Entanglement in quantum impurity problems is nonperturbative

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We study the entanglement entropy of a region of length $2L$ with the remainder of an infinite one-dimensional gapless quantum system in the case where the region is centered on a quantum impurity. The coupling to this impurity is not scale invariant, and the physics involves a crossover between weak- and strong-coupling regimes. While the impurity contribution to the entanglement has been computed numerically in the past, little is known analytically about it, since in particular the methods of conformal invariance cannot be applied because of the presence of a crossover length. We show in this paper that the small coupling expansion of the entanglement entropy in this problem is quite generally plagued by strong infrared divergences, implying a nonperturbative dependence on the coupling. The large coupling expansion turns out to be better behaved, thanks to powerful results from the boundary CFT formulation and, in some cases, the underlying integrability of the problem. However, it is clear that this expansion does not capture well the crossover physics. In the integrable case—which includes problems such as an XXZ chain with a modified link, the interacting resonant level model or the anisotropic Kondo model—a nonperturbative approach is in principle possible using form factors. We adapt in this paper the ideas of Cardy *et al*. [J. Stat. Phys. **130**, 129 (2008)] and Castro-Alvaredo and Doyon [J. Stat. Phys. **134**, 105 (2009)] to the gapless case and show that, in the rather simple case of the resonant level model, and after some additional renormalizations, the form-factors approach yields remarkably accurate results for the entanglement all the way from short to large distances. This is confirmed by detailed comparison with numerical simulations. Both our form factor and numerical results are compatible with a nonperturbative form at short distance.

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I. INTRODUCTION

Quantum entanglement has given rise to much work in the condensed-matter community as a new way to explore interesting aspects of physical systems. The Kondo problem, for instance, has been revisited along these lines, with studies addressing the interplay between the impurity screening and the information shared between the impurity and the bath.[1,2] It is certainly reasonable to expect that entanglement—together with other quantities inspired by quantum information theory, such as the Loschmidt echo or the work distribution—might shed new light on, and offer new experimental/numerical probes of, the key physical features of the Kondo and other problems.[1,3] A particularly interesting question in this direction is whether the Kondo screening cloud—which has had so elusive an appearance in standard thermodynamic quantities[4]—might play a bigger role in quantum information aspects. Other aspects of interest in the context of two-level systems interacting with gapless excitations—generalizing the Kondo problem—apply to the decoherence of qubits interacting with the environment.[5–7]

A large part of the work combining entanglement and quantum impurities has been numerical so far. Indeed, apart from the scale invariant situations, where conformal invariance techniques have led to spectacular progress,[8,9] the general situations involving crossover are very difficult to tackle. This is mostly because the entanglement is a different kind of quantity, not amenable to simple Bethe-ansatz calculations, for instance. There is, however, another reason for the relative lack of analytical results in this area: entanglement, being a zero-temperature quantity, is naturally plagued by IR divergences, which make it nonperturbative in the impurity strength. In that respect, it does behave somehow like some properties of the Kondo screening cloud studied in Refs. 4 and 10.

In order to clarify the main features of entanglement in the presence of impurities—in particular its scaling properties, and flow from small to strong coupling—we focus in this paper on a couple of representative situations, which we handle by a mix of analytical and numerical techniques. The lessons learned will be put to use in forthcoming papers, with applications of more direct physical interest.

The paper is organized as follows. In Sec. II we discuss the basic models we want to study, and define precisely the entanglement entropy. In Sec. III we put together the perturbative calculation of the entanglement at small coupling, and show that it is plagued by strong IR divergences. In Sec. IV we discuss this difficulty in a more general context. In Sec. V we show how the nonperturbative nature of the entanglement entropy can be obtained using general conformal field-theoretic arguments. In Sec. VI we recall the principles of the large coupling expansion proposed in Ref. 2 and carried out to high order in Ref. 11. When the dimension of the perturbation is $h = \frac{1}{2}$, we develop in Sec. VII the form-factor approach using the results of Refs. 12 and 13, and obtain nonperturbative approximations for the entanglement extrapolating all the way from the UV to the IR limit. Finally, in Sec. VIII we compare our results with those of exact numerical calculations on large spin chains. The conclusion contains some last comments and prospect for future work. Finally, the Appendix contains a discussion of the equivalence between our impurity models when the dimension of the perturbation is $h = \frac{1}{2}$ to the boundary Ising model with a boundary magnetic field at special values of the coupling.

II. MODELS AND QUESTIONS

The main problem we study in this paper—though it has various, mathematically equivalent formulations (see below)—is the calculation of the entanglement of a region of length $2L$ centered on an "impurity" in an otherwise one dimensional, gapless quantum system. We characterize this entanglement by the von Neumann entropy $S = -\mathrm{Tr}\rho \ln \rho$, where ρ is the reduced density matrix that has been formed by tracing over the degrees of freedom outside of the segment of length $2L$.

An example of this setup is obtained by taking two semi-infinite XXZ chains coupled by a weak link:

$$H = \sum_{-\infty}^{-1} J\left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right] + \sum_{1}^{\infty} J\left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right] + J'\left[S_0^x S_1^x + S_0^y S_1^y + \Delta S_0^z S_1^z\right]. \quad (1)$$

The bulk chains are in a gapless Luttinger liquid phase for $-1 < \Delta \leqslant 1$. We shall consider the case of anisotropy $\Delta < 0$, where the tunneling between the two half infinite chains is a relevant perturbation, and one observes healing at large scales. The case $\Delta = 0$ is exactly marginal. We parametrize $\Delta = -\cos\frac{\mu\pi}{2}$, $\mu \in [0,1]$. We focus on the physics at energies much smaller than the bandwidth, where field-theoretic results can be applied.

Consider then the entanglement of a region of length $2L$ centered on the modified link. We can easily surmise what this entanglement will look like in the high- and low-energy limits from the existing literature. Indeed, at high energy, the system is effectively cut in half. Using the well-known formula for the entropy of a region *on the edge* of a conformal invariant system we have

$$S_{\mathrm{UV}} = 2 \times \left[\frac{1}{6}\ln\frac{2L}{\epsilon} + \frac{s_1}{2} + \ln g\right] = \frac{1}{3}\ln\frac{2L}{\epsilon} + s_1 + \ln g_{\mathrm{UV}}, \quad (2)$$

where we used that the central charge is unity, ϵ is a UV cutoff of the order of the lattice spacing a, and $\ln g_{\mathrm{UV}} = 2\ln g$ where $\ln g$ is the boundary entropy[14] associated with the conformal boundary condition corresponding to an open XXZ spin chain. The remaining constant term s_1 is nonuniversal as it obviously depends on the definition of the cutoff ϵ.

On the other hand, at low energy, healing has taken place, the system behaves just as one ordinary quantum spin chain, and the entropy obeys the general form for a region of length $2L$ in the bulk of a conformal invariant system:

$$S_{\mathrm{IR}} = \frac{1}{3}\ln\frac{2L}{\epsilon} + s_1 + \ln g_{\mathrm{IR}}. \quad (3)$$

Here, we have allowed for a term $\ln g_{\mathrm{IR}}$, which can be thought of as a residual contribution of the weak link at low energy. In general, comparing entanglements for bulk and boundary theories is indeed difficult, since the dependency of the cutoff ϵ on the physical cutoff (the lattice spacing in the spin chain a, which is the same in both geometries) is not universal, and not necessarily the same in the bulk and boundary cases. This important aspect is discussed in detail in Ref. 13; see in particular Sec. 6.2.1 in that reference. The point for us is that the quantity $\ln g_{\mathrm{UV}} - \ln g_{\mathrm{IR}}$ is well defined, and its value $\ln g_{\mathrm{UV}} - \ln g_{\mathrm{IR}} = -\frac{1}{2}\ln\mu$ can be easily obtained from the folded version of the system [see Eq. (6) below].

More generally, since the bulk behavior of the entanglement entropy is not modified, it is natural to expect the existence of a scaling relation

$$S(L) - S_{\mathrm{IR}} = \mathcal{S}_{\mathrm{imp}}(LT_B), \quad (4)$$

where the crossover scale T_B is expected to be related to the coupling J'. $\mathcal{S}_{\mathrm{imp}}$ should be a monotonic function extrapolating between $-\frac{1}{2}\ln(\mu)$ at small values of the argument and 0 at large values.

To proceed, and conveniently describe the field theory limit,[15] we first observe that the problem, at low energy, can be turned into a purely chiral one. Indeed, in the low-energy limit, each half chain is equivalent to a combination of L and R moving excitations, and we formally map via a canonical transformation the L moving sector into a R moving one so as to have two chiral "wires" representing the two half chains. The additional tunneling between the two chains becomes, in this language, a hopping term between two chiral wires. Bosonizing, forming odd and even combinations of the bosons for each wire, one finds that the odd combination decouples, while the even one obtains the simple Hamiltonian

$$H = \int_{-\infty}^{\infty} dx\, (\partial_x\phi_R)^2 + \lambda\cos\beta\phi_R(0), \quad (5)$$

where $\frac{\beta^2}{8\pi} = \mu \equiv h$ is the conformal weight of the perturbation, and we have set the Fermi velocity $v_F = 1$. The dimension of the perturbation being $[\mathrm{length}]^{-\mu}$, we see that $T_B \propto \lambda^{1/(1-\mu)} \propto (J')^{1/(1-\mu)}$. One can also fold back this problem into the boundary sine-Gordon model (BSG) with Hamiltonian

$$H_{\mathrm{BSG}} = \int_{-\infty}^{0} dx \frac{1}{2}[(\partial_x\Phi)^2 + \Pi^2] + \lambda\cos\frac{\beta}{2}\Phi(0). \quad (6)$$

This shows equivalence to a large variety of other problems, including the one of tunneling between edge states in the fractional quantum Hall effect (FQHE).[16,17] In this case, $\mu = \nu$ is the filling fraction. The RG flows from Neumann ($\lambda = 0$) to Dirichlet ($\lambda = \infty$) boundary conditions (BCs), and the boundary entropy associated with these conformally invariant BCs satisfy $\ln g_{\mathrm{UV}} - \ln g_{\mathrm{IR}} = -\frac{1}{2}\ln\mu$, as claimed earlier.

