Fano resonances and entanglement entropy

Viktor Eisler
Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark

Savannah Sterling Garmon
Chemical Physics Theory Group, Department of Chemistry and Center for Quantum Information and Quantum Control, University of Toronto, 80 St. George Street, Toronto, Ontario, Canada M5S 3H6

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We study the entanglement in the ground state of a chain of free spinless fermions with a single side-coupled impurity. We find a logarithmic scaling for the entanglement entropy of a segment neighboring the impurity. The prefactor of the logarithm varies continuously and contains an impurity contribution described by a one-parameter function while the contribution of the unmodified boundary enters additively. The coefficient is found explicitly by pointing out similarities with other models involving interface defects. The proposed formula gives excellent agreement with our numerical data. If the segment has an open boundary, one finds a rapidly oscillating subleading term in the entropy that persists in the limit of large block sizes. The particle-number fluctuation inside the subsystem is also reported. It is analogous with the expression for the entropy scaling, however, with a simpler functional form for the coefficient.

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I. INTRODUCTION

The entanglement properties of many-body systems have attracted considerable attention and have become the topic of a large number of studies in the last decade.[1,2] In particular, the study of a suitable measure of entanglement such as the entanglement entropy was triggered by the need to understand ground-state properties that lead to the emergence of area laws.[3] This keyword refers to a rather generic property of ground states of bipartitioned systems in which the entropy S of a subsystem scales as the number of contact points with the environment. The most notable and well-understood counterexamples are represented by one-dimensional (1D) critical quantum systems with an underlying conformal symmetry where the area law is violated in the form of universal terms, scaling as the logarithm of the subsystem size.[4] In the translationally invariant case this can be written as

$$S = \frac{c}{3}\ln L + k_0 \quad (1)$$

with c being the central charge of the conformal field theory (CFT) and k_0 a nonuniversal constant.

The presence of impurities has interesting effects on the entanglement entropy.[5] An example is given by critical lattice models where single defective links separate the two subsystems. This can lead to a modified prefactor for the logarithm varying continuously with the defect strength in models with free fermions[6–9] while for interacting electrons the defect either renormalizes to a cut or to the homogeneous value in the $L\to\infty$ scaling limit.[10,11] In the more general context of a conformal interface separating two CFTs the effective central charge has been calculated recently and was shown to depend on a single parameter.[12]

Another broad and intensively studied class of impurity problems is related to the Kondo effect.[13] From the viewpoint of block entropies a spin-chain version of the Kondo model has been studied[14,15] using density-matrix renormalization-group (DMRG) methods.[16,17] Here a different geometry was considered with an impurity spin coupled to one end of a finite chain. The induced change in the entropy varies between zero and ln 2 and its qualitative behavior for various system sizes and coupling values can be described in terms of an impurity valence-bond picture.

A counterpart of the Kondo effect can be found in a single-impurity model introduced by Anderson.[18] A similar, exactly solvable model was studied independently by Fano[19] where the interaction of a discrete state with a continuum of propagation modes leads to scattering resonances. The exact form of these resonances is controlled by the couplings between the modes. Here we consider a simple geometry where an impurity is side coupled to a linear chain of electron-conduction sites. This setting can also be realized experimentally with gated semiconductor heterostructure quantum dots. In accordance with theoretical predictions,[20] Fano resonances were detected as dips in the conductance measurements at low temperatures.[21] Despite the large amount of theoretical and experimental work on Fano resonances,[22] the question how they affect entanglement properties is still unanswered.

In the present paper we address this question by investigating the simplest model capturing the main features of the Fano resonance. The Fano-Anderson model[23] is described by a free fermion Hamiltonian, thus standard techniques are available for the study of its entanglement properties.[24] We find that the entropy scaling of a block neighboring the impurity is of the form in Eq. (1) with a prefactor c_{eff} which decreases monotonously as the parameters are tuned toward the Fano resonance and depends only on a well-defined scattering amplitude. The numerical analysis leads to the same functional form of c_{eff} that has recently been derived for simpler fermionic models with interface defects[9] and also seems to be closely related to the one found for conformal interfaces.[12] If the subsystem contains an open boundary we find a rapidly oscillating subleading term in the entropy that persists even in the large L limit.

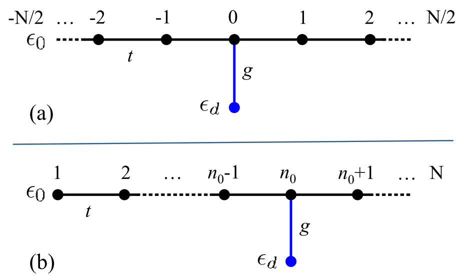

FIG. 1. (Color online) Model geometry for (a) the infinite case and (b) the semi-infinite case.

In the following we first introduce the model and the geometries considered, along with the methods used to calculate the entropy. In Sec. III we treat an impurity attached to an infinite hopping model, determine the correlation matrix and present results on the scaling of the entropy as well as the particle-number fluctuations. The effects of an open boundary will be detailed in Sec. IV followed by our concluding remarks in Sec. V. The derivation of an asymptotic form of the correlation functions and some of the necessary formulas for the semi-infinite case are presented in Appendices A and B, respectively.

II. MODEL AND METHODS

We consider a model of noninteracting spinless electrons described by a 1D tight-binding chain that is coupled to an impurity. The impurity is represented by an additional site from which tunneling events can only occur to a specific site n_0 of the chain. The Hamiltonian is

$$H = -\frac{t}{2}\sum_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \epsilon_0 \sum_n c_n^\dagger c_n - g(c_{n_0}^\dagger d + d^\dagger c_{n_0}) + \epsilon_d d^\dagger d, \qquad (2)$$

where c_n and d are the fermion annihilation operators along the chain and at the impurity site, respectively, while t and g are the corresponding tunneling strengths. The potential ϵ_0 sets the filling of the chain and ϵ_d is the site energy of the impurity.

We will consider two different geometries: (1) in the *infinite geometry* the $N+1$ sites are indexed as $n=-N/2,\ldots,N/2$ while the impurity is located at the center of the chain ($n_0=0$) and we take periodic boundary conditions and (2) in the *semi-infinite geometry* one has N sites with $n=1,\ldots,N$ while n_0 is arbitrary and we have open boundary conditions.

The two geometries are depicted in Fig. 1. In the following we set $t=1$. After a Fourier transformation one has

$$H = \sum_q \epsilon_q c_q^\dagger c_q + \sum_q t_q(c_q^\dagger d + d^\dagger c_q) + \epsilon_d d^\dagger d, \qquad (3)$$

where $\epsilon_q = \epsilon_0 - \cos q$. The couplings and the allowed wave numbers are $t_q = -\frac{g}{\sqrt{N+1}}$ with $q=\frac{2\pi}{N+1}n$ for the infinite and $t_q = -g\sqrt{\frac{2}{N+1}}\sin n_0 q$ with $q=\frac{\pi}{N+1}n$ for the semi-infinite case, respectively, where n runs over the corresponding site indices. The Fermi-level ϵ_{q_F} is set to zero by applying a potential $\epsilon_0 = \cos q_F$.

Hamiltonian (3) is known as the Fano-Anderson model and is diagonalized by introducing new fermionic operators f_q by the transformation[23]

$$d = \sum_q \nu_q f_q, \quad c_q = \sum_{q'} \mu_{qq'} f_{q'}, \qquad (4)$$

where

$$\nu_q = \frac{t_q}{\eta_-(\epsilon_q)} \quad \eta_\pm(\epsilon_q) = \epsilon_q - \epsilon_d - \Sigma(\epsilon_q \pm i\delta), \qquad (5)$$

$$\mu_{qq'} = \delta_{qq'} - \frac{t_q \nu_{q'}}{\epsilon_q - \epsilon_{q'} + i\delta} \qquad (6)$$

with the self-energy term defined as

$$\Sigma(\epsilon_q \pm i\delta) = \sum_{q'} \frac{t_{q'}^2}{\epsilon_q - \epsilon_{q'} \pm i\delta}. \qquad (7)$$

The infinitesimal terms $\pm i\delta$ are needed to regularize the sum. Note that the number of different q values equals the number of all sites, including the impurity. In the limit $N\to\infty$ one has a continuum of the unmodified single-particle spectrum ϵ_q of the chain while additional bound states can emerge as real solutions ϵ of the equation

$$\epsilon - \epsilon_d - \Sigma(\epsilon) = 0. \qquad (8)$$

Our aim is to calculate the entanglement entropy $S=-\mathrm{Tr}(\rho \ln \rho)$ of a block of L sites neighboring the impurity, where ρ denotes the corresponding reduced density matrix. Since one is dealing with free fermions, this can be obtained through the eigenvalues ζ_l of the correlation matrix $C_{mn} = \langle c_m^\dagger c_n\rangle$ restricted to the block $1\le m,n\le L$ as[25]

$$S = -\sum_l \zeta_l \ln \zeta_l - \sum_l (1-\zeta_l)\ln(1-\zeta_l). \qquad (9)$$

III. INFINITE GEOMETRY

We first consider the infinite geometry and calculate the matrix C_{mn} analytically; this result is, in turn, used to numerically obtain the entropy. The particle-number fluctuations are also considered where explicit calculations are performed using an asymptotic form of the correlations.

A. Correlation functions

The correlations $\langle c_m^\dagger c_n\rangle$ are calculated by first going over to Fourier modes c_q and subsequently applying the transformation Eq. (4). The expectation values to be evaluated are then trivial and read $\langle f_q^\dagger f_{q'}\rangle = \delta_{qq'}\chi(q)$, where in the ground state $\chi(q)=1$ for the modes $\epsilon_q<0$ and zero otherwise. Moreover, in the infinite geometry it was shown that Eq. (8) always gives two real solutions with $\epsilon_+>1$ and $\epsilon_-<-1$ corresponding to bound states above and below the band.[26] The energies $\epsilon_\pm$ are obtained numerically by solving the quartic Eq. (8) with

$$\Sigma(\epsilon_{\pm}) = \pm \frac{g^2}{\sqrt{\epsilon_{\pm}^2 - 1}}. \tag{10}$$

These modes $f_{\pm}$ have to be dealt with separately in the transformation Eq. (4) with the factors

$$\nu_{\pm} = \sqrt{N_{\pm}} \quad \mu_{q\pm} = \sqrt{N_{\pm}} \frac{t_q}{\epsilon_{\pm} - \epsilon_d}, \tag{11}$$

where $N_{\pm}$ is set by the normalization condition $|\nu_{\pm}|^2 + \Sigma_q |\mu_{q\pm}|^2 = 1$. Since $\langle f_-^{\dagger} f_- \rangle = 1$, one has a contribution $C_{mn}^b = C^b(m+n)$ to the correlations coming from the lower bound state. Setting $t_q = -g/\sqrt{N+1}$ and taking $N \to \infty$ the sums are replaced with integrals over the full band $[-\pi, \pi]$ and can be rewritten as contour integrals over the complex plane. Evaluating the residues one has

$$C^b(l) = \frac{g^2}{2\epsilon_-^2 - \epsilon_- \epsilon_d - 1} e^{-l/\xi_-} \tag{12}$$

with $l = m+n$ for $m,n \geq 0$ while the correlation length is defined by $\xi_-^{-1} = \text{arcosh}(-\epsilon_-)$.

There are two contributions from the conduction band. First we have the translationally invariant terms

$$C_{mn}^0 = C^0(m-n) = \frac{\sin q_F(m-n)}{\pi(m-n)} \tag{13}$$

that give the correlations without the impurity arising from the $\delta_{qq'}$ term in Eq. (6). The remaining term gives rise to the correlation contributions $C_{mn}^1 = C^1(m+n)$; these can be evaluated by applying the same methods used for determining $C^b(l)$. The calculation yields the simple form

$$C^1(l) = \int_0^{q_F} \frac{dq}{\pi} \sin \delta(q) \sin[lq + \delta(q)], \tag{14}$$

where the scattering phases for $q > 0$ are defined as

$$\tan \delta(q) = \frac{\Sigma_q}{\epsilon_q - \epsilon_d} = \frac{g^2}{\sin q(\epsilon_d - \epsilon_q)}. \tag{15}$$

Here $\Sigma_q = \text{Im}\, \Sigma(\epsilon_q + i\delta)$ is the imaginary part of the retarded self-energy with the real part being zero.

Collecting all the contributions, the correlation matrix is given by

$$C_{mn} = C_{mn}^0 - C_{mn}^1 + C_{mn}^b. \tag{16}$$

The integrals in Eq. (14) must be evaluated numerically and are shