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▶ **To cite this version:**

Sergei L. Lukyanov, Hubert Saleur, Jesper L. Jacobsen, Romain Vasseur. Exact overlaps in the Kondo problem. Physical Review Letters, 2015, 114 (8), pp.080601. 10.1103/PhysRevLett.114.080601 . cea-01229970

HAL Id: cea-01229970

https://cea.hal.science/cea-01229970

Submitted on 11 Apr 2023

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Exact Overlaps in the Kondo Problem

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(Received 12 December 2014; published 24 February 2015)

It is well known that the ground states of a Fermi liquid with and without a single Kondo impurity have an overlap that decays as a power law of the system size, expressing the Anderson orthogonality catastrophe. Ground states with two different values of the Kondo couplings have, however, a finite overlap in the thermodynamic limit. This overlap, which plays an important role in quantum quenches for impurity systems, is a universal function of the ratio of the corresponding Kondo temperatures, which is not accessible using perturbation theory or the Bethe ansatz. Using a strategy based on the integrable structure of the corresponding quantum field theory, we propose an exact formula for this overlap, which we check against extensive density matrix renormalization group calculations.

DOI: 10.1103/PhysRevLett.114.080601 PACS numbers: 05.70.Ln, 72.15.Qm, 74.40.Gh

Introduction.—The Anderson orthogonality catastrophe (AOC) is one of the cornerstones of modern many body physics. In its simplest formulation, this "catastrophe" states that the ground states of two Fermi seas with different local scattering potentials become (if the orthogonality exponent is nonzero) orthogonal in the thermodynamic limit. This fact has many important consequences, and is at the root of the physics of Mahan excitons [1], the Fermi edge singularity in absorption spectra [2], the nonlinear I_V characteristics in quantum dots, or the Kondo effect [3] in magnetic alloys. More recently, the AOC has played a central role in understanding the postquench dynamics induced by optical absorption in quantum dots tunnel coupled to Fermi seas [4,5].

The simplest manifestation of the AOC occurs in the case of a free Fermi sea involving a single channel of noninteracting electrons that experience two different local scattering potentials. If the corresponding phase shifts at the Fermi energy are $\delta_F^{(1)}$, $\delta_F^{(2)}$, a simple argument [6] shows that the scalar product of the ground states vanishes as

$$\langle \Omega_2 | \Omega_1 \rangle \propto N^{-(\delta_F^{(1)}-\delta_F^{(2)})^2/2\pi^2}, \qquad (1)$$

where N is the total number of electrons. The AOC occurs as well in interacting systems. In the k-channel Kondo problem for instance, it is known that the scalar product of the system with and without a Kondo impurity behaves as $\langle \Omega(J)|\Omega(J=0)\rangle \propto N^{-d_K}$ where [7] $d_K = 3/4(k+2)$ and J is the (antiferromagnetic) Kondo coupling. The simplest one-channel case, to which we will restrict ourselves in this Letter, corresponds then to $d_K = \frac{1}{4}$. In this case, the orthogonality of the ground states expresses the fact that at very low energy, spin up and spin down electrons see a phase shift of $0(\pi/2)$ with zero (nonzero) Kondo coupling. An easy generalization of this argument gives the exponent in the anisotropic Kondo case as well: in the Toulouse limit in particular, $d_K^{(\mathrm{Tou})} = \frac{1}{8}$. No such simple Fermi liquid calculation exists for $k > 1$, and sophisticated techniques have to be used to calculate the overlap, such as integrability or conformal invariance. In the latter setup, the orthogonality exponent d_K is interpreted as the scaling dimension of a boundary condition changing operator [7]. Note that such exponents are directly related to the power law tail in the so-called work distribution [8,9] for quenches when a coupling is suddenly turned on, such as those studied in Refs. [4,5] in the Kondo case.