An interesting variant involves modifying two successive links on the chain:

$$H = \sum_{-\infty}^{-2} J\left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right] + \sum_{1}^{\infty} J\left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z\right] + J'\left[S_{-1}^x S_0^x + S_{-1}^y S_0^y + \Delta S_{-1}^z S_0^z + S_0^x S_1^x + S_0^y S_1^y + \Delta S_0^z S_1^z\right]. \quad (7)$$

This is equivalent to tunneling through a resonant level at the origin. This time, the dimension of the tunneling operator is half what it is in the previous situation, J' is always relevant for $-1 < \Delta \leqslant 1$, and the system is always healed at low energy. The same series of manipulations—"unfolding the two half chains," forming odd and even combinations, decoupling the odd one and bosonizing—leads to the Hamiltonian formulation

$$H = \int_{-\infty}^{\infty} dx (\partial_x \phi_R)^2 + \lambda[e^{i(\beta/\sqrt{2})\phi_R(0)} S^- + e^{-i(\beta/\sqrt{2})\phi_R(0)} S^+], \quad (8)$$

where we recall that $\frac{\beta^2}{8\pi} = \mu$. In this case, the dimension of the perturbation is $h = \frac{\mu}{2}$ (note the factor $\frac{1}{2}$ compared with the first case). The problem can also be folded back into the anisotropic Kondo problem

$$H_{\text{AK}} = \int_{-\infty}^{0} dx \frac{1}{2}[(\partial_x \Phi)^2 + \Pi^2] + \lambda[e^{i(\beta/2\sqrt{2})\Phi(0)} S^- + e^{-i(\beta/2\sqrt{2})\Phi(0)} S^+]. \quad (9)$$

Of particular interest is the case $\Delta = 0$, $\mu = 1$ which corresponds to free fermions. While the chain with one weak link is marginal, the chain with two weak links describes an interesting flow, and is in fact equivalent to a widely studied problem—that of the resonant level model (RLM). Indeed, fermionization in this case leads to

$$H = -J\left(\sum_{-\infty}^{-2} c_{m+1}^\dagger c_m + \text{H.c.}\right) - J\left(\sum_{1}^{\infty} c_{m+1}^\dagger c_m + \text{H.c.}\right) - J'(c_{-1}^\dagger c_0 + c_0^\dagger c_{-1} + c_0^\dagger c_1 + c_1^\dagger c_0), \quad (10)$$

where we have redefined the couplings $J \to -2J$ and $J' \to -2J'$. When going to the continuum limit, the $i = 0$ site behaves like a two-level impurity, and the Hamiltonian reads

$$H = \int_{-\infty}^{0} i[\psi_{1L}^\dagger \partial_x \psi_{1L} - \psi_{1R}^\dagger \partial_x \psi_{1R}]dx + \int_{0}^{\infty} i[\psi_{2L}^\dagger \partial_x \psi_{2L} - \psi_{2R}^\dagger \partial_x \psi_{2R}]dx + \lambda[(\psi_1^\dagger(0) + \psi_2^\dagger(0))d + \text{H.c.}], \quad (11)$$

with $\psi_{1L}(0) = \psi_{1R}(0) \equiv \psi_1(0)$, same for the second species, $\lambda \propto J'$.[18] In contrast with the case of the XX chain with a single defect, this noninteracting problem is *not scale invariant*. The coupling λ flows, and the system again exhibits *healing*: at low energy, the impurity level is completely hybridized with the two half chains.

Let us go back to the general case $\Delta = -\cos\frac{\pi\mu}{2}$. Proceeding like before, we can write the limiting behaviors of the entanglement entropy. At low energy, the impurity is hybridized, the system behaves just as *one* nonchiral wire and a hybridized impurity, and the entropy obeys the general form for a region of length $2L$ in the bulk of a conformal invariant system decoupled from the two baths, so

$$S_{\text{IR}} = \frac{1}{3}\ln\frac{2L}{\epsilon} + s_1 + \ln g_{\text{IR}}, \quad (12)$$

where once again, we included a term g_{IR} that accounts for the remaining boundary condition at $x = 0$ of the hybridized impurity. Meanwhile, at high energy, the impurity is completely decoupled from the wires, and one gets

$$S_{\text{UV}} = 2 \times \left[\frac{1}{6}\ln\frac{2L}{\epsilon} + \frac{s_1}{2} + \ln g\right] = \frac{1}{3}\ln\frac{2L}{\epsilon} + s_1 + \ln g_{\text{UV}}. \quad (13)$$

Using the folded (boundary) version of the system (9), one can easily argue that $\ln g_{\text{UV}} - \ln g_{\text{IR}} = \ln 2$, as a decoupled impurity has two degrees of freedom. One thus expects a behavior entirely similar to (4), where the crossover scale T_B is expected to be proportional to a power of the coupling square, $T_B \propto \lambda^{2/(2-\mu)}$, and $\mathcal{S}_{\text{imp}}$ should be a monotonic function extrapolating between $\ln 2$ at small values of the argument and 0 at large values.

Finally, we note that in the boundary versions (6) and (9), the entanglement impurity we have discussed is now the entanglement of a region of length L on the edge of the system with the rest. If one were to start from an (anisotropic) Kondo version, this would be the most natural point of view.[1]

There are of course other variants of the problem, for instance involving a slightly modified link in the antiferromagnetic XXZ chain with $\Delta > 0$, interactions in the RLM model, etc. In all these cases, we should stress that the geometry we are considering is probably not the most interesting: considering the entanglement of the two halves connected by a weak link or a quantum dot is probably more physical. This latter problem is however significantly more difficult technically. We will discuss it in our next paper, relying on the present work as a stepping stone.

III. UV PERTURBATION

The most natural way to explore the behavior of $\mathcal{S}_{\text{imp}}(LT_B)$ between the fixed points is to use perturbation theory. The required calculation is a modification of the one proposed in Refs. 8,9, and 19. Using the well-known replica trick, one first observes that the entanglement entropy S can be obtained from the Renyi entropies $R_n = \text{Tr}\rho^n$ by considering $S = -\lim_{n\to 1}\frac{\partial}{\partial n}R_n$.The Renyi entropies in turn can be obtained as $R_n = \frac{Z_n}{(Z_1)^n}$, where Z_n is the partition function on a n-sheeted Riemann surface $\mathcal{R}_{n,1}$ with the sheets joined at a cut corresponding to the segment of length $2L$. The difference between the problem at hand and the conformal case is that now there is a perturbation inserted at the origin in the Hamiltonian formulation, which corresponds to the insertion of a perturbation along an imaginary time line for each of the n sheets. The modified partition functions Z_n can in principle be expanded in powers of the coupling constant, and perturbative corrections to the Renyi entropies and the entanglement entropies finally obtained.

To see what happens in more detail, we consider first Hamiltonian (5). We start with $n=2$ sheets, and write formally the Renyi entropy as a functional integral for a pair of chiral bosons as

$$R_2 = \frac{Z_2}{(Z_1)^2} = \frac{\int_{\text{twist}}[\mathcal{D}\phi_1][\mathcal{D}\phi_2]\exp\left\{-A[\phi_1]-A[\phi_2]-\lambda\int_{-\infty}^{\infty}[V_1(x=0,y)+V_2(x=0,y)]\,dy\right\}}{\left(\int[\mathcal{D}\phi]\exp\left\{-A[\phi]-\lambda\int_{-\infty}^{\infty}V(x=0,y)dy\right\}\right)^2}, \tag{14}$$

where $V_i = \cos\beta\phi_i$ is the perturbation, and $A[\phi] = \int d^2x\mathcal{L}[\phi]$ is the free action. Note that we are working in the chiral version, but have suppressed the "R" label in the fields for simplicity of notation. Finally, the label twist means the functional integral is evaluated with conditions around the cut,

$$\begin{aligned}\phi_1(-L\leqslant x\leqslant L, y=0^+) &= \phi_2(-L\leqslant x\leqslant L, y=0^-),\\ \phi_2(-L\leqslant x\leqslant L, y=0^+) &= \phi_1(-L\leqslant x\leqslant L, y=0^-).\end{aligned} \tag{15}$$

If $\lambda=0$, the ratio (14) is nothing but the correlation function of an (order 2) twist operator corresponding to (15), which we will write then as[8,19]

$$R_2(\lambda=0) = \frac{z_2}{z_1^2} = \langle\tau_2(L,0)\tilde{\tau}_2(-L,0)\rangle_{\mathcal{L}^{(2)},\mathbb{C}} \propto L^{-1/8}, \tag{16}$$

where $\langle\cdots\rangle_{\mathcal{L}^{(2)},\mathbb{C}}$ means that the correlator is to be evaluated in the plane $\mathbb{C}=\mathbb{R}^2$ (worldsheet) with the Lagrangian $\mathcal{L}^{(2)} = \mathcal{L}[\phi_1]+\mathcal{L}[\phi_2]$. We also recall that in general, the scaling dimension of the twist operator τ_n reads $h_n = \frac{c}{24}(n-1/n)$. We now consider the perturbation expansion in powers of λ. For the denominator, we have immediately

$$D = d^2;\quad d = z_1\left[1+\frac{\lambda^2}{2}\int dy dy'\frac{1}{2|y-y'|^{2\mu}}+\cdots\right], \tag{17}$$

where the factor 1/2 in the integral comes from the 1/2's in the cosines, and we recall that μ is the conformal weight $\mu=\frac{\beta^2}{8\pi}$ of the perturbation.

