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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, 3, 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, 6, 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, 13, 14, 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 a the form $\Delta \sim \delta^{2/3}/|\ln \delta|^{1/2}$. Such logarithmic behavior was confirmed by numerical calculations in [18, 19, 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 dimerization not too small, 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 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:

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

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, 13, 14, 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:

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

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

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

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

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

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

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

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:

$$\begin{aligned} \frac{1}{a} \mathbf{S}_n \cdot \mathbf{S}_{n+1} &= (\text{uniform}) + \\ &(-)^n a [-(\mathbf{J}_+ + \mathbf{J}_-)(na) \cdot \mathbf{n}((n+1)a) \\ &+ \mathbf{n}(na) \cdot (\mathbf{J}_+ + \mathbf{J}_-)((n+1)a)] \end{aligned} \quad (10)$$

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 Eqs. (5) and (7) with Glauber identities, one finds the following expressions:

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

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

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 Eqs. (6) and (8) the two following short distance expansion:

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

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

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 Eqs. (11)–(12) are compatible with spin rotational invariance. Combining the expressions (11) and (12) in (10), and using the value of λ in Eq. (9) we finally obtain that:

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

Therefore, 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 $\phi \rightarrow \phi + \pi/\sqrt{2}$. 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, the Hamiltonian (14) becomes the sine-Gordon model. This model is integrable, and the expression of the gap can be found in [31], or in [32] Eq. (12). In the notations of [32], $\beta^2 = K/4 = 1/4$, 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:

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

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

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

We note that the formula (16) has already been applied to calculate the gap of the dimerized spin 1/2 chain in [33], but the value of λ , Eq. (9) was not known. 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 Ref.[24], $\Delta/J = 1.94\delta^{0.73}$,

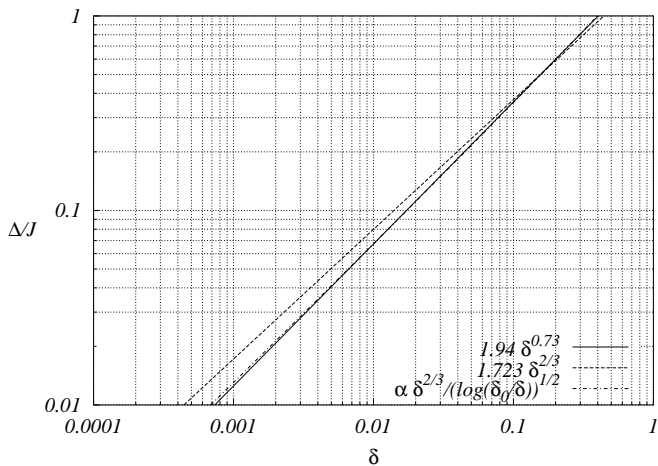


Fig. 1. Comparison of the gap obtained in Ref.[24] (solid line) with the expressions (17) without logarithmic corrections(dashed line) and the expression (29) including logarithmic corrections with $y_2(0) = -0.22$ i.e. $\alpha = 4.499$ and $\delta_0 = 148$ (dash dotted line). Equation (17) gives a result nearly indistinguishable from the result of Ref.[24].

we find that they are in agreement within a 10% relative error when $\delta \geq 0.03$ as represented on Fig. 1. For lower values of δ , the two results deviate sensibly. As we shall see, this is the result of the logarithmic corrections.

In [32], the expression of the ground state energy was also given in dimensionless units in Eq. (14). Using this expression, we obtain for the ground state energy:

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

This expression is compared to the one quoted in [24], $E_0/J = -0.39\delta^{1.45}$ on Fig. 2. The two energy formulas are in better agreement than the gap formulas at low dimerization. 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[14,5] induced by this operator in the gap formula, are responsible for the discrepancies between the numerical and the analytical results. The renormalization group equations associated with the Hamiltonian (14) read[13]:

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

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

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

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[34] $dy_2/dl = y_2^2$. We see that for $y_2 < 0$, this equation flows to the fixed point $y_2^* = 0$, with the follow-

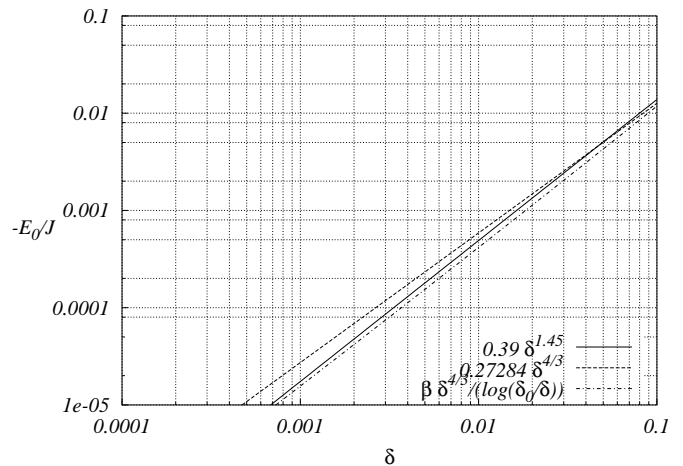


Fig. 2. Comparison of the expression of ground state energy of Ref. [24] with the expression derived in this paper without logarithmic corrections (18) (dashed line) and with logarithmic corrections (30) for $y_2(0) = -0.22$ i.e. $\beta = 1.86$ and $\delta_0 = 148$ (dash-dotted line). Including logarithmic corrections leads to a better agreement for small dimerization. However, deviations are still significant in contrast with the case of the gap.

ing flow equation:

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

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:

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

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

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, the equation (24) is trivially integrated, leading to:

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

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

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

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:

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

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

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

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 $y_1 \rightarrow 0$, 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 Eq. (15) imply $y_1 = 1.3612\delta$, we obtain that $\mathcal{C} = 0.8932$.

We are lead to the following expressions of the gap:

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

and of the ground state energy difference:

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

These equations are trivially reduced to the Eqs. (7) and (8) in [24], by expressing $\alpha, \alpha_{gap}, \delta_0$ as a function of $y_2(0)$. A good fit to the power-law expression of the gap quoted in [24] is obtained using Eq. (29) with $y_2(0) = -0.22$ (see Fig. 1). The corresponding fit for the ground state energy using Eq. (30) with the same value of $y_2(0) = -0.22$ is better than the fit obtained without logarithmic corrections (see Fig. 2), however it is not as good as the fit obtained for the gap, especially for $\delta > 0.01$. This could be due to the non-singular part of the free-energy which is not taken into account in the Renormalization Group calculation. The value of $y_2(0) = -0.22$ compares reasonably well with the one quoted in [5, 35] $y_0 = -0.25$.

To summarize, we have shown that the results of Ref.[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[36]. 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, 37].

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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:

$$:\partial_x \phi(x'):: V(\phi(x)) :=: \partial_x \phi(x')V(\phi(x)) : + : \frac{dV}{d\phi}(\phi(x)) : \partial_x(\phi(x'))\phi(x)$$

which is easily obtained by expanding $V(\phi)$ as a power series and applying Wick's theorem[38]. In the case of the massless free boson, we have:

$$\langle \phi(x')\phi(x) - \phi^2 \rangle = \frac{1}{2} \ln \left| \frac{x - x'}{a} \right|, \quad (32)$$

which leads to the expansion:

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

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

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