The ground state overlap exemplifies the nonperturbative quantities occurring in quantum impurity problems. An interesting variant is provided by the overlap $\langle \Omega_2|\Omega_1\rangle$ between ground states corresponding to two different nonvanishing Kondo couplings $J^{(1)}$, $J^{(2)}$. This overlap is not expected to vanish when both $J^{(1)}, J^{(2)} \neq 0$, even in the thermodynamic limit. This is because, for any nonzero Kondo coupling, fermions at very low energy now see the same phase shift of $\pi/2$. Nevertheless, this overlap is nontrivial, even in the noninteracting Toulouse limit, because it is determined by the behavior of the whole Fermi sea, and not just by what happens at the Fermi energy. This overlap is also nonperturbative: any attempt to calculate it by expanding in $J^{(1)}$, $J^{(2)}$ is plagued by infrared divergences precisely because of the AOC. Overlaps such as $\langle \Omega_2|\Omega_1\rangle$ arise in quantum quenches where one suddenly

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changes the Kondo coupling $J^{(1)} \mapsto J^{(2)}$. The system then has a finite probability of remaining in the ground state at large times, which translates into a delta function in the corresponding work distribution [8]: this probability is precisely the square modulus $P_{1\mapsto 2} = |\langle \Omega_2 | \Omega_1 \rangle|^2$, and it could be measured in optical absorption experiments realizing such quantum quenches [4,5].

Now, the Kondo problem exhibits universal properties at energy scales much smaller than the bandwidth D. In this limit, physical quantities depend only on the temperature, the magnetic field, and a crossover scale that encodes the Kondo coupling J (see their precise relationship below)—the Kondo temperature T_K. Different (proportional) definitions of T_K exist, but this will not matter for us. Indeed, provided $T_K^{(1)}, T_K^{(2)} \ll D$, scaling arguments show that the overlap becomes a universal function of the ratio

$$\langle \Omega_2 | \Omega_1 \rangle = F(T_K^{(1)}/T_K^{(2)}) = F(T_K^{(2)}/T_K^{(1)}). \tag{2}$$

In this Letter, we obtain an exact formula for this quantity, which we also check with extensive density matrix renormalization group (DMRG) calculations.

Anisotropic Kondo model.—The anisotropic Kondo problem is initially formulated as a three-dimensional problem of noninteracting fermions coupled to a local magnetic impurity. After a spherical waves decomposition, only the s channel interacts with the impurity, and the problem can be transformed into one-dimensional gapless fermions on the half line (the radial coordinate) coupled to a spin at the origin. "Unfolding" the half line one obtains a problem of chiral fermions with

$$\boldsymbol{H} = -iv_F \sum_{\alpha=\uparrow,\downarrow} \int_{-\infty}^{\infty} dx \psi_\alpha^\dagger \partial_x \psi_\alpha + J[j^+(0)\sigma^- + j^-(0)\sigma^+] + J_z j^z(0)\sigma^z, \tag{3}$$

where the spin currents are $j^+ = \psi_\uparrow^\dagger \psi_\downarrow$, $j^- = \psi_\downarrow^\dagger \psi_\uparrow$, $j^z = \psi_\uparrow^\dagger \psi_\uparrow - \psi_\downarrow^\dagger \psi_\downarrow$. We bosonize the fermionic fields $\psi_\sigma \sim e^{i\sqrt{4\pi}\phi_\sigma}$ [10], which allows us to separate charge and spin modes $\phi_{c/s} = (\phi_\uparrow \pm \phi_\downarrow)/\sqrt{2}$. The charge boson decouples, and the interacting part involves only the spin boson $\phi = \phi_s$. After a canonical transformation, $\boldsymbol{H} \to \boldsymbol{U}^\dagger \boldsymbol{H} \boldsymbol{U}$ with $\boldsymbol{U} = \exp(iJ_z \phi(0)\sigma^z)$, one can then rewrite the Hamiltonian as

$$\boldsymbol{H} = \int_{-\infty}^{\infty} dx (\partial_x \phi)^2 + J(e^{i\beta\phi(0)}\sigma^- + e^{-i\beta\phi(0)}\sigma^+) \tag{4}$$

with $\beta = \sqrt{8\pi} - 2J_z$ and the equal time commutation relations $[\phi(x), \phi(x')] = (i/4)\mathrm{sgn}(x - x')$. The scaling dimension of the perturbation is $\beta^2/(8\pi) = [1 - (J_z/\sqrt{2\pi})]^2 \equiv \xi/(\xi+1)$, where the last equality defines the coupling constant ξ. The Kondo temperature in this framework varies as $T_K \propto J^{\xi+1}$.