For the numerator, things are a little more complicated since we have two types of fields on the plane, with $1-1$, $1-2$, and $2-2$ contractions, in the presence of the gluing conditions along the cut. To proceed, we uniformize. We start with the complex coordinates $w=x+iy$, and introduce

$$z = \left(\frac{w-u}{w-v}\right)^{1/2}, \tag{18}$$

where $u=L$ and $v=-L$ are the complex coordinates of the cut's extremities. This maps the whole two-sheeted Riemann surface $\mathcal{R}_{2,1}$ to the z-complex plane $\mathbb{C}$. We then write (14) as

$$\frac{R_2}{R_2(\lambda=0)} = \frac{1+\frac{\lambda^2}{2}\int dw dw'\langle\cos\beta\phi(w)\cos\beta\phi(w')\rangle_{\mathcal{R}_{2,1}}}{\left(1+\frac{\lambda^2}{2}\int dy dy'\frac{1}{2|y-y'|^{2\mu}}\right)^2} + \cdots, \tag{19}$$

where the spatial integrals in the numerator are now over $\mathcal{R}_{2,1}$ (worldsheet), and we have a unique boson ϕ instead of ϕ_1 and ϕ_2. Here the integrals in the numerator correspond to insertions along *two* lines, corresponding to the two copies of the theory, so overall there are four possible terms (contractions). The perturbation $V=\cos\beta\phi$ is a primary operator, so we can calculate the correlations on $\mathcal{R}_{2,1}$ by using the conformal mapping (18). We have

$$\begin{aligned}&2\times 2^{2\mu}\langle\cos\beta\phi(w)\cos\beta\phi(w')\rangle_{\mathcal{R}_{2,1}}\\ &\quad= \frac{(u-v)^{2\mu}}{N_{12}^{2\mu}(w-u)^{\mu/2}(w-v)^{\mu/2}(w'-u)^{\mu/2}(w'-v)^{\mu/2}}.\end{aligned} \tag{20}$$

Here,

$$N_{12} = (w-u)^{1/2}(w'-v)^{1/2}-(w'-u)^{1/2}(w-v)^{1/2}. \tag{21}$$

In (19) we have to integrate w,w' both over the imaginary axis $w=iy$, but also over the second sheet, which is obtained by sending $(w-u)\to e^{2i\pi}(w-u)$ and the same for w'. This means we end up with two integrals where w,w' are on the same sheet, and two where they are on different sheets.

Replacing everything by the particular choice of coordinates, and expanding the denominator in (19) we get

$$\begin{aligned}\frac{R_2}{R_2(\lambda=0)} &= 1+\frac{\lambda^2}{4}\times 2\int_{-\infty}^{\infty}dy dy'[G_{\text{same}}(y,y')\\ &\quad+G_{\text{diff}}(y,y')]+\cdots,\end{aligned} \tag{22}$$

where the factor 2 comes since there are two sheets, and insertions can be on the same or different sheets, so

$$\begin{aligned}&G_{\text{same}}(y,y')\\ &\quad= \frac{1}{2^{2\mu}|y-y'|^{2\mu}}\\ &\qquad\times\frac{[(iy-L)^{1/2}(iy'+L)^{1/2}+(iy'-L)^{1/2}(iy+L)^{1/2}]^{2\mu}}{(y^2+L^2)^{\mu/2}[(y')^2+L^2]^{\mu/2}}\\ &\qquad-\frac{1}{|y-y'|^{2\mu}},\end{aligned} \tag{23}$$

while G_{diff} will be the same expression with a minus in the numerator's bracket, and no subtraction (the two point function of the fields in different copies in the denominator of course vanish identically).

It is convenient to introduce new variables via $\tan\theta = \frac{y}{L}$, so the integral becomes

$$L^{2-2\mu}\int_{-\pi/2}^{\pi/2} d\theta d\theta' (\cos^2\theta)^{\mu-1}(\cos^2\theta')^{\mu-1}\frac{\left(\cos^2\frac{\theta-\theta'}{2}\right)^{\mu}-1}{[\sin^2(\theta-\theta')]\mu}. \tag{24}$$

The second integral reads similarly

$$L^{2-2\mu}\int_{-\pi/2}^{\pi/2} d\theta d\theta' (\cos^2\theta)^{\mu-1}(\cos^2\theta')^{\mu-1}\frac{1}{\left(\cos^2\frac{\theta-\theta'}{2}\right)^{\mu}}. \tag{25}$$

Both integrals are UV convergent for a relevant perturbation $\mu < 1$. They are however both IR divergent (here the IR region being $\theta \approx \pm\frac{\pi}{2}$). This means that, although formally the perturbation at small coupling looks like it should be an expansion in powers of $\lambda^2 L^{2-2\mu}$, this might actually not be the case and, as we shall see later, is not. In fact, we will see that the entanglement is simply nonperturbative in λ^2, and cannot be obtained via this perturbation theory.

This result could appear as a surprise. On the one hand, the entanglement is a $T = 0$ quantity, and such quantities are often plagued by IR divergences. On the other hand, we are looking for an L-dependent quantity, and it would be natural to expect that L would act as an effective IR cutoff, rendering the perturbation expansion finite. This is however definitely not what happens. The situation is reminiscent of similar divergences encountered in the Kondo screening cloud problem.[4]

We stress finally that the argument applies almost without modification to the Hamiltonian (8). All that changes is that the perturbation is of the form $e^{i\beta\phi}S^- + \text{H.c.}$ instead of $e^{i\beta\phi} + \text{H.c.}$, so exponentials of opposite signs have to alternate in the imaginary time insertions, modifying some of the numerical coefficients, but not the integrals or their divergences.

IV. IR DIVERGENCES IN QUANTUM IMPURITY PROBLEMS

To gain a better understanding of the situation, it is useful to start by discussing another observable[20] than the entanglement entropy for (5). We turn briefly to the boundary formulation (6), and consider the one point function $\langle \cos\frac{\beta\Phi}{2}(x)\rangle$ which appears, for instance, in the determination of Friedel oscillations for impurities in Luttinger liquids. Simple scaling arguments suggest the general form

$$\left\langle :\cos\frac{\beta\Phi}{2}:\right\rangle = \left(\frac{2}{|x|}\right)^{\mu/2} F(\lambda|x|^{1-\mu}), \tag{26}$$

where F is a universal function obeying $F(\infty) = 1$, so the field sees Dirichlet boundary conditions, and the bulk normalization has been chosen appropriately.

Determining the function F is also a difficult problem. The most natural is once again to attempt perturbation theory in λ. This would share many features of the calculation of one and two point functions in the bulk sine-Gordon theory.[21] There, it is well known that (in fact, the result essentially goes back to Coleman), provided $h \leqslant 1$ (that is, the perturbing operator is not irrelevant), there are *no UV divergences* in the calculation. All divergences coming from bringing together two insertions of the perturbing term $\cos\frac{\beta\Phi}{2}$ are exactly canceled by similar divergences coming from the expansion of the denominator (the partition function and associated bubble diagrams). In general, the divergences are indeed controlled by the operator product expansion (OPE),

$$e^{i\beta\Phi(y)/2}e^{-i\beta\Phi(y')/2} = |y-y'|^{-2\mu}(1+\cdots-\pi\mu(y-y')^2[\partial\Phi(y)]^2+\cdots),$$

with all fields at $x = 0$, y the coordinate along the boundary. The leading order comes from the contribution of the identity operator and leads to a disconnected piece subtracted off by a similar term in the denominator. The $\cdots$ stand for higher orders, or lower orders that vanish after integration. The overall singularity at order $O(\lambda^{2n-1})$ thus behaves as $\sim \int \prod_{i=0}^{n-1} d(y_{2i}-y_{2i+1}) \times (y_{2i}-y_{2i+1})^{2-2\mu}$, it comes with dimension $d_{\rm UV} = n(3-2\mu)$, and for $\mu \leqslant 1$ the integrals are UV finite. Other singularities (when several points are brought together at once, etc.)[21] behave similarly.

However, there will always appear IR divergences at a certain order, depending on the exact value of the conformal weight h. Of course, we expect in the end the scaling form to hold, and thus to depend only on xT_B, $T_B \propto \lambda^{1/1-\mu}$. What will happen in general is that the divergences in the perturbative expansion have to be resummed before the proper scaling form can be obtained. The latter, in general, will thus behave nonperturbatively in the coupling λ.

This is nicely illustrated in the case $\mu = \frac{1}{2}$, where the exact form of the one point function is known, thanks to a mapping to the boundary Ising model (see below), together with a very clever argument by Chatterjee and Zamolodchikov.[22] One finds[23]

$$\left\langle :\cos\frac{\beta\Phi}{2}:\right\rangle(x) = 4\lambda\sqrt{\pi}\left(\frac{x}{2}\right)^{1/4}\Psi(1/2,1;8\pi\lambda^2 x), \tag{27}$$

where Ψ is the degenerate hypergeometric function. The asymptotics follows from $\Psi(1/2,1;2x) = \frac{e^x}{\sqrt{\pi}}K_0(x)$, where K_0 is the usual modified Bessel function, so that we find

$$\left\langle :\cos\frac{\beta\Phi}{2}:\right\rangle(x) \sim \left(\frac{2}{x}\right)^{1/4}, \quad x \gg 1,$$
$$\left\langle :\cos\frac{\beta\Phi}{2}:\right\rangle(x) \sim x^{-1/4}2^{7/4}\lambda x^{1/2} \times -\ln(\lambda^2 x), \quad x \ll 1. \tag{28}$$

We thus see that this function exhibits a nonperturbative dependence at small coupling λ. The nonanalyticity in λ arises from the IR divergence of the first perturbative integral.

There is a general way to understand the nonanalyticity of course. Whenever a bulk operator (of conformal weights h,h) is sent to the boundary where it becomes a boundary field of weight h_B, one has

$$O(x) \approx x^{h_B-2h}O_B + \cdots. \tag{29}$$

In our case, the cosine of the bulk field simply goes over to the cosine of the boundary field. We have thus $h = \frac{\mu}{4}$ and $h_B = \mu$, while $[O_B] = L^{-h_B} \propto T_B^{h_B} \propto \lambda^{h_B/1-\mu}$. We thus expect that $\langle O_B\rangle = \langle :\cos\frac{\beta\Phi(0)}{2}:\rangle \propto \lambda^{\mu/1-\mu}$. The dependence of the one point function of the boundary field on λ is nonanalytic in λ, and nonperturbative—of course, because again of IR divergences. This problem is the cousin of a similar problem in bulk massive theories, and has been studied in Refs. 24 and 25. We deduce from this that, to leading order,

$$\langle O(x)\rangle \propto x^{h_B-2h}\lambda^{h_B/1-\mu} \tag{30}$$

More generally, we can write

$$O(x) \approx \sum_i x^{h_B^i-2h} O_B^i \tag{31}$$

so

$$\begin{aligned}\langle O(x)\rangle &\approx \sum_i x^{h_B^i-2h} c_B^i T_B^{h_B^i} = x^{-2h}\sum_i x^{h_B^i} c_B^i T_B^{h_B^i}\\ &\equiv x^{-2h} G(xT_B)\end{aligned} \tag{32}$$

with $G(xT_B) \equiv F(\lambda x^{1-\mu})$,

$$F(y) \propto y^{h_B} \propto \lambda^{h_B/1-\mu} x^{h_B}. \tag{33}$$

Going back to the case of Friedel oscillations, we have therefore $F(y) \propto y^{\mu} \propto x^{\mu}\lambda^{\mu/1-\mu}$. This leading dependence in λ replaces the expected perturbative one, which would be linear in λ.

The foregoing argument applies in the generic case. Whenever there are "resonances" and the parameter μ takes special rational values $\mu = 1 - \frac{1}{2n}$, extra logarithmic terms appear in the one point functions of the operators right on the boundary, which translates in logarithms in the one point functions of operators at $x \neq 0$ as well. This is the case precisely when $\mu = \frac{1}{2}$.

It is important to stress also that the IR divergences naturally disappear at finite temperature, $1/T$ providing a natural cutoff. Once again this is illustrated in the $\mu = \frac{1}{2}$ case, where one finds,[23,26] for Friedel oscillations at finite temperature,

$$\begin{aligned}&\left\langle : \cos\frac{\beta\Phi}{2} : \right\rangle(x)\\ &\quad = f(2\lambda^2/T)\left(\frac{4\pi T}{\sinh(2\pi T x)}\right)^{1/4}\\ &\quad\times F\left(\frac{1}{2},\frac{1}{2};1+2\frac{\lambda^2}{T},\frac{1-\coth 2\pi x T}{2}\right).\end{aligned} \tag{34}$$

Here F is the usual hypergeometric function, f is a function whose existence and value were determined in Ref. 26. The right-hand side admits a perturbative expansion in powers of λ, whose leading term, at fixed x, goes as $\lambda/\sqrt{T}$ when $T \to 0$. The coefficient of λ thus diverges in the zero-temperature limit, in agreement with the fact that the true expansion is then in $\lambda \ln \lambda$.

The general IR behavior can easily be investigated. One finds that at order $O(\lambda^{2n+1})$, there is no IR divergence provided $\mu > \frac{n+1/2}{n+1}$. Only when $\mu = 1$—that is, the boundary perturbation is exactly marginal, and the bulk is a Fermi liquid—are all orders finite. In this case, the Friedel oscillations admit a perturbative expansion in powers of λ.[27]

While the nature of the divergences is quite generic, the quantities for which they occur depend on the problem at hand. For instance, for the screening cloud in the (anisotropic) Kondo model, divergences occur even when the boundary perturbation has dimension 1—in that case, it is marginally relevant.[4]

V. SMALL COUPLING BEHAVIOR OF THE ENTANGLEMENT ENTROPY

We now go back to the calculation of the entanglement entropy for Hamiltonian (5). We see that, to obtain the nonperturbative UV behavior, we must discuss twist fields and their OPEs. We follow the paper[28] but focus more directly on the question at hand. Imagine that we have a single interval for which we want to calculate the entanglement with the rest of the system, and introduce accordingly the n-sheeted Riemann surface (n replicas) $\mathcal{R}_{n,1}$. In the limit where the interval of length L shrinks, we expect the presence of the two sewing points to decompose like an operator product expansion of the form

$$I = \sum_{\{k_j\}} C_{\{k_j\}} \prod_{j=1}^{n} \Psi_{k_j}(z_j), \tag{35}$$

where we allowed for fields inserted at points z_j, the point z on the jth sheet, and the set $\{\Psi_k\}$ denotes a complete set of local fields for one copy of the CFT. Recall that the cut in the Riemann surface $\mathcal{R}_{n,1}$ corresponds to the insertion of twist fields in the complex plane, so that $I \sim \tau_n(L)\tilde{\tau}_n(-L)$ and (35) should be considered as the OPE of these twist fields. What (35) means more precisely is that, if we have other operators inserted elsewhere, we can expect to have

$$\begin{aligned}&\frac{Z_n(L)}{Z_1^n}\left\langle \prod_{j=1}^{n} O_j \right\rangle_{\mathcal{R}_{n,1}}\\ &\quad = \left\langle I \prod_{j=1}^{n} O_j \right\rangle_{\mathbb{C}^n} = \sum_{\{k_j\}} C_{\{k_j\}} \prod_{j=1}^{n} \left\langle \Psi_{k_j}(z_j) O_j \right\rangle_{\mathbb{C}_j},\end{aligned} \tag{36}$$

where O_j designates operators inserted on the jth sheet, and $\mathbb{C}_j$ is the jth copy of the complex plane. Note indeed that the expectation on the right is taken in a fully factorized theory.

Restricting now to the Ψ_k that make an orthonormal basis (so in particular they are all quasiprimary), and choosing $O_j = \Psi_{k_j}$ shows that the structure constant $C_{\{k_j\}}$ will not vanish only if the average of $\prod_j O_j$ on the Riemann surface $\mathcal{R}_{n,1}$ does not vanish. It is useful to make things concrete now, so for instance we see that there is no term with a single primary operator on the right-hand side of (35) since the corresponding one point function on $\mathcal{R}_{n,1}$ vanishes. There is, however, at least one term with a single operator, the stress energy tensor, since we know that $\langle T\rangle_{\mathcal{R}_{n,1}} \neq 0$. Apart from this, the most important terms will be those involving the same primary operator on two different sheets $\prod_{j=1}^{n} \Psi_{k_j} = \Psi_1\Psi_2$, whose average on $\mathcal{R}_{n,1}$ will be nonzero in general. If the field Ψ has conformal weights $h,\bar{h}$, we will thus have that

$$C \propto L^{-4h_n} L^{2\times(h+\bar{h})}, \tag{37}$$

where $h_n = \frac{c}{24}(n - \frac{1}{n})$ is the conformal weight of the twist field. The crucial point is that C involves *twice* the scaling dimension of primary fields, in contrast with ordinary OPEs where only the scaling dimension would appear.

The discussion carries over to the boundary case. One can, for instance, think of it after unfolding the system so as to keep only chiral fields as in (5). Everything then formally goes through after setting $\bar{h} = 0$. The question is then, what kind of fields ψ (the chiral part of Ψ) can appear in the OPE of two twist fields? The one copy bulk theory is a compact boson which allows for the fields $\exp(\pm i\frac{\beta}{2}\Phi)$ on the boundary. This means that the radius is $R = \frac{2}{\beta}$, and thus the bulk conformal weights are given by

$$\Delta_{wk} = 2\pi\left(\frac{\beta k}{8\pi} - \frac{w}{\beta}\right)^2, \quad \bar{\Delta}_{wk} = 2\pi\left(\frac{\beta k}{8\pi} + \frac{w}{\beta}\right)^2. \quad (38)$$

Restricting to scalar operators we get $\Delta = \frac{k^2\beta^2}{32\pi}$ or $\Delta = \frac{2\pi}{\beta^2}w^2$. For instance, the first values of Δ correspond to fields $\exp(\pm ik\frac{\beta}{2}\Phi)$, or, for the chiral part, $\exp(\pm ik\frac{\beta}{2}\phi_R)$.

We now go back to the entropy calculation in the folded, nonchiral theory (6). Upon folding, the chiral vertex operators $e^{\pm ik(\beta/2)\phi_R(0)}$ become $e^{\pm ik(\beta/4)\Phi(0)}$, as $\Phi(0) = \phi_R(0) + \phi_L(0) = 2\phi_R(0)$. Recall also that the nonchiral twist field in the folded version can be thought of as the chiral part of I in the unfolded theory. Hence, going through the discussion of short-distance expansions we find, for the nonchiral twist field,

$$\tau_n(L) \approx L^{-2h_n} \times \left(1 + \sum_k L^{2\Delta_k} c_n \sum_{\substack{i,j=1\\ i\neq j}}^{n} e^{ik\frac{\beta}{4}\Phi_i(0)} e^{ik\frac{\beta}{4}\Phi_j(0)} + \cdots\right) \quad (39)$$

where we used the fact[28] that the two fields ψ in the twist OPEs must belong to different copies. We are only interested in terms whose one point function acquires a nonzero value in the presence of the perturbation. This means the first term with $k = 1$ cannot contribute, and thus we need $k = 2$, $\Delta_2 = \mu$. Taking derivative with respect to n gives then the leading term for the entanglement correction, which should go as

$$\mathcal{S}_{\rm imp} - \ln 2 \propto (LT_B)^{2\mu} \propto L^{2\mu}\lambda^{2\mu/(1-\mu)}. \quad (40)$$

For $\mu = \frac{1}{2}$ in particular, this can be corrected by a resonance, and it is tempting to speculate then that one has

$$\mathcal{S}_{\rm imp} - \ln 2 \propto LT_B\left[{\rm cst} + {\rm cst}\ln(LT_B)\right]. \quad (41)$$

Finally, we note once again that the RLM or the various (anisotropic) Kondo versions will behave identically, the presence of the operators S^+, S^- not modifying in any essential way the OPE argument—but one will have to be careful with the dimensions of the operators involved, and their relationship with μ. In the end, we find that for the RLM (41) is expected to hold as well.

