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Quantitative expression of the spin gap via bosonization for a dimerized spin-1/2 chain

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Abstract. Using results on the mass gap in the sine-Gordon model combined with the exact amplitudes in the bosonized representation of the Heisenberg spin-1/2 chain and one-loop renormalization group, we derive a *quantitative* expression for the gap in a dimerized spin-1/2 chain. This expression is shown to be in good agreement with recent numerical estimates when a marginally irrelevant perturbation is taken into account.

PACS. 75.10.Pq Spin chain models

Low dimensional antiferromagnets have been the subject of intense scrutiny both theoretical and experimental for the last twenty years. The simplest model, the spin-1/2 Heisenberg antiferromagnet, is integrable [1] and can be mapped onto a continuum field theory [2–4] which allows the full determination of its zero temperature critical behavior. The presence of a marginally irrelevant operator in the continuum theory induces logarithmic corrections to the critical scaling [5]. The corrections to scaling of the correlation functions [5–7], NMR relaxation rates [8,9], and susceptibilities [10,11] in this model have been investigated in details. Further, when the Heisenberg spin-1/2 chain model is perturbed by a relevant operator such as an alternation of the exchange coupling, the marginal operator gives rise to a logarithmic correction to the power law dependence of the gap on the perturbation [5]. Such logarithmic corrections to scaling in the gap in the context of two dimensional statistical mechanics of the four state Potts model whose transfer matrix is related to the Hamiltonian of the alternating Heisenberg chain [12–15]. In [14] in particular, it was shown that the dependence of the gap Δ on the dimerization δ, was changed from the form $\Delta \sim \delta^{2/3}$ [16,17] to the form $\Delta \sim \delta^{2/3}/|\ln\delta|^{1/2}$. Such logarithmic behavior was confirmed by numerical calculations in [18–20]. Alternatively, the dependence of the gap on the dimerization can be described by an effective power law form with an exponent that deviates from 2/3 [21,22]. For a not too small dimerization, it is found that the resulting effective exponent is close to 2/3 [21]. Further, by considering a Heisenberg chain with an additional next-nearest neighbor coupling finely tuned to cancel the marginal operator, a pure power law with exponent 2/3 can be obtained obtained for the gap [23]. Recently, the logarithmic corrections were investigated in greater details using the DMRG [24]. The data for the gap could be fitted to the form:

$$\Delta = \alpha_{gap}^{1/2} \frac{\delta^{2/3}}{(\ln \delta_0/\delta)^{1/2}}, \tag{1}$$

with $\alpha_{gap} = 19.4$ and $\delta_0 = 115$ or alternatively by the power law form $\Delta = 1.94\delta^{0.73}$. A difficulty that arises when comparing the predictions of the Renormalization Group approach [5,12–15] with the numerical results is that the former approach can only predict the exponents, and not the non-universal prefactors. However, exact results for the sine-Gordon model combined with recent progress [25,26] on the bosonization treatment of the Heisenberg spin 1/2 chain using integrability make it possible to overcome these two difficulties and obtain the prefactor in the expression of the gap at least in the absence of logarithmic corrections. Assuming that the gap varies continuously as the marginally irrelevant is turned on, it is then possible to obtain an expression of the gap as a function of the marginally irrelevant operator, with no further unknowns. Fitting the data of [24] then allows the determination of the order of magnitude of the marginally irrelevant interaction. The obtained value can then be checked against the one obtained in [5]. A similar approach has been used previously in [27] to estimate the gaps induced by a staggered field in an anisotropic spin 1/2 chain.

The Hamiltonian of the dimerized spin-1/2 chain reads:

$$H = J\sum_n (1 + (-)^n\delta)\mathbf{S}_n \cdot \mathbf{S}_{n+1} \tag{2}$$

For $\delta = 0$, this Hamiltonian reduces to the one of the uniform antiferromagnetic Heisenberg chain ($J > 0$) the low

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energy properties of which are described by the following continuum Hamiltonian [4,14]:

$$H = \int \frac{dx}{2\pi}\left[uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x\phi)^2\right] - \frac{2g_2}{(2\pi a)^2}\int dx \cos\sqrt{8}\phi, \quad (3)$$

where $[\phi(x), \Pi(x')] = i\delta(x-x')$, $u = \frac{\pi}{2}Ja$ and $K = 1 - \frac{g_2}{2\pi u}$. The latter conditions ensures $SU(2)$ symmetry, and for $g_2 < 0$ the operators $(\pi\Pi)^2 - (\partial_x\phi)^2$ and $\cos\sqrt{8}\phi$ are both marginally irrelevant resulting a gapless fixed point. The exact bare value of g_2 has been estimated in [5].