Perturbative results.—It is first natural to try to evaluate the universal function (2) using perturbation theory. To this end, we fold the chiral problem (4) to obtain a nonchiral boson on the half line $(-\infty, 0]$, scattering off the spin impurity at $x = 0$. We then map this $(1+1)$D quantum impurity system onto a 2D classical statistical mechanics problem in the half plane, critical in the bulk (corresponding to the $c = 1$ free boson theory), with the impurity now acting as a boundary condition (see Fig. 1). We then calculate the partition function $\mathcal{Z}(J^{(1)}, J^{(2)})$ of a half-infinite system with the boundary condition corresponding to the Kondo temperature $T_K^{(1)}$ everywhere except on a part of the boundary of length τ where the boundary field is taken to correspond to $T_K^{(2)}$. It gives a term linear in imaginary time (corresponding to a boundary free energy contribution), a term exponential in imaginary time (corresponding to excited states propagating along the boundary), and a term of order 1 that can be seen to be $|\langle \Omega_2 | \Omega_1 \rangle|^2$ in the Hamiltonian formalism.

Expanding the overlap $|\langle \Omega_2 | \Omega_1 \rangle|^2$ in $J^{(1)} - J^{(2)}$ from the ratio $\mathcal{Z}(J^{(1)}, J^{(2)})/\mathcal{Z}(J^{(1)}, J^{(1)})$ is extremely complicated, since the two-point function of the boundary perturbation in Eq. (4) is not known in general. At the Toulouse point ($\xi = 1$), however, the perturbation can be refermionized, so the spin-spin propagator at a finite value of J is easily found, and expanding the partition function yields [11]

$$|\langle \Omega_2 | \Omega_1 \rangle|_{\xi=1} = 1 - \frac{\alpha_{12}^2}{8\pi^2} + \mathcal{O}(\alpha_{12}^4), \tag{5}$$

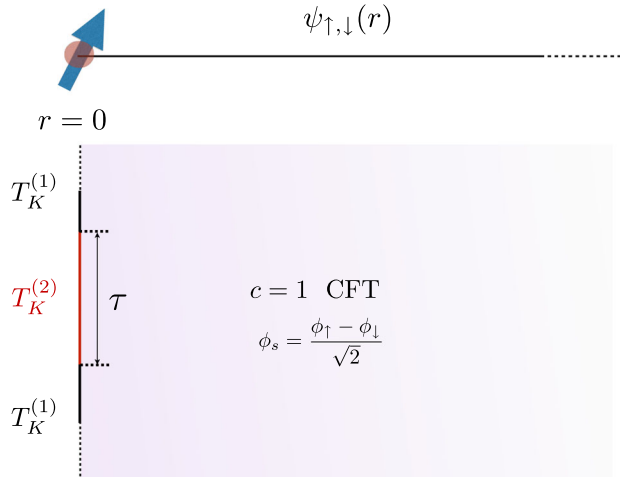


FIG. 1 (color online). The overlap $|\langle \Omega_2 | \Omega_1 \rangle|$ can be extracted from the partition function of the system with the insertion of a Kondo impurity and two different values of the coupling. In this picture, the boundary condition corresponds to the spin impurity while the bulk describes a critical statistical mechanics problem associated with the spin mode ϕ_s.

where $e^{\alpha_{12}} = T_K^{(2)}/T_K^{(1)}$. Even for this noninteracting case, going beyond this first order expansion becomes quickly involved, and capturing the full behavior of the function (2) seems hopeless.

Semiclassical analysis.—The overlap can also be calculated perturbatively in the semiclassical limit, where $\xi \simeq \beta^2/(8\pi) \ll 1$. In this case, it is convenient to implement yet another canonical transformation, and bring the Hamiltonian into the form

$$\boldsymbol{H} = \frac{1}{2}\int_{-\infty}^{0} dx[(\partial_x\Phi)^2 + (\partial_t\Phi)^2] + J\sigma^x + \frac{\beta}{4}\partial_t\Phi(0)\sigma^z. \tag{6}$$

Using perturbation theory in β, we now calculate the partition function $\mathcal{Z}$ in imaginary time of a system with two different values of J as shown in Fig. 1. The leading contribution comes from the configuration where $\sigma^x = -1$ everywhere but between a pair of insertions, spaced by τ, of the $\partial_t\Phi(0)\sigma^z$ term. Discarding terms that depend on τ and encode the nonuniversal boundary free energy, we find [11]

$$|\langle\Omega_2|\Omega_1\rangle| = 1 + \frac{\xi}{2}\left(1 - \frac{\alpha_{12}}{2}\coth\frac{\alpha_{12}}{2}\right) + \mathcal{O}(\xi^2). \tag{7}$$

Once again, going beyond this first order is extremely involved, and there is, in particular, no chance to capture the crossover between the two extreme behaviors, $T_K^{(1)} \sim T_K^{(2)}$ and $T_K^{(1)} \gg T_K^{(2)}$.

