ground-
state configurations differ locally from the ground state
of an even site ring only at the wall, i.e. the energy-density
with respect to the ground-state is non-zero only on one
bond, we can regard the excitation as localized there. As
the $x-y$ coupling is turned on these degenerate ground
states evolve into a band of states with well-defined en-
ergy momentum relation. Thinking in terms of an odd-
site ring also explains why these domain-wall excitations
have half-integer spin for spin-half chains and integer spin
for integral spin-chains. In the Ising limit a spin-chain
has recently been formulated in terms of a cluster expan-
sion by Gelfand [9]. The magnon calculation is similar to
that in higher dimension [10], but the solitons are special
to one-d as discussed in the previous paragraph. For the
purpose of our calculation we only need to focus on the
vicinity of the excitation. The boundaries can be con-
sidered to be infinitely far away and do not matter. The
degenerate perturbation theory, allows us to construct an
effective hamiltonian in the space of these localized Ising
states, which can then be diagonalized straightforwardly
by Fourier transformation. The recursive procedure for
obtaining the effective Hamiltonian has been discussed
by Gelfand [11].

We consider the Heisenberg-Ising Hamiltonian:

$$
\mathcal{H} = J \sum_i S_i^x S_{i+1}^x + \lambda (S_i^z S_{i+1}^z + S_i^y S_{i+1}^y).
$$

(1)

For the $S = 1/2$ case it is most convenient to present
the square of the spinon dispersion, which we calculate via
the cluster expansion to order $\lambda^{12}$

$$
16\epsilon(q)^2 = 4 + 20\lambda^2 - 6\lambda^4 - \frac{3}{2} \lambda^6 + \frac{3}{8} \lambda^8 - \frac{9}{16} \lambda^{12} + \cos 2q(16\lambda + 4\lambda^3 - \frac{2}{3} \lambda^7 - \frac{3}{4} \pi \lambda^9 + \frac{1}{4} \pi \lambda^{11}) + O(\lambda^{13})
$$

(2)

A closed form expression for the spinon dispersion can be
read off from the work of Johnson and McCoy [4]:

$$
\epsilon(q) = (1 - \lambda^2)^{1/2} \frac{K}{\pi} (1 - k^2 \sin^2 q)^{1/2}
$$

(3)

Here $K$ (and similarly $K'$) is a complete elliptic integral
of the first kind with modulus $k$. The latter is determined
as a function of $\lambda$ from the relation

$$
\frac{K'(k)}{K(k)} = \frac{\cosh^{-1}(1/\lambda)}{\pi}
$$

(4)

We have verified that to the order calculated our expansion
coefficients agree term by term with a direct expansion
of the above expressions [11].

In general, this expansion shows excellent convergence. By simply adding the
terms in Eq. 2, one obtains the dispersion for the Heisen-
berg model as shown in Figure 1 and compared with the
exact Heisenberg spectrum. Except very near $q = \pi/2$,
where the spectrum becomes gapless at the Heisenberg
point, the convergence is excellent. It is also evident that
the maximum of the spectra at $q = 0$ is much less sensi-
tive to small anisotropy than the spectrum near $q = \pi/2$.

For $S = 1$, the soliton states can have $S^z = 0, \pm 1$.
While all three are degenerate in the Ising limit, the $S^z = 0$
soliton becomes the lowest energy one for $\lambda \neq 0$. We
have calculated the full spectrum for the solitons. The
minimum energy soliton corresponds to $q = \pi$, unlike the
spin-half case where the minimum energy is at $q = \pi/2$.
The mass gap is given by:

$$
m = 2 - 2\lambda - \frac{1}{2} \lambda^2 + \frac{9}{2} \lambda^3 - 1.207407 \lambda^4 + 1.971667 \lambda^5
- 2.723225 \lambda^6 + 3.294886 \lambda^7 - 3.400478 \lambda^8
+ 2.240766 \lambda^9 + 1.571335 \lambda^{10} + \ldots
$$

(5)

Since we expect a $2D$ Ising critical point, with $\nu = 1$,
where the soliton becomes massless, we use simple Pade
approximants to obtain the location of this critical point.
We estimate $\lambda_c = 0.842\pm0.002$, which compares well
with previous studies of this phase transition using ground
state properties [12].

In order to calculate the magnon spectra in the Heisen-
berg limit we consider the Hamiltonian:

$$
\mathcal{H} = J \sum_i S_i^z S_{i+1}^z + \lambda (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)
+ (1 - \lambda) \sum_i (-1)^i S_i^z.
$$

(6)

The addition of the last term ensures that for $\lambda \neq 1$, only
one of the two Neel states is the ground state of the system
and the other Neel state (and the solitons) have infi-
nite excitation energies. Exactly at the Heisenberg point
($\lambda = 1$) the staggered field term goes to zero and one
recovers the Heisenberg hamiltonian. Because we have
introduced the staggered field and doubled the unit cell,
the magnon spectra is also doubled. Since there is no long
range order in the Heisenberg limit, only the calculated
spectra between wavevectors $(\pi/2, \pi)$ will survive and the
spectral weights for those between $(0, \pi/2)$ will vanish as
$\lambda \rightarrow 1$. The effective Hamiltonian, whose fourier trans-
form gives the excitation spectra is given complete to
order $\lambda^{10}$ in table 1. The convergence of the series for
$\lambda = 1$ is excellent. In Figure 2 we show simply the sum
of terms from 8, 9 and 10 term series. Pade approximants
can be used to improve convergence slightly. They lead
to estimates for the energy gap of $0.42\pm0.01J$. The entire
spectrum is within a few percent of those calculated earlier by exact numerical diagonalization of finite systems [6].