VI. LARGE COUPLING EXPANSION

While the small coupling expansion is plagued with IR divergences, a large coupling expansion is possible. It is now finite in the IR, and exhibits UV divergences which are easily taken care of using integrability and analyticity. Let us recall how the calculation goes at leading order in the anisotropic Kondo case[29] (see also, e.g., Ref. 30). The leading IR perturbation is nothing but the stress energy tensor $H = H_{\rm IR} + \frac{1}{\pi T_B}T(0) + \cdots$. The correction to the Renyi entropy can therefore be expressed as

$$\begin{aligned}-\delta Z_n &= \frac{n}{\pi T_B}\int_{-\infty}^{+\infty} d\tau \langle T(w = i\tau)\rangle_{\mathcal{R}_{n,1}} \\ &= \frac{n - n^{-1}}{24\pi T_B}\int_{-\infty}^{+\infty} \frac{(2L)^2}{(i\tau - L)^2(i\tau + L)^2} d\tau \\ &= \frac{1}{12LT_B}\left(n - \frac{1}{n}\right). \end{aligned} \quad (42)$$

The first correction to the entanglement entropy thus reads

$$\mathcal{S}_{\rm imp} = \frac{1}{6LT_B} + \cdots. \quad (43)$$

It is quite remarkable that this result does not depend on the anisotropy parameter $\frac{\mu}{2}$ (recall that $\Delta = -\cos\pi\frac{\mu}{2}$ in the XXZ language). It turns out that this IR expansion can be generalized to higher orders.[11] The results for the Kondo case are as follows:

$$\begin{aligned}\mathcal{S}_{\rm imp} &= \frac{1}{6}\ln\left(1 + \frac{1}{LT_B}\right) - \frac{18}{35}\frac{(\pi g_4)^2}{(2LT_B)^6}(4\alpha^4 - 8\alpha^2 + 9) \\ &\quad + O[(LT_B)^{-7}], \end{aligned} \quad (44)$$

where the coefficient g_4 has the following dependence on the dimension $h = \frac{\mu}{2}$ of the tunneling operator:

$$\begin{aligned} g_4 &= \frac{\mu}{12\pi^2}\left(\frac{\Gamma[\mu/2(2-\mu)]}{\Gamma[1/(2-\mu)]}\right)^3 \frac{\Gamma[3/(2-\mu)]}{\Gamma[3\mu/2(2-\mu)]}, \\ \alpha &= \frac{(2-\mu)}{\sqrt{2\mu}}. \end{aligned} \quad (45)$$

Note that in (44), the first term in the right-hand side has to be truncated at order 6.

While in principle higher orders in the IR expansion could be determined, the complexity of the calculations increases considerably. Moreover, the convergence properties of this expansion are not clear. Finally, we observe that, in this point of view, the pure BSG case turns out to be quite different, because different operators appear in the IR effective description. The corresponding result has not even been worked out yet.

Making analytical progress therefore requires developing nonperturbative approaches. The problems we are interested in are indeed integrable, at least in their boundary versions. While it is natural to expect that this can be used in some way, integrability has been mostly used to calculate local properties such as magnetization, energy, or impurity entropies. von Neumann entanglement is nonlocal, and therefore much harder to obtain in general.

VII. FORM FACTOR APPROACH TO THE ENTANGLEMENT ENTROPY

We will in what follows restrict to the case where the dimension of the perturbation is $h = \frac{1}{2}$: this corresponds to $\Delta = -\frac{\sqrt{2}}{2}$ ($\mu = \frac{1}{2}$) for the problem of tunneling between XXZ chains, and to $\Delta = 0$—the RLM ($\mu = 1$)—for the tunneling through an impurity. These cases are closely related to the boundary Ising model with a boundary magnetic field (see Appendix). While the problem of calculating the entanglement nonperturbatively remains extremely difficult—entanglement still involving nonlocal observables in the fermionic language—it can be tackled using the idea of form factors.

It has been known for many years that correlation functions of local observables in massive integrable theories can be calculated using the form-factors approach, where the integrable quasiparticles provide a basis of the Hilbert space, and the form factors (FFs)—that is, the matrix elements of the operators in that basis—can be obtained using an axiomatic approach based on the knowledge of the S matrix and the bootstrap. It is a natural idea to extend this approach to the case of entanglement entropy. Indeed, the von Neumann entanglement is obtained form the Renyi entropy by taking an n derivative at $n = 1$, and the Renyi entropies can be considered formally as correlation functions of twist operators that live in n copies of the theory of interest. The integrability of a single theory carries over to integrability of the n copies, and a calculation similar to the one of ordinary correlators can be set up, after some additional work to determine the form factors of the twist operators $\tau,\tilde{\tau}$.[12,13]

We are interested here in a variant where the bulk is massless. The form-factors technique in this case is more delicate to use, since particles can have arbitrarily low energies, and the convergence of the approach is not guaranteed. Various regularization tricks have to be used in the calculation of local quantities (e.g., the charge density for Friedel oscillations),[31,32] and we will see below that the situation for the entanglement is not better. Nevertheless, $\mathcal{S}_{\text{imp}}(LT_B)$ can be calculated for $h = \frac{1}{2}$, by using the Ising model formulation, and relying heavily on the work.[12,13]

To fix ideas, and explore the feasibility of form-factors calculations in our problem, we first discuss briefly the bulk case and the massless limit. One can find in[12,13] the first order contribution to the two point function of the bulk Ising model twist field in the bulk,

$$\langle\tau(r)\tilde{\tau}(0)\rangle = \langle\tau\rangle^2 + \frac{1}{2}\sum_{i,j=1}^{n}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\left|F_2^{\tau|ij}(\theta_{12},n)\right|^2 \times e^{-mr(\cosh\theta_1+\cosh\theta_2)} + \cdots, \tag{46}$$

where n is the number of copies, θ_i is the rapidity of the ith particle with energy $e = m\cosh\theta_i$ and momentum $p = m\sinh\theta_i$, and $F_2^{\tau|ij}(\theta_{12},n)$ is the two-particle form factor of the twist field τ,

$$F_2^{\tau|ij}(\theta_{12},n) = \langle 0|\tau(0)Z_i^{\dagger}(\theta_1)Z_j^{\dagger}(\theta_2)|0\rangle. \tag{47}$$

In this last expression, we have used the notation $Z_j^{\dagger}$ for the usual Faddeev-Zamolodchikov creation operators (here, the fermions) living in the jth copy. Since the theory is integrable, the form factors $F_2^{\tau|ij}(\theta_{12},n)$ can be computed exactly and are conveniently expressed using the function

$$K(\theta) = \frac{F_2^{\tau|11}}{\langle\tau\rangle} = -i\frac{\cos\frac{\pi}{2n}\sinh\frac{\theta}{2n}}{n\sinh\frac{i\pi+\theta}{2n}\sinh\frac{i\pi-\theta}{2n}}, \tag{48}$$

which vanishes when $n = 1$. The other form factors $F_2^{\tau|ij}(\theta_{12},n)$ can then be obtained from $F_2^{\tau|11}(\theta_{12},n)$ by shifting appropriately θ_{12} by a factor of $2\pi i$. Going to variables $\theta_1 \pm \theta_2$ one can perform one integration, and be left with

$$\langle\tau(r)\tilde{\tau}(0)\rangle = \langle\tau\rangle^2\left(1 + \frac{n}{4\pi}\int_{-\infty}^{\infty}d\theta f(\theta,n)K_0[2mr\cosh(\theta/2)]\right) + \cdots, \tag{49}$$

where

$$\langle\tau\rangle^2 f(\theta) \equiv \left|F_2^{\tau|11}(\theta)\right|^2 + \sum_{j=1}^{n-1}\left|F_2^{\tau|11}(\theta + 2i\pi j)\right|^2. \tag{50}$$

Doyon *et al.* then argue the crucial result that

$$\left.\frac{d}{dn}nf(\theta,n)\right|_{n=1} = \frac{\pi^2}{2}\delta(\theta). \tag{51}$$

Taking the derivative of the two point twist correlation function meanwhile should give, at short distances, the entanglement entropy of the CFT. Since (46) is only a first-order approximation where contributions with a larger number of particles have not been included, we get an approximation to the entanglement entropy of a segment of length r in the bulk with the rest of the system,[12]

$$S_A = \cdots - \frac{K_0(2mr)}{8} + \cdots \approx \cdots + \frac{\ln r}{8} + \cdots, \tag{52}$$

and thus the expected factor $\frac{c}{3} = \frac{1}{6}$ is approximated by $\frac{1}{8}$ at this order.