Exact results from integrability.—For many other questions in the Kondo problem—such as the study of thermodynamics properties [12,13], correlation functions [14], quantum quenches [15], or entanglement [16]—nonperturbative techniques have led to analytic expressions in the crossover regions, when the physical scale of interest (temperature, magnetic field, etc.) is comparable with T_K. Although exact Bethe ansatz wave functions are in principle known for different values of T_K, overlaps such as $\langle\Omega_2|\Omega_1\rangle$ have however proven, so far, impossibly hard to calculate directly. We report here another approach to the problem based on an axiomatic determination of the overlaps directly in the field theory limit. This approach is similar in philosophy to the S-matrix bootstrap from Ref. [17]. We give the relevant details in the Supplemental Material [11], and move directly to the main result.

We find that the overlap is given by

$$\langle\Omega_2|\Omega_1\rangle = (\xi+1)\frac{\sinh\frac{\alpha_{12}}{2(\xi+1)}}{\sinh\frac{\alpha_{12}}{2}}g_\xi(\alpha_{12}) \tag{8}$$

with

$$g_\xi(\alpha) = \exp\left(\int_0^\infty \frac{dt}{t}\frac{\sin^2(\alpha t/\pi)}{\sinh 2t\cosh t}\frac{\sinh t\xi}{\sinh t(\xi+1)}\right), \tag{9}$$

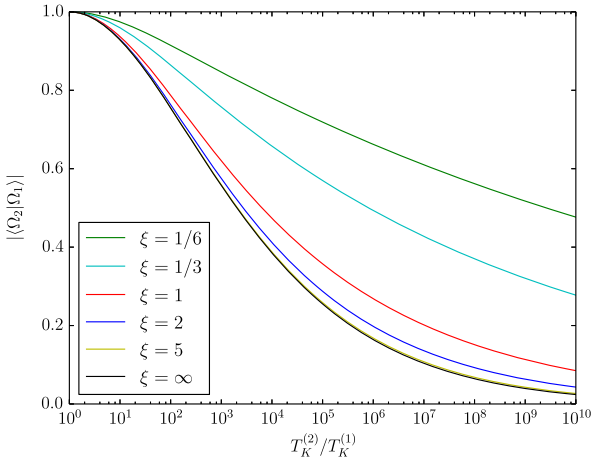


FIG. 2 (color online). Theoretical result for the overlap for various anisotropies as a function of the ratio $T_K^{(2)}/T_K^{(1)}$. The isotropic Kondo problem then corresponds to $\xi = \infty$. Note the extreme values on the x axis.

where we recall that $e^{\alpha_{12}} = T_K^{(2)}/T_K^{(1)}$. See Fig. 2 for a plot of this exact solution, illustrating the variation of the overlap with the anisotropy, as well as the incredibly large values of the ratio $T_K^{(2)}/T_K^{(1)}$ necessary to bring this overlap down to 10^{-1} or less. It is worth mentioning here that the function $g_\xi(\alpha_{12})$ coincides with properly normalized matrix elements of the operators $e^{\pm i\beta\phi(0)}\sigma^\mp$:

$$\frac{\langle\Omega_2|e^{\pm i\beta\phi(0)}\sigma^\mp|\Omega_1\rangle}{\sqrt{\langle\Omega_2|e^{-i\beta\phi(0)}\sigma^+|\Omega_2\rangle\langle\Omega_1|e^{+i\beta\phi(0)}\sigma^-|\Omega_1\rangle}} = g_\xi(\alpha_{12}). \tag{10}$$