The spin operators can be expressed as a function of Π, ϕ as:

$$\frac{\mathbf{S}_n}{a} = (\mathbf{J}_+ + \mathbf{J}_-)(na) + (-)^{x/a}\mathbf{n}(na), \quad (4)$$

$$J_r^+(x) = (J_r^x + iJ_r^y)(x) = \frac{1}{2\pi a}e^{-i\sqrt{2}(\theta - r\phi)(x)}\eta_\uparrow\eta_\downarrow, \quad (5)$$

$$J_r^z = \frac{1}{2\pi\sqrt{2}}\left[r\Pi - \partial_x\phi\right], \quad (6)$$

$$n^+(x) = (n^x + in^y)(x) = \frac{\lambda}{\pi a}e^{-i\sqrt{2}\theta(x)}\eta_\uparrow\eta_\downarrow, \quad (7)$$

$$n^z(x) = \frac{\lambda}{\pi a}\sin\sqrt{2}\phi_\sigma(x), \quad (8)$$

where a is a lattice spacing, $\eta_{\uparrow/\downarrow}$ represent Majorana fermion operators that can be omitted in some cases (see e.g. Ref. [28] for a discussion of this point), and θ is defined by $\theta(x) = \pi\int_{-\infty}^{x} dx'\Pi(x')$. The constant λ is a non-universal parameter that depends on the lattice model being considered. Recently, this parameter has been determined in the case of the isotropic Heisenberg spin-1/2 chain [25,26], and it was found that:

$$\lambda = \left(\frac{\pi}{2}\right)^{1/4}. \quad (9)$$

In order to determine the bosonized Hamiltonian of the dimerized spin-1/2 chain (2), all we need is a bosonized expression of the dimerization operator $\sum_n (-)^n \mathbf{S}_n\cdot\mathbf{S}_{n+1}$. Using (4), the corresponding expression is easily extracted from:

$$\frac{1}{a}\mathbf{S}_n\cdot\mathbf{S}_{n+1} = (\text{uniform}) + (-)^n a\left[-(\mathbf{J}_+ + \mathbf{J}_-)(na)\cdot\mathbf{n}((n+1)a) + \mathbf{n}(na)\cdot(\mathbf{J}_+ + \mathbf{J}_-)((n+1)a)\right]. \quad (10)$$

The bosonized expression of the dimerization operator, is thus obtained from the the short distance expansion of $\mathbf{J}_{R,L}$ and $\mathbf{n}$. Using equations (5) and (7) with Glauber identities, one finds the following expressions:

$$n^\pm(x)(J_+ + J_-)^\mp(x+a) = \frac{\lambda}{(\pi a)^2}\cos\sqrt{2}\phi(x) + \ldots \quad (11a)$$

$$(J_+ + J_-)^\pm(x)n^\mp(x+a) = -\frac{\lambda}{(\pi a)^2}\cos\sqrt{2}\phi(x) + \ldots \quad (11b)$$

The change of sign is a consequence of the application of the Glauber identity taking into account the commutation relation $[\phi(x), \theta(x')] = i\pi Y(x'-x)$, Y being the Heaviside step function. Finally, $n^z(x+a)(J_+^z + J_-^z)(x)$ and $n^z(x)(J_+^z + J_-^z)(x+a)$ are respectively obtained from equations (6) and (8) the two following short distance expansion:

$$-\frac{1}{2\pi\sqrt{2}}\partial_x\phi(x+a)\sin\sqrt{2}\phi(x) = \frac{1}{2\pi a}\cos\sqrt{2}\phi(x) + \ldots \quad (12a)$$

$$-\frac{1}{2\pi\sqrt{2}}\partial_x\phi(x)\sin\sqrt{2}\phi(x+a) = -\frac{1}{2\pi a}\cos\sqrt{2}\phi(x) + \ldots \quad (12b)$$

which can be derived by normal ordering the product of the two operators [29,30]. A sketch of the derivation is given in the appendix. It is easily seen that equations (11, 12) are compatible with spin rotational invariance. Combining the expressions (11, 12) in (10), and using the value of λ in equation (9) we finally obtain that:

$$\frac{1}{a}\mathbf{S}_n\cdot\mathbf{S}_{n+1} = \text{uniform} + (-)^n\frac{3}{\pi^2 a}\left(\frac{\pi}{2}\right)^{1/4}\cos\sqrt{2}\phi. \quad (13)$$

Actually, the bosonized expression of the spin operator is more complicated than equation (4). It can be found for instance in [31]. Ignoring the contribution of the descendant fields in the expressions (2.35) and (2.36) and requiring that at the point with SU(2) symmetry the correlators $\langle S_m^a S_n^a\rangle$ are the same for all a, the expansion reduces to (4). However, when descendant fields are taken into account, no such reduction takes place, and the full expansion has to be considered. The expression (13) is then only the first term of an expansion of the dimerization operator [32], and the coefficient of the term $\cos\sqrt{2}\phi$ could be modified by the higher order terms of the expansion. However, we shall see in the following that retaining only the first term of this expansion (13), already yields a rather good estimate of the gap when compared to numerical calculations. Using equation (13), the continuum Hamiltonian describing the dimerized spin 1/2 chain at low energy reads:

$$H = \int \frac{dx}{2\pi}\left[uK(\pi\Pi)^2 + \frac{u}{K}(\partial_x\phi)^2\right] - \frac{2g_1}{(2\pi a)^2}\cos\sqrt{2}\phi - \frac{2g_2}{(2\pi a)^2}\int dx\cos\sqrt{8}\phi. \quad (14)$$

Note that in (14), the sign of g_1 does not matter as it can always been rendered positive by the shift $\phi \to \phi + \pi/\sqrt{2}$. In (14), we have:

$$g_1 = 6J\left(\frac{\pi}{2}\right)^{1/4}\delta a. \quad (15)$$

As we noted before, g_2 is a marginally irrelevant field which flows to 0 if $g_1 = 0$. Let us assume for a moment that we can neglect completely the presence of this marginally irrelevant operator and take $K = 1, g_2 = 0$ in (14). Then,

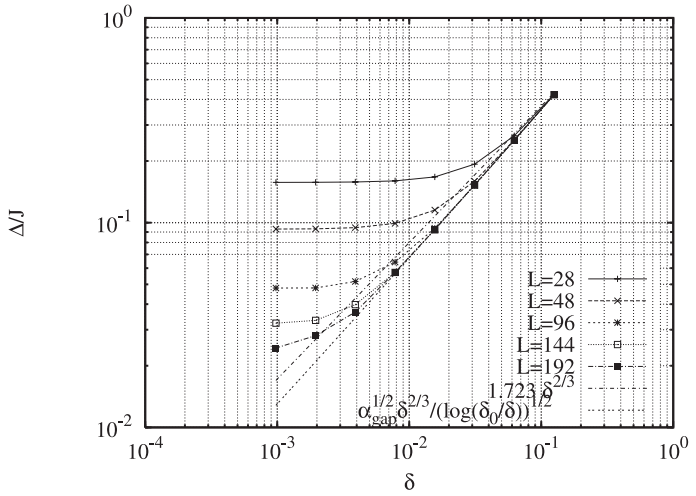

Fig. 1. Comparison of the gap $\Delta(\delta, L) = (1+\delta)(e_1(\delta, L) - e_0(\delta, L))$ obtained from the data of Table 1 of reference [24] for $L = 28, 48, 96, 144, 192$ with the expressions (17) without logarithmic corrections (dash-dotted line) and the expression (29) including logarithmic corrections with $y_2(0) = -0.22$ i.e. $\alpha_{gap} = 20.2$ and $\delta_0 = 148$ (dotted line). For large L, the gap extrapolates to the expression (29).

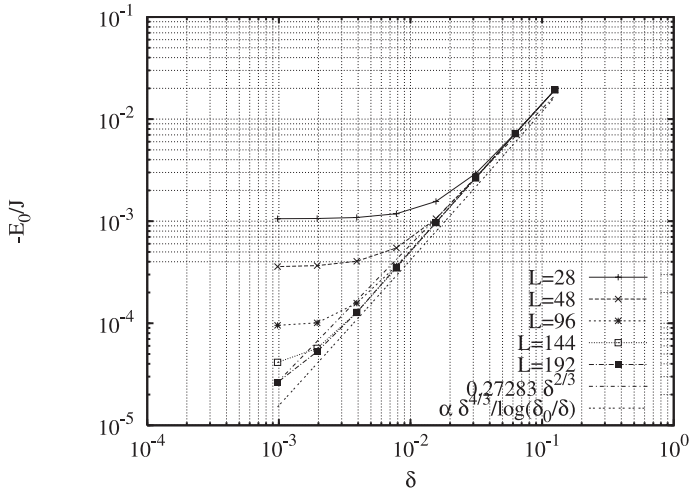

Fig. 2. Comparison of the expression of ground state energy per spin $e_0 - \tilde{e}_0(\delta, L) = -E_0(\delta, L)$ taken from Table 1 of reference [24] for $L = 28, 48, 96, 144, 192$ with the expression derived in this paper without logarithmic corrections (18) (dash-dotted line) and with logarithmic corrections (30) for $y_2(0) = -0.22$ i.e. $\alpha = 1.86$ and $\delta_0 = 148$ (dotted line). Including logarithmic corrections leads to a better agreement for small dimerization as L is increased. However, deviations are still significant in contrast with the case of the gap.

the Hamiltonian (14) becomes the sine-Gordon model. This model is integrable, and the expression of the gap can be found in [33], or in [34] equation (12). In the notations of [34], $\beta^2 = K/4 = 1/4$, and $\mu = 3/\pi^3(\pi/2)^{1/4}\delta$ (where we have used the fact that the velocity $u = \frac{\pi}{2}Ja$). The dimensionless gap M is then given by:

$$M = \frac{2}{\sqrt{\pi}}\frac{\Gamma(1/6)}{\Gamma(2/3)}\left[\frac{\Gamma(3/4)}{\Gamma(1/4)}\frac{3}{\pi^2}\left(\frac{\pi}{2}\right)^{1/4}\delta\right]^{2/3} \simeq 1.097\delta^{2/3}, \tag{16}$$

and the energy gap is given by $\Delta = \frac{u}{a}M$ i.e.

$$\frac{\Delta}{J} = \frac{\pi}{2}M \simeq 1.723\delta^{2/3}. \tag{17}$$

We note that the formula (16) has already been applied to calculate the gap of the dimerized spin 1/2 chain in [35], but the value of λ, equation (9) was not known. A formula similar to (16) has also been derived in the case of a spin$-\frac{1}{2}$ chain in a staggered magnetic field [36]. The formula (17) is in reasonable agreement with the result quoted in [21] who reported that $\Delta/J = 1.5\delta^{0.65}$ as two expression differ at most by 6% for $0.01 \leq \delta \leq 0.1$. Comparing our expression (17) to the one of reference [24], $\Delta/J = 1.94\delta^{0.73}$, we find that they are in agreement within a 10% relative error when $\delta \geq 0.03$. For lower values of δ, the two results deviate sensibly. It can also be seen in Figure 1 that for low dimerization the extrapolation of the numerical results of reference [24] deviates significantly from the prediction of (17). As we shall see, this is the result of the logarithmic corrections.

In [34], the expression of the ground state energy was also given in dimensionless units in equation (14). Using this expression, we obtain for the ground state energy:

$$\frac{E_0}{J} = -\frac{\pi}{2}J\frac{M^2}{4}\tan\frac{\pi}{6} \simeq -0.2728\,\delta^{4/3} \tag{18}$$

This expression is compared to the one quoted in [24], $E_0/J = -0.39\delta^{1.45}$. For low dimerization $\delta < 0.01$, these two expressions start to deviate by more than 20%. Also, as can be seen in Figure 2, the equation (18) does not provide a good extrapolation of the numerical results of reference [24]. Till now, we have totally neglected the presence of the marginally irrelevant operator $\cos\sqrt{8}\phi$. As we shall now see, the corrections to scaling [5,14] induced by this operator in the gap formula, are responsible for the discrepancies between the numerical and the analytical results. Similar results have been obtained in the case of a staggered magnetic field [37], albeit with a different exponent for the logarithmic corrections. The renormalization group equations associated with the Hamiltonian (14) read [13]:

$$\frac{d}{dl}\left(\frac{1}{K}\right) = \frac{1}{8}y_1^2 + \frac{1}{2}y_2^2, \tag{19}$$

$$\frac{dy_1}{dl} = \left(2 - \frac{K}{2} + y_2\right)y_1, \tag{20}$$

$$\frac{dy_2}{dl} = (2-2K)y_2 + \frac{y_1^2}{4}, \tag{21}$$

where we have introduced $y_i = g_i/(\pi u)$. For $y_1 = 0$, the $SU(2)$ symmetric flow is recovered for $K = 1 - y_2/2$. Then, the equations (19) reduce to the single Kosterlitz-Thouless [38] $dy_2/dl = y_2^2$. We see that for $y_2 < 0$, this

equation flows to the fixed point $y_2^* = 0$, with the following flow equation:

$$y_2(l) = \frac{y_2(0)}{1 - y_2(0)l}. \tag{22}$$

Let us now assume [13] that we have turned on a very small y_1. Using the initial conditions with $SU(2)$ symmetry, we can easily show that the RG equations reduce to:

$$\frac{dy_2}{dl} = y_2^2 + \frac{1}{4}y_1^2, \tag{23}$$

$$\frac{dy_1}{dl} = \left(\frac{3}{2} + \frac{3}{4}y_2\right) y_1. \tag{24}$$

If we assume that $y_1(0) \ll y_2(0)$, we can assume that in (23), we can take $y_1 = 0$, so that the flow of y_2 is given by (22). Then, equation (24) is trivially integrated, leading to:

$$y_1(l) = y_1(0)\frac{e^{\frac{3}{2}l}}{(1 + |y_2(0)|l)^{3/4}}. \tag{25}$$

This equation should break down for a scale l_0 such that $y_1(l_0) \sim y_2(l_0)$. One has:

$$e^{l_0}(1 + y_2(0)l_0)^{1/6} = \frac{|y_2(0)|^{2/3}}{y_1(0)^{2/3}}. \tag{26}$$

For $l > l_0$ the contribution of y_2 to the renormalization of y_1 being negligible, $y_1(l) = e^{3/2(l-l_0)}y_1(l_0)$. The scale l^* at which $y_1(l) \sim 1$ is thus given by:

$$e^{-l^*} = e^{-l_0}\frac{(1 + |y_2(0)|l_0)^{2/3}}{|y_2(0)|^{2/3}} = \frac{|y_1(0)|^{2/3}}{(1 + |y_2(0)|l_0)^{1/2}}, \tag{27}$$

An approximate form of l_0 can be obtained by iterating (26) leading to:

$$e^{-l^*} \simeq \frac{|y_1(0)|^{2/3}}{\left(1 + \frac{2}{3}|y_2(0)| \ln\left|\frac{y_2(0)}{y_1(0)}\right|\right)^{1/2}}. \tag{28}$$

Since the scaling of the gap is $\Delta \sim e^{-l^*}$ and the scaling of the ground state energy is $E_0 \sim e^{-2l^*}$, for $y_1 \to 0$, these formulas are in agreement with the scaling predicted in [5].

We now make an important assumption. We assume that in the formulas (17, 18), we can replace M with $\mathcal{C}e^{-l^*}$, l^* being given by (28), with $\mathcal{C}$ being chosen in such a way that for $y_2 = 0$, the resulting M agrees with (16). This is a uncontrolled approximation as the model (14) is non-integrable but it is partially justified by the fact that the energy and the correlation length evolve continuously as a function of the parameter y_2 in the vicinity of the integrable point. With this assumption, and noting that the definition of y_1 and equation (15) imply $y_1 = 1.3612\delta$, we obtain that $\mathcal{C} = 0.8932$.