Since in this paper we are interested in bulk CFTs, we need to take an $m \to 0$ limit. This corresponds formally to describing the CFT using massless particles and massless scattering. We thus set $\frac{m}{2} = Me^{-\theta_0}$ and send $\theta_0 \to \infty$. Only two types of excitations remain at finite energies: those for which $\theta = \pm\theta_0 \pm \beta$ with β finite. In the first case, one obtains right moving particles with $e = p = Me^{\beta}$ and in the second case left moving particles with $e = -p = Me^{\beta}$. Conformal fields factorizing into left and right components are not expected to mix the L and R sectors. Indeed,

$$\lim_{\theta\to\infty}K(\theta) = 0, \tag{53}$$

so only the LL and RR sectors will contribute in the massless limit of (46). Therefore, setting (say for the R sector)

$$\theta_{1,2} = \theta_0 + \beta_{1,2}, \tag{54}$$

and introducing $\beta_{\pm} \equiv \beta_1 \pm \beta_2$, we obtain

$$\langle\tau(r)\tilde{\tau}(0)\rangle = \langle\tau\rangle^2 + \frac{1}{2}\sum_{i,j=1}^{n}\int\frac{d\beta_+}{2\pi}\frac{d\beta_-}{2\pi}\left|F_2^{\tau|ij}(\beta_-,n)\right|^2 \times e^{-2Mre^{\beta_+/2}\cosh(\beta_-/2)} + \cdots, \tag{55}$$

where the $1/2$ coming from the Jacobian was canceled by the fact that there are two integrals, the L and the R one. Using (51) we get the correction to the entanglement entropy as

$$S_A = \cdots - \frac{1}{16}\int_{-\infty}^{\infty}d\beta_+ e^{-2Mre^{\beta_+/2}} = \cdots - \frac{1}{8}\int_0^{\infty}\frac{dx}{x}e^{-2Mrx}. \tag{56}$$

This integral is divergent at small energy, a feature which is quite general in the use of massless form factors. We regularize by considering the integral

$$\int_0^\infty dx x^{\alpha-1} e^{-2Mrx} = \frac{1}{(2Mr)^\alpha}\Gamma(\alpha) = \left(\frac{1}{\alpha}+\cdots\right)[1-\alpha\ln(2Mr)+\cdots] \tag{57}$$

so the finite part of the integral is $-\ln(2Mr)$ and thus we recover

$$S_A = \cdots + \tfrac{1}{8}\ln r + \cdots. \tag{58}$$

Let us now consider the Ising model with a boundary magnetic field as in (A5), and to start assume that the bulk is massive. The form-factors approach can be applied to this case as well. The first nontrivial contribution reads then[13]

$$\langle 0|\tau(r)|B\rangle = \langle\tau\rangle + \frac{1}{2}\sum_{i=1}^n \int \frac{d\theta}{2\pi} R\left(\frac{i\pi}{2}-\theta\right) e^{-2mr\cosh\theta} \times F_2^{\tau|11}(-\theta,\theta,n) + \cdots \tag{59}$$

coming from the boundary state

$$|B\rangle = \exp\left[\frac{1}{4\pi}\sum_{j=1}^n \int d\theta R\left(\frac{i\pi}{2}-\theta\right) Z_j^\dagger(-\theta) Z_j^\dagger(\theta)\right]|0\rangle, \tag{60}$$

where we recall that $Z_j^\dagger$ are the usual Faddeev-Zamolodchikov creation operators living in the jth copy, and $R(\theta)$ is the reflection matrix[33] of the Ising field theory with a boundary magnetic field h_b [proportional to λ in (A5)]. Ultimately, we want once again to take the massless limit $m \to 0$. Notice that (59) involves F_2 instead of $|F_2|^2$. We write

$$\langle 0|\tau(r)|B\rangle = \langle\tau\rangle + \frac{n}{4\pi}\int d\theta R\left(\frac{i\pi}{2}-\theta\right) F_2^{\tau|11}(-\theta,\theta) \times e^{-2mr\cosh\theta} + \cdots \tag{61}$$

and observe that the analytical continuation in n is trivial because the particle and its reflection must belong to the same copy. To every order, contributions are linear in F. But there is a lot of similarity—e.g., between the term with four particles here, and the term with two particles in the bulk entropy. In the massless limit case, since the boundary produces as many L as R particles, and since we need both these numbers to be even, only the terms with $2l$ R movers and $2l$ L movers contribute.

Indeed, the first correction to the entanglement, after taking derivative with respect to n at $n=1$, reads explicitly

$$s_1 = -\frac{1}{4}\int_0^\infty d\theta \left(\frac{\kappa+\cosh\theta}{\kappa-\cosh\theta}\right)\left(\frac{\cosh\theta-1}{\cosh^2\theta}\right) e^{-2mL\cosh\theta}, \tag{62}$$

with $\kappa = 1 - h_b^2/(2m)$. To obtain a scaling expression in the massless limit, we boost rapidities like in the bulk case, and we obtain

$$s_1 \approx \frac{1}{4}\int_{-\infty}^\infty d\beta \frac{e^\beta - \frac{h_b^2}{2M}}{e^\beta + \frac{h_b^2}{2M}} \times 2e^{-\theta_0} e^{-\beta} e^{-2LMe^\beta} \to 0, \tag{63}$$

a vanishing result—natural, since in this limit, the two-particle form factor factorizes onto one-particle form factors (one for the left, one for the right), which both vanish. We thus need to go to the next order (corresponding to four particles), where we use formula (3.25) in Ref. 13:

$$s_2 = \frac{1}{16}\int_0^\infty d\theta \left(\frac{\kappa+\cosh\theta}{\kappa-\cosh\theta}\right)^2\left(\frac{1-\cosh\theta}{1+\cosh\theta}\right) e^{-4mL\cosh\theta}. \tag{64}$$

We obtain then

$$s_2 \approx -\frac{1}{16}\int_{-\infty}^\infty d\beta \left(\frac{e^\beta - \frac{h_b^2}{2M}}{e^\beta + \frac{h_b^2}{2M}}\right)^2 e^{-4LMe^\beta} = -\frac{1}{16}\int_{-\infty}^\infty d\beta \left(\frac{e^\beta - T_B}{e^\beta + T_B}\right)^2 e^{-4Le^\beta}, \tag{65}$$

where we have set

$$T_B \equiv \frac{h_b^2}{2} \tag{66}$$

and we have shifted the β integral. Now the expression (65) is divergent at low energies, just like (56). To regularize it, we consider the difference:

$$s_2(LT_B) - s_2(\infty) = \frac{1}{4}\int_{-\infty}^\infty d\beta \frac{e^\beta}{(1+e^\beta)^2} e^{-4LT_B e^\beta} = \frac{1}{4}\int_0^\infty \frac{du}{(1+u)^2} e^{-4LT_B u}. \tag{67}$$

The UV value is $\frac{1}{4} = 0.25$, to be compared with the exact value $\frac{1}{2}\ln 2 = 0.346\,574\ldots$. This indicates that we are on the right track.

To proceed, we now take Eq. (3.54) in Ref. 13 and perform the appropriate limits and rescalings to get

$$s_4 \approx \frac{1}{2^8\pi^2}\int \prod_i d\beta_i \delta\left(\sum \beta_i\right)\left[e^{-2L\sum e^{\beta_i}} \prod_i \frac{e^{\beta_i}-T_B}{e^{\beta_i}+T_B} \times \prod_i \frac{1}{\cosh\frac{\beta_i-\beta_{i+1}}{2}} - \begin{matrix}\beta_{1,3}\to\beta_{1,3}\pm\frac{i\pi}{4}\\ \beta_{2,4}\to\beta_{2,4}\mp\frac{i\pi}{4}\end{matrix}\right], \tag{68}$$

where products and sums run over $i = 1,\ldots,4$ and we have set $\beta_{4+1} \equiv \beta_1$. The second term is obtained by shifting the contours of integration in the imaginary direction as indicated. We observe the same divergence at low energy, and the same regularization [subtracting the formal expression for $s_4(\infty)$] also works like for s_2. We find

$$s_4(LT_B) - s_4(\infty) = \int_0^\infty \frac{du_1 du_2 du_3}{16\pi^2}\left[e^{-2LT_B(u_1+u_2)(u_2+u_3)/u_2} \times \frac{u_2}{(u_1+u_2)^2(u_2+u_3)^2}\left(\prod_i \frac{1-u_i}{1+u_i} - 1\right) - \ldots\right], \tag{69}$$

where the dots correspond to the two other terms obtained by shifting the contours of integration as in (68). The UV value is $s_4(0) - s_4(\infty) = \frac{1}{24}$, so at second order we have the UV value $\frac{1}{4}+\frac{1}{24} = 0.291\,667\ldots$, to be compared once again with the value $\frac{1}{2}\ln 2 = 0.346\,574\ldots$.

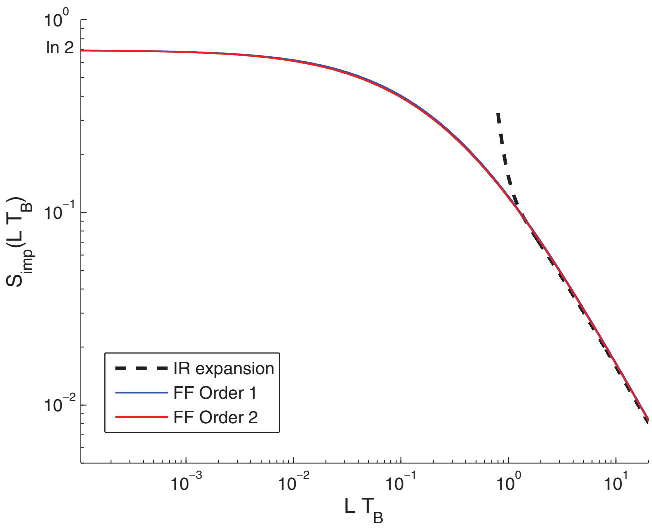

FIG. 1. (Color online) The form factor approximations together with the IR expansion.

We find that higher orders can be dealt with in the same way, and that the UV values can be resummed exactly to yield the exact result,

$$S_{\rm UV} - S_{\rm IR} = \sum_{l=1}^{\infty}[s_{2l}(0) - s_{2l}(\infty)] = \sum_{l=1}^{\infty} \frac{1}{4l(2l-1)} = \frac{1}{2}\ln 2, \tag{70}$$

as expected.