An immediate check is to study the behavior at large $T_K^{(2)}/T_K^{(1)}$, where we find

$$\langle\Omega_2|\Omega_1\rangle \simeq \begin{cases} C_\xi\left(\frac{T_K^{(2)}}{T_K^{(1)}}\right)^{-\xi/4(\xi+1)} & (\xi < \infty), \\ C_\infty\left(\log\frac{T_K^{(2)}}{T_K^{(1)}}\right)^{(3/4)}\left(\frac{T_K^{(2)}}{T_K^{(1)}}\right)^{-(1/4)} & (\xi = \infty) \end{cases} \tag{11}$$

for $T_K^{(2)} \gg T_K^{(1)}$. This is in agreement with the dimension of the boundary condition changing operator for the anisotropic Kondo problem, $d_K = \frac{1}{4}\xi/(\xi+1)$. For the isotropic Kondo case ($\xi = \infty$) we recover the dimension, $d_K = \frac{1}{4}$, of the $j = \frac{1}{2}$ $SU(2)$ primary. Notice that, since in Eq. (8) we assume the conventional normalization condition $\langle\Omega|\Omega\rangle = 1$, the constants in asymptotic formulas (11) are universal amplitudes. Their expression can be found in the Supplemental Material [11]. Of course, one can also verify that Eq. (8) is consistent with the perturbative results (5) and (7).

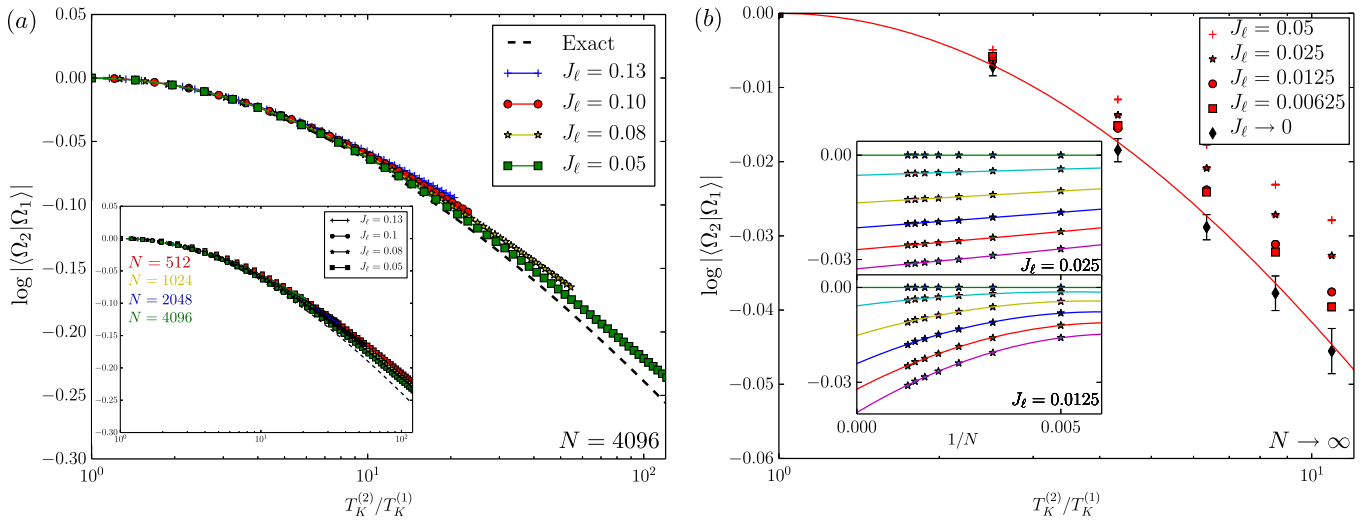


FIG. 3 (color online). Numerical checks of the main result (8). Note that the comparison between numerical and field theory results does not involve any free parameter. (a) Measures of the overlap in the free-fermion Toulouse case $\xi = 1$, modeled by a spinless noninteracting resonant level, tunnel coupled with parameter J_ℓ to two metallic reservoirs with $N = 4096$ sites each. The dashed line is the analytical result, with $T_K \propto J_\ell^2$. Inset: finite size scaling. (b) DMRG results for the overlap in the interacting case $\xi = 1/3$, modeled by an XXZ spin chain with anisotropy $\Delta = -1/\sqrt{2}$ and N sites, with an extra site at the edge characterized by a weak link J_ℓ, corresponding to the impurity. The numerical results for $N = 200, \ldots, 800$ are extrapolated in the thermodynamic limit $N \to \infty$. The red line is the analytical result, with $T_K \propto J_\ell^{4/3}$, and the black symbols correspond to the extrapolation $J_\ell \to 0$. Inset: examples of finite size extrapolations for fixed $J_\ell \equiv J_\ell^{(1)}$ and different values of $J_\ell^{(2)}$.