For \( S = 3/2 \) we have also calculated the effective hamiltonian for the magnon excitation spectra. It is presented in table 2. In Figure 3 we show the estimated dispersion for \( \lambda = 1 \) obtained by simply adding terms upto 4th, 6th and 8th order. Except very near \( q = 0 \), where the dispersion should become linear and gapless at the Heisenberg point, we find that this simple addition converges rapidly. By assuming a linear dispersion near \( q = 0 \), and using series extrapolation methods we can directly estimate the spin-wave velocity. However, if we assume that the spin-wave spectrum is uniformly renormalized with respect to the classical spectrum, the quantum renormalization of the spin-wave spectrum can be estimated from the value of the excitation energy at \( q = \pi/2 \). The latter measure, involving the maximum spin-wave energy, is insensitive to anisotropy, whereas the linear spectrum at small \( q \) is clearly very sensitive to anisotropy. Using the latter measure, we estimate the quantum renormalization of the spectrum to be approximately 1.16. This is somewhat larger than the order 1/\( S \) spin-wave estimate of 1.12 [6]. Recently, this quantum renormalization of the spin-wave spectra has also been determined experimentally in the material CsVCl\(_3\) from the energy of the zone-boundary magnons [6]. They obtain a spin-wave renormalization of 1.26 \( \pm \) 0.2, the large uncertainties resulting from the lack of accurate determination of the exchange constant \( J \).

In conclusion, we have shown that topological excitations such as spinons and solitons as well as magnons in one-dimensional Heisenberg-Ising antiferromagnets can be studied by a straightforward application of Raleigh-Schrodinger perturbation theory. This expansion gives nearly the complete answer for systems with significant Ising anisotropy, but is also highly accurate for the Heisenberg model. We have used this method here to verify the spinon spectrum for \( S = 1/2 \), to calculate the soliton spectrum for \( S = 1 \) and show that it becomes gapless at the Ising critical point, as well as to calculate the magnon spectra for \( S = 1 \) and \( S = 3/2 \) chains. The application of a staggered field, whose coefficient goes to zero in the Heisenberg limit allows one to study the magnon spectra for the Haldane-gap Heisenberg systems as well.

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FIG. 1. The spinon excitation spectra for the spin-half Heisenberg model obtained by adding terms upto order 10 (crosses), 11 (circles) and 12 (squares) in Eq. 2. The solid line is the exact result

FIG. 2. The magnon spectra for the spin-1 Heisenberg model obtained by adding terms upto order 8 (squares), 9 (circles) and 10 (crosses) in table 1.

FIG. 3. The spin-wave spectra for the spin-3/2 Heisenberg model obtained by adding terms upto order 4 (crosses), 6 (circles) and 8 (squares) in table 2.

| Table I. Effective Hamiltonian for the \( S = 1 \) Heisenberg-Ising model (Eq. 6). To get the magnon dispersion at wavevector \( q \) one needs to sum the series over \( r \) with a factor \( \cos(qr) \). |
| r Series |
|----------------------------------|
| 0 \( -\lambda - 0.2\lambda^2 - 0.18\lambda^3 - 0.0530357\lambda^4 + 0.0088342\lambda^5 + 0.0109158\lambda^6 + 0.0015458\lambda^7 + 0.0021357\lambda^8 + 0.0008055\lambda^9 + 0.0105825\lambda^{10} \) |
| 2 \( -4\lambda^2 - 4\lambda^3 - 1.1904048\lambda^4 + 0.6644654\lambda^5 - 0.0528568\lambda^6 - 0.0318666\lambda^7 - 0.0176628\lambda^8 - 0.0020513\lambda^9 + 0.0025792\lambda^{10} \) |
4 \(-0.019375\lambda^4 - 0.0245625\lambda^5 - 0.0212035\lambda^6 - 0.0177130\lambda^7 - 0.0153450\lambda^8 - 0.0132463\lambda^9 - 0.0114761\lambda^{10}\)
6 \(-0.0016698\lambda^6 - 0.0035734\lambda^7 - 0.0046995\lambda^8 - 0.0054470\lambda^{10}\)
8 \(-0.0001682\lambda^8 - 0.0004937\lambda^9 - 0.0008462\lambda^{10}\)
10 \(-0.0000195\lambda^{10}\)

**TABLE II. Effective Hamiltonian for** \(S = 3/2\) **Heisenberg Ising model.** To get the magnon dispersion at wavevector \(q\) one needs to sum the series over \(r\) with a factor \(\cos(qr)\).

| \(r\) | \(\text{Series}\) |
|---|---|
| 0 | \(3 - 0.825\lambda^2 - 0.0529051\lambda^4 + 0.0195540\lambda^6 + 0.0186877\lambda^8\) |
| 2 | \(-1.125\lambda^2 - 0.2552099\lambda^6 - 0.0900226\lambda^8 - 0.0174543\lambda^{10}\) |
| 4 | \(-0.0980859\lambda^4 - 0.0691161\lambda^6 - 0.0454369\lambda^8\) |
| 6 | \(-0.0190201\lambda^6 - 0.0229853\lambda^8\) |
| 8 | \(-0.0043107\lambda^8\) |