We now return to the RLM, whose results are obtained simply by multiplying those for Ising by a factor of 2. In the following, we will allow for an extra multiplicative renormalization to obtain the UV result exactly, that is consider, at lowest order, the ratio

$$\mathcal{S}^{(2)}_{\rm imp}(LT_B) \equiv \ln 2 \frac{s_2(LT_B) - s_2(\infty)}{s_2(0) - s_2(\infty)} = \ln 2 \int_0^{\infty} \frac{du}{(1+u)^2} e^{-4LT_B u}. \tag{71}$$

It is then interesting to consider the IR expansion of this quantity. Using

$$s_2(LT_B) - s_2(\infty) = \tfrac{1}{2}[\alpha e^{\alpha}\mathrm{Ei}(-\alpha) + 1], \quad \alpha = 4LT_B, \tag{72}$$

where Ei is the usual exponential integral function. One finds

$$\mathcal{S}^{(2)}_{\rm imp}(LT_B) = 2\ln 2 \sum_{k=1}^{n} (-1)^{k-1} \frac{k!}{2(4LT_B)^k} + O\left(\frac{1}{(LT_B)^{n+1}}\right), \tag{73}$$

where the expansion is only asymptotic. We see thus that our "renormalized" first-order approximation interpolates between ln 2 and to $\frac{\ln 2}{4LT_B} = 0.173\,287/(LT_B)$, while the exact result goes from ln 2 to $\frac{1}{6LT_B} = 0.166\,66/(LT_B)$, which is quite good. The next order approximation can be handled similarly, and we will simply provide the corresponding results on the curves below.

We plot our results for the FF approach in Fig. 1 where the dashed line is the IR expansion (see above and Ref. 11), and the full colored lines are form factors approximations. Clearly, on this scale, the (renormalized) FF expansion has converged very quickly. We shall soon see how close it is to the real data from numerical simulations on the XX chain.

We now discuss briefly the UV behavior. For s_2, the standard tables give

$$\mathcal{S}^{(2)}_{\rm imp}(LT_B) = \ln 2 + 4\ln 2 \times (LT_B)\,[\ln 4 + \gamma + \ln(LT_B)] + \cdots, \tag{74}$$

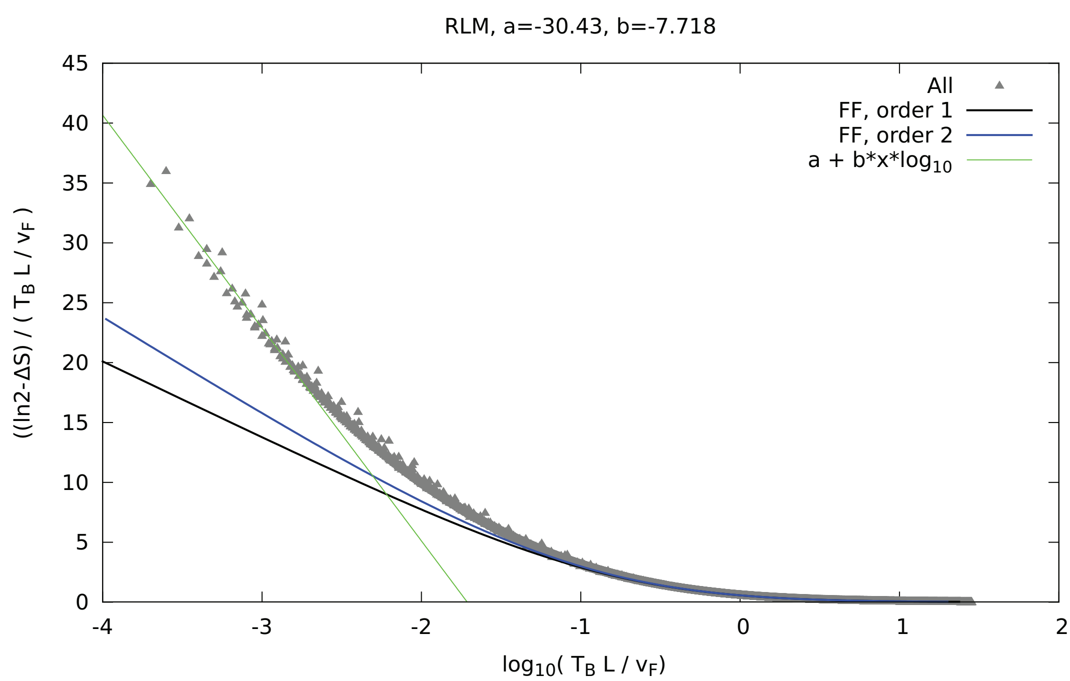

FIG. 2. (Color online) Singularity in the UV, with $\Delta S \equiv \mathcal{S}_{\rm imp}(LT_B)$.

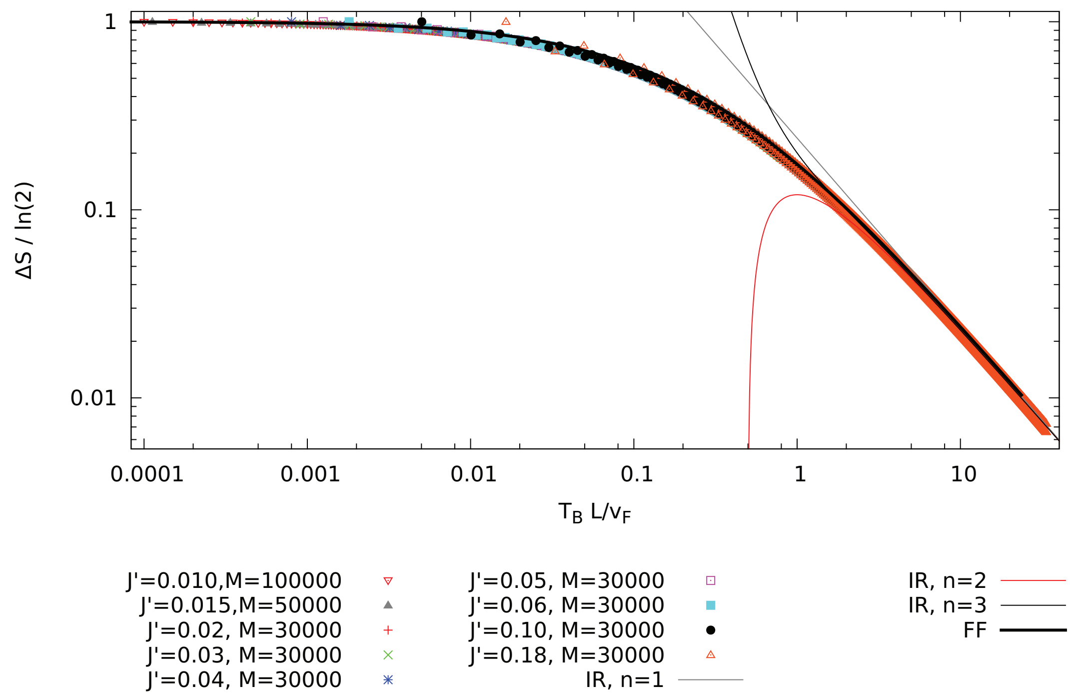

FIG. 3. (Color online) Comparison of numerical results and various approximations (recall that $\Delta S = S_{\mathrm{imp}}(LT_B)$).

where $\gamma \simeq 0.5772\ldots$ is the Euler constant. This provides a leading-order correction in the UV which reads $4\ln 2(LT_B)\ln(LT_B)$. Note that this is compatible with what was expected from the general discussion about the nonperturbative behavior in the UV: we get a term linear in LT_B, decorated by logarithmic corrections. The next order is more difficult to handle analytically, but very accurate numerics shows that it does behave similarly, only leading to a correction of the slope which goes from $4\ln 2 = 2.772\,59$ to 3.53. We plot in Fig. 2 the leading correction divided by LT_B as a function of $-\ln(LT_B)$, together with numerical data that shall be discussed in the next section. We see that the FF expansion converges very well except in the UV, where it seems to still converge, but more slowly, giving us only a rough approximation of the exact leading singularity.

Finally, the results for the entanglement for the problem of weakly coupled XXZ chains at $\Delta = -\frac{\sqrt{2}}{2}$ would be identical but for an overall normalization by a factor 1/2.

VIII. NUMERICS

We now turn to a numerical determination of the entanglement entropy in the RLM, going back to the formulation (10) where we will now also have to be careful with the overall finite size of the system. We write

$$H = -J\sum_{m=-M'}^{-2}(c_m^\dagger c_{m+1} + \text{H.c.}) - J\sum_{m=1}^{M'-1}(c_m^\dagger c_{m+1} + \text{H.c.}) - \tilde{J}(c_{-1}^\dagger c_0 + c_0^\dagger c_{-1} + c_0^\dagger c_1 + c_1^\dagger c_0). \tag{75}$$

So the left and right leads have M' sites, and the impurity sits at site 0. We can now switch to a representation of symmetric and antisymmetric combination of the lead sites, $C(\tilde{C}) = (c_j \pm c_{-j})/\sqrt{2}$. Since the antisymmetric combination decouples from the rest, its contribution to the impurity entanglement will drop out. It is therefore sufficient to study a system of $M \equiv M' + 1$ sites:

$$H = -J\sum_{m=1}^{M'-1}(C_m^\dagger C_{m+1} + \text{H.c.}) - \tilde{J}\sqrt{2}(C_1^\dagger C_0 + C_0^\dagger C_1). \tag{76}$$

Here a single resonant level couples to a single chain of M sites. In order to compare with field theory we use the exactly half filled system to exploit the linear regime of the cosine band. In return we have to use an even number of $M = M' + 1$ sites.

The scale of the resonant level with a coupling of $J' = \sqrt{2}\tilde{J}$ is

$$T_{\mathrm{B}}/v_{\mathrm{F}} = \frac{J'^2}{2\sqrt{1 - J'^2}}, \tag{77}$$

with $v_F = 2$ as we have chosen the normalization $J = 1$. Following the recipe of Ref. 34 we now calculate the reduced single-particle matrix $\rho_{\mathrm{I},L+1}$ for the last $L+1$ sites, where the first site (labeled 0) corresponds to the impurity. In order to obtain the bulk result we determine the reduced density matrix $\rho_{\mathrm{B},L}$ for the first L sites of the chain. The reason for taking the bulk result from the opposite end of the chain is that we cannot just study a chain of M' sites, as we would then have a degenerate ground state as M' is odd. The diagonalization is performed within double precision, while the trace for the entropy is performed using quadruple (128 bit) precision.