We are lead to the following expressions of the gap:

$$\frac{\Delta}{J} = \frac{1.723\delta^{2/3}}{\left(1 + \frac{2}{3}|y_2(0)| \ln\left|\frac{y_2(0)}{1.3612\delta}\right|\right)^{1/2}}, \tag{29}$$

and of the ground state energy difference:

$$-\frac{E_0}{J} = \frac{0.2728\delta^{4/3}}{1 + \frac{2}{3}|y_2(0)| \ln\left|\frac{y_2(0)}{1.3612\delta}\right|}. \tag{30}$$

These equations are trivially reduced to the form of the equations (7, 8) in [24], with:

$$\alpha_{gap}^{1/2} = \frac{1.723}{\sqrt{\frac{2}{3}|y_2(0)|}} \tag{31}$$

$$\alpha = \frac{0.2728}{\frac{2}{3}|y_2(0)|} \tag{32}$$

$$\ln \delta_0 = \frac{3}{2|y_2(0)|} + \ln\left(\frac{|y_2(0)|}{1.3612}\right). \tag{33}$$

A good extrapolation for large L of the numerical data for the gap obtained in reference [24] is obtained using equation (29) with $y_2(0) = -0.22$ (see Fig. 1). This leads to $\delta_0 = 148$, $\alpha_{gap} = 20.2$ and $\alpha = 1.86$, whereas the values reported by Papenbrock et al. are $\delta_0 = 115$, $\alpha_{gap} = 19.4$ and $\alpha = 2.2$. The corresponding extrapolation for the ground state energy using equation (30) with the same value of $y_2(0) = -0.22$ is better than the one obtained without logarithmic corrections (see Fig. 2). However for large system sizes, the numerical results of [24] do not extrapolate to the form (30) but to a higher value. This could be due to the non-singular part of the free-energy which is not taken into account in the Renormalization Group calculation. Further, comparing the expressions (29) with the expression quoted in reference [24], $\Delta = 1.94\delta^{0.73}$, it is seen that in the range $10^{-4} \leq \delta \leq 0.1$ they differ by less than 10%. For the energy, the agreement is slightly worse with the two expression differing by about 16%. The value of $y_2(0) = -0.22$ also compares reasonably well with the one quoted in [5,39] $y_0 = -0.25$. Thus, taking into account the logarithmic corrections leads to a clear improvement of the estimation of the gap and the ground state energy.

To summarize, we have shown that the results of reference [24] could be recovered from a bosonization approach including the appropriate operator renormalizations, and using exact results for the sine-Gordon model combined with a one-loop RG. The amplitude of the marginally relevant operator was found to be in reasonable agreement with an independent estimate coming from logarithmic corrections to the dependence of the gaps in a spin-1/2 chain. Given the relatively large value of the coupling constant, we are at the limit of applicability of the one-loop RG. Better agreement might be obtained by going beyond the one-loop approximation [40] and finding the contribution of the descendent fields to equation (13). The present approach does not depend crucially on integrability as it is also possible to determine the parameter λ in (4) for a non-integrable model via numerical calculations [27,41].

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Appendix A: Derivation of the short distance expansion

The short distance expansion (12) has been derived in [29,30] using a fermionic representation. In this appendix, we give an alternative derivation using the bosonic representation. We start from the equation:

$$:\partial_x\phi(x'):V(\phi(x)):=:\partial_x\phi(x')V(\phi(x)):\\ +:\frac{dV}{d\phi}(\phi(x)):\partial_x\langle\phi(x')\phi(x)-\phi^2\rangle, \quad (34)$$

which is easily obtained by expanding $V(\phi)$ as a power series and applying Wick's theorem [42]. In the case of the massless free boson, we have:

$$\langle\phi(x')\phi(x)-\phi^2\rangle=\frac{1}{2}\ln\left|\frac{x-x'}{a}\right|, \quad (35)$$

which leads to the expansion:

$$:\partial_x\phi(x'):V(\phi(x)):=:\partial_x\phi(x')V(\phi(x)):\\ +\frac{-1}{2(x'-x)}:\frac{dV}{d\phi}(\phi(x)): \quad (36)$$

Applying this formula in the case of $V(\phi)=\sin\sqrt{2}\phi$ leads to equation (12).

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