NOVEL EXTRAPOLATION FOR STRONG COUPLING EXPANSIONS*

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We present a novel extrapolation scheme for high order series expansions. The idea is to express the series, obtained in orders of an external variable, in terms of an internal parameter of the system. Here we apply this method to the 1-triplet dispersion in an antiferromagnetic $S = 1/2$ Heisenberg ladder. By the use of the internal parameter the accuracy of the truncated series is enhanced tremendously.

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1. Introduction

High order series expansions have become a powerful tool in the field of strongly correlated electron systems [1]. Especially in low dimensional quantum spin systems significant progress has been achieved, see *e.g.* [2-6]. Usually the obtained truncated series must be extrapolated using various extrapolation schemes in order to obtain results for the physically interesting regions [7]. Albeit these extrapolations are a standard technique they always introduce some uncertainty about the results. Therefore, a general transformation scheme which allows to read off the information content of the high order series more directly is highly desirable. Here we will propose such a general scheme. Its usefulness will be demonstrated for the 1-triplet dispersion in antiferromagnetic 2-leg $S = \frac{1}{2}$ Heisenberg ladders. The series was obtained previously by various techniques [2,4,5]; we used a perturbative continuous unitary transformation (CUT) [3].

The Hamiltonian for the antiferromagnetic 2-leg Heisenberg ladder reads

$$H = \sum_i \left[J_{\parallel} \left(\boldsymbol{S}_{1,i} \boldsymbol{S}_{1,i+1} + \boldsymbol{S}_{2,i} \boldsymbol{S}_{2,i+1} \right) + J_{\perp} \boldsymbol{S}_{1,i} \boldsymbol{S}_{2,i} \right] , \tag{1}$$

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where $J_\parallel$ and $J_\perp$ are the exchange couplings on the legs and on the rungs, respectively. The subscript i denotes the rungs and the subscript $1,2$ the legs of the ladder.

We use a CUT to map the Hamiltonian H to an effective Hamiltonian H_{eff} which conserves the number of rung-triplets, *i.e.* $[H_0, H_{\text{eff}}] = 0$ where $H_0 := H|_{J_\parallel=0}$ [3]. The ground state of H_{eff} is the rung-triplet vacuum. The effective Hamiltonian H^{eff} is calculated in the 1-triplet subspace of the Hilbert space to order 14 in $x := J_\parallel/J_\perp$. The ground state energy $E_0 = \langle 0|H_{\text{eff}}|0\rangle$ and the 1-triplet dispersion $\omega(k) = \langle k|H_{\text{eff}}|k\rangle - E_0$ is obtained [2,4,5]. The 1-triplet dispersion is expressed in terms of the 1-triplet hopping amplitudes $t_n(x) = \langle i|H_{\text{eff}}|i+n\rangle$ where $|i\rangle$ denotes the state with one triplet on rung i

$$\frac{\omega(k)}{J_\perp} = \sum_n t_n(x)\cos(nk)\,. \tag{2}$$

The 1-triplet dispersion has a minimum for $k = \pi$, *i.e.* the 1-triplet gap $\Delta(x)$ given by $\omega(\pi)$. In Fig. 1(a), the results for $\Delta(x)$ are shown. The truncated series for $\Delta(x)$ yields a satisfactory agreement up to $x \approx 0.6$. Beyond this value it cannot be used as estimate for the value of the gap. More sophisticated extrapolation schemes, however, still work fine.

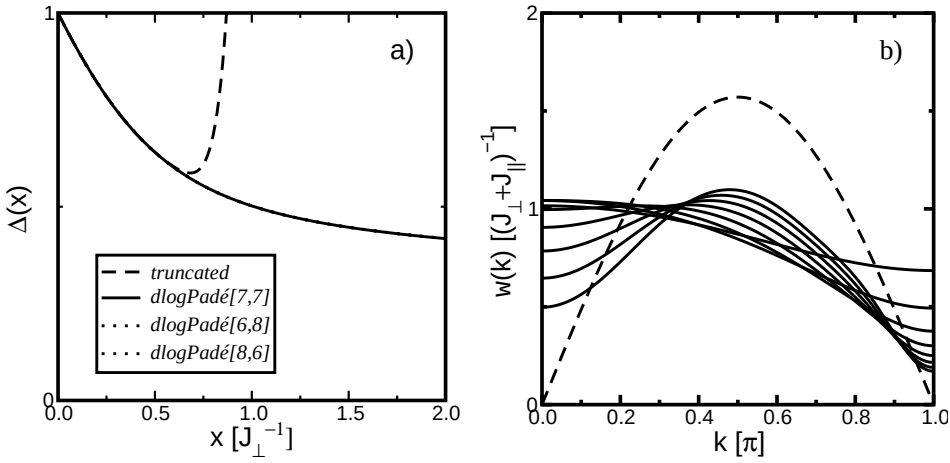

Fig. 1. (a) Gap $\Delta(x)/J_\perp$. The solid and the dotted curves result from a [7,7], [6,8] and a [8,6] dlogPadé approximant, respectively, assuming constant behavior on $x \to \infty$. The long-dashed curve depicts the truncated series. (b) Dispersion relation $\omega(k)$ in units of $J_\perp + J_\parallel$ for the couplings $x = J_\parallel/J_\perp = 0.2, 0.4, \ldots, 1.6$. The highest plot at $k = \pi$ is $x = 0.2$ and the lowest plot is $x = 1.6$. The long-dashed curve is the limit of isolated chains ($x = \infty$), *i.e.* the Cloizeaux–Pearson result $(\pi/2)\sin(k)$ [10].

2. Extrapolation scheme and results

Generically, the various physical quantities in a given system depend in a complicated way on the external control parameters. Expanding the quantities under study in terms of one of the external control parameters, let us say x, yields the bare, truncated series which can only rarely be directly used to compute the quantities. This is so since singularities induced by phase transitions easily spoil the convergence of the series. For instance, a correlation length diverges and the corresponding energy gap closes rendering an expansion about the gapped phase difficult.

If the convergence of the series is deteriorated due to an incipient phase transition it is reasonable to assume that *all* quantities in the particular system behave in a similar fashion. If this is so we may proceed in two separate steps: *(i)* We extrapolate an internal parameter which may serve as a measure of the distance to the phase transition as reliably as we can. Thereby, we can attribute reliably to a given value of x the corresponding value of the internal parameter. *(ii)* We express all *other* quantities as functions of the internal parameter. According to our argument the latter functional dependencies are expected to be much simpler, *i.e.* they are much less singular. The canonical candidate for the internal parameter measuring the distance to a phase transition or, more generally, to some singular situation is the energy gap Δ. It is inversely proportional to the correlation length ξ which plays the role of the internal control parameter in standard renormalization group treatments.

In the following, we illustrate for the 1-triplet dispersion of the model in (1) that this scheme works indeed stunningly well. The gap $\Delta(x)$ can be extrapolated reliably up to $x \approx 2$ using dlogPadé-approximants, Fig. 1(a). In this extrapolation we can exploit additional properties of the gap such as its positivity and its asymptotic behavior for $x \to \infty$. In this way, very reliable extrapolations are possible (Fig. 1(a)) so that step *(i)* is successfully solved. Note that $\Delta(x)$ in units of $J_\perp$ does not vanish on $x \to \infty$ but rests finite [8,9].

For step *(ii)* we define

$$p(x) = 1 - \Delta(x)/((1+x)J_\perp) = 1 - \Delta(x)/(J_\parallel + J_\perp)\,. \tag{3}$$

In units of $J_\parallel + J_\perp$ the gap is unity at $x = 0$ and it goes to zero on $x \to \infty$. So $p(x)$ varies monotonically between 0 and 1 when x is increased from 0 to ∞. Note that $p = 1$, *i.e.* $x = \infty$, constitutes the limit where the spin ladder becomes a system of two isolated spin chains. Since one has $p \propto x$ for small x any expansion in x can be rewritten as expansion in p of the same order as the series in x, yet with other coefficients! This is done by inverting Eq. (3), thus completing the second step.

We applied the extrapolation scheme proposed above to the expansions of the 1-triplet hopping amplitudes t_n in Eq. (2) which yields the 1-triplet dispersion $\omega(k,p)$. In Fig. 1(b) the results are depicted for the truncated series in p without any further extrapolation! For $x < 0.6$ the dispersion is a monotonic decreasing function in k whereas for larger values of x a characteristic dip at $k = 0$ appears. For comparison, the limiting case of isolated chains is also included [10]. The main point is that the truncated series in p gives a quantitatively correct 1-triplet dispersion up to $x \approx 1.2$ (*cf.* Ref. [2]) and qualitatively good results up to $x \approx 2$ while the truncated series in x can be trusted only up to $x \approx 0.6$.

3. Conclusion

We presented a novel generally applicable extrapolation scheme for high order series expansions. The basic idea is to use an *internal* control parameter instead of an *external* control parameter as expansion variable. All difficulties stemming from singularities are dealt with in the determination of the dependence of the internal parameter on the external one.

The power of the novel scheme was demonstrated for the 1-triplet dispersion of the antiferromagnetic $S = \frac{1}{2}$ 2-leg Heisenberg ladder. Further investigations on other quantities and systems are in progress. In addition, the use of standard extrapolation techniques on the series in the internal parameter constitutes a very promising route to extend the applicability of strong coupling expansions.

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