The entanglement entropy corresponding to the single-particle reduced density matrix is now given by

$$S = -\mathrm{Tr}\rho\ln\rho - \mathrm{Tr}(1-\rho)\ln(1-\rho), \tag{78}$$

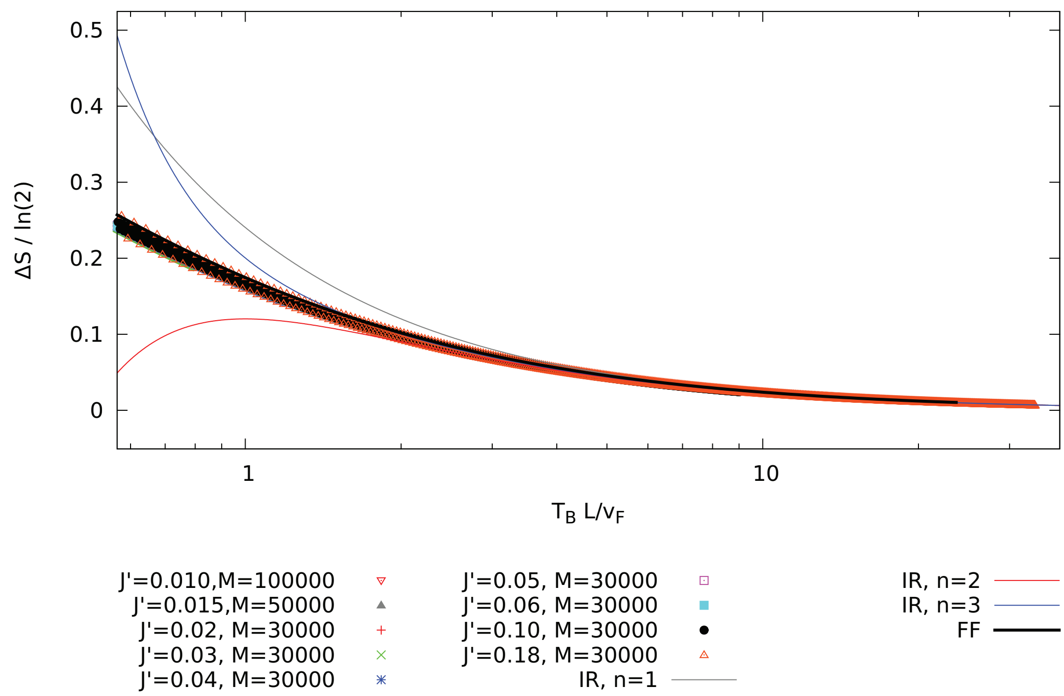

FIG. 4. (Color online) Comparison of numerical results and various approximations: focus on the IR.

which finally leads to

$$\mathcal{S}_{\text{imp},L} = S_{\text{I},L+1} - S_{\text{B},L}. \tag{79}$$

In Fig. 3 we plot the numerical results together with the first three orders of the IR expansion and the first order of the FF expansion. We would like to remark that on the lattice we get small $2k_\text{F}$ oscillations on top of the continuum result. Figure 4 is a similar plot emphasizing the IR behavior.

Finally, in Fig. 2—as commented on already—we focus on the singularity in the UV, comparing slopes obtained from the FF expansion. Our numerics on system sizes $M = 3 \times 10^4 \cdots 10^5$ is consistent with a singularity

$$\mathcal{S}_{\text{imp}} = \ln 2 + \alpha L T_B \ln(L T_B) + \cdots, \tag{80}$$

with a slope $-7.5 \lesssim \alpha \lesssim -8$. By applying damped boundary conditions (DBCs),[35] one can access very small energy scales on system sizes which are accessible by numerics. By looking at systems of $M = 4000$ sites where we scale down the bulk hopping elements by a factor of $\Lambda = 0.98$ on each bond from site 2000 to 3000 and using a bulk hopping element of $J\Lambda^{1000}$ on the last 1000 sites we find an indication that the singularity is even slightly stronger. While we can exclude an L^2 behavior, we cannot rule out the possibility of an $LT_B \ln^2(LT_B)$ contribution. Note that the DBCs change the form of the density of states at the Fermi surface; for details see Ref. 36. It is therefore possible that this additional increase is due to this modification of the level spacing at the Fermi surface. Due to the slow increase of the logarithm such a clarification is asking for multiprecision arithmetic.

IX. CONCLUSION

This study shows that the entanglement entropy of quantum impurities involved in an RG flow is a quantity which is difficult to access. It is nonperturbative in the UV, and the IR perturbation, while well defined, does not capture the crossover regime very well. The form-factors approach, on the other hand, is remarkably successful. It is, however, difficult to develop except in the simple case of the Ising model, and more work will have to be done in that direction. Nevertheless, we believe that the essential features of $\mathcal{S}_{\text{imp}}$ are under control, although it would be useful to check the UV singularities for other values of the coupling (anisotropy).

In conclusion, we emphasize that the geometry considered in this paper where the interval for the entropy is centered on the impurity is probably not the most natural physically. To characterize the Kondo physics, one would rather be interested in the entanglement of the two wires tunneling through an impurity. This could be characterized physically by the entropy of an interval with the impurity at its boundary or, for example, by the negativity of two intervals in the different wires (see, e.g., Refs. 37–39 for examples related to the Kondo problem). This situation is unfortunately much more complicated technically, mostly because the folding procedures described in this paper no longer apply. However, we still expect the conclusions of this paper to hold in that case as well, namely, we expect the entanglement entropy (or other entanglement estimators) to depend nonpertubatively on the coupling to the impurity when this is weak. We believe that improper regularizations of the IR divergences encountered in perturbation theory led to some confusion in the literature.[40] We will report on this—together with a correct calculation—in a subsequent paper.

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APPENDIX: RELATIONSHIP BETWEEN THE CASE $h = \frac{1}{2}$ AND THE BOUNDARY ISING MODEL

Let us begin by discussing the relationship between the RLM and the Ising model with a boundary magnetic field. This can be seen in various ways. Start from the Hamiltonian (11), unfold the wires to get only right movers, and form the combinations

$$\Psi_R \equiv \frac{1}{\sqrt{2}}(\psi_{1R} + \psi_{2R}), \quad \tilde{\Psi}_R \equiv \frac{1}{\sqrt{2}}(\psi_{1R} - \psi_{2R}). \quad \text{(A1)}$$

The fermion $\tilde{\Psi}_R$ decouples from the impurity entirely, and we will mostly discard it from now on. The remaining dynamics is then encoded in the Hamiltonian

$$H = -i\int_{-\infty}^{\infty} \Psi_R^\dagger \partial_x \Psi_R dx + \lambda\sqrt{2}[\Psi_R^\dagger(0)d + \text{H.c.}]. \quad \text{(A2)}$$

We then refold this Hamiltonian to map back to a boundary problem, introducing a Ψ_L component:

$$H = -i\int_{-\infty}^{0} [\Psi_R^\dagger \partial_x \Psi_R - \Psi_L^\dagger \partial_x \Psi_L]dx + \lambda\sqrt{2}[\Psi^\dagger(0)d + \text{H.c.}], \quad \text{(A3)}$$

where $\Psi(0) \equiv \Psi_L(0) = \Psi_R(0)$. The next—and almost final step—is to go to a Majorana version of this problem. We decompose the fermions into real and imaginary parts as

$$\Psi_R = \frac{1}{\sqrt{2}}(\xi_R + i\eta_R), \quad \Psi_L = \frac{1}{\sqrt{2}}(\xi_L + i\eta_L), \quad \text{(A4)}$$

where ξ,η are real and obey $\{\xi_R(x),\xi_R(x')\} = \delta(x - x')$, etc. We set similarly $d = \frac{a+ib}{\sqrt{2}}$ with $\{a,a\} = \{b,b\} = 1$. The problem then decouples into *two independent* Majorana problems $H = H_1 + H_2$, with

$$H_1 = -\frac{i}{2}\int_{-\infty}^{0} [\xi_R \partial_x \xi_R - \xi_L \partial_x \xi_L]\, dx + \frac{i}{\sqrt{2}}\lambda\xi(0)b,$$
$$H_2 = -\frac{i}{2}\int_{-\infty}^{0} [\eta_R \partial_x \eta_R - \eta_L \partial_x \eta_L]\, dx - \frac{i}{\sqrt{2}}\lambda\eta(0)a, \quad \text{(A5)}$$

and $\xi(0) \equiv \xi_R(0) + \xi_L(0)$, the same for η. The problems correspond of course to two Ising models with a boundary magnetic field proportional to $\pm\lambda$ (up to normalizations), the boundary spin operator being $\sigma_B(0) = i(\xi_R + \xi_L)(0)b$.

Note that this result is compatible with boundary entropy counting. The flow from UV to IR in the original problem leads to $g_{\text{UV}}/g_{\text{IR}} = 2$ since a dot with two states is screened. In each of the Ising models meanwhile, we have a flow from free to fixed, with $g_{\text{free}}/g_{\text{fixed}} = \sqrt{2}$, so the product of the two ratios—one for each Ising copy—is 2 indeed.

Turning now to entanglement entropy, we see that the RLM entanglement for a region of size $2L$ centered around the impurity is exactly twice the entanglement for a region of length L on the edge of the system in the boundary Ising model. This has been studied numerically, e.g., in Refs. 2 and 41, and Sec. VII presents an analytical calculation of this quantity.

The boundary sine-Gordon problem at $\mu = \frac{1}{2}$ is also well known to be equivalent to two boundary Ising models,[23] where this time only one of these models experiences a nonzero boundary magnetic field. Hence, we shall also be able to obtain the entanglement entropy for (1) for this value of μ, that is $\Delta = -\frac{\sqrt{2}}{2}$.

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