Numerical results.—We now turn to a detailed numerical exploration of our result. There are various lattice models where the overlap (8) can be measured. We have focused on the XXZ chain with a weak boundary coupling

$$H = \sum_{i=0}^{N} t_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \qquad (12)$$

where $t_i = 1$ for $i \neq 0$ and $t_0 = J_\ell$. Standard bosonization [18] shows that this Hamiltonian is equivalent, at low energy, to Eq. (4) with the Kondo coupling $J \propto J_\ell$ and $\beta^2/(8\pi) = 1 - (1/\pi)\arccos\Delta$ [19]. From a numerical point of view, the easiest case to check is of course the Toulouse point where $\Delta = 0$, for which the overlap (2) can be expressed as a determinant of a matrix whose size scales linearly with the number of sites (see, e.g., Ref. [20]). Results are presented in Fig. 3(a). While the agreement with the theoretical value is clearly good—note that there is no free parameter in Eq. (8)—several aspects are important to notice. First, the overlap varies very slowly with the ratio of Kondo temperatures. This requires exploring ratios $T_K^{(2)}/T_K^{(1)}$ of the order of 10^2 or more. Since the analytical result is only true in the scaling limit where $J_\ell \ll 1$, this forces us to explore extremely small values of the bare coupling. For these values, the Kondo screening length $1/T_K \propto (J_\ell)^{-2}$ is in turn very large. To avoid finite size effects—which seem quite important for the determination of the overlaps—we finally have to study larger systems than one would have expected—of the order of 10^4 sites, forbidding us in particular from testing the region where the overlap becomes very small.

The interacting case requires use of the DMRG technique [21]. We use here a two-site version in the matrix product state language [22]. In this case, we have been limited to chains of about 800 sites, for which finite size effects in the scaling limit remain unfortunately important. In order to obtain usable results, we have had to perform a double extrapolation. For finite, small J_ℓ we have first extrapolated results for different sizes to $N = \infty$. These results are represented in Fig. 3(b) for $\xi = 1/3$. We have then performed a second extrapolation for different values of J_ℓ to $J_\ell = 0$, represented by the black symbols in the figure. The result of these extrapolations is found to be consistent with the analytical result (8). Note that in principle, one would also need to extrapolate the bond dimension χ of the variational matrix product state used in the DMRG calculations to infinity, but we find that keeping $\chi \sim 100$–300 was enough for the finite χ effects to be negligible compared with the more important finite N and finite J_ℓ effects. We also note that our formula can be verified very efficiently in the isotropic case ($\xi = \infty$) [23] using the numerical renormalization group (NRG) [24].

Discussion.—It is clear *a posteriori*—in view of its extremely slow variation with the ratio of Kondo temperatures—that the overlap in the crossover would be impossible to obtain perturbatively. It is also difficult to measure it numerically. The slow variation quantifies the weak

dependency of the Kondo ground state on the impurity coupling. It would be interesting to obtain a more qualitative understanding of this effect in terms of the screening cloud. Technically, the exact formula for the ground states overlap is the building stone for the calculation of general overlaps between quantum impurity systems with different boundary conditions. Exact calculations of Loschmidt echoes and work distributions in quantum quenches then follow using more traditional techniques [25], which will be discussed elsewhere.

Despite their importance in the context of quantum information, the thermodynamic limit of similar ground state overlaps (fidelities) remains extremely difficult to access exactly—even for noninteracting systems—and are often nonperturbative in the relevant expansion parameters. Our result opens the door to the calculation of such overlaps in integrable systems.

We thank I. Affleck, N. Andrei, J. Dubail, F. H. L. Essler, A. M. Tsvelick, and A. B. Zamolodchikov for useful discussions. We also thank A. Weichselbaum for checking our formula in the isotropic case using the NRG. H. S. gratefully acknowledges the hospitality of the Rutgers Physics Department where this work was started. The work of H. S. and J. L. J. was supported by the French Agence Nationale pour la Recherche (ANR Projet 2010 Blanc SIMI 4: DIME); the research of J. L. J. was also supported by the Institut Universitaire de France. The work of H. S. was also supported by the U.S. DOE under Grant No. DE-FG03-01ER45908. The work of R. V. was supported by the Quantum Materials program of Lawrence Berkeley National Laboratory, and the work of S. L. L. was supported by the NSF under Grant No. NSF-PHY-1404056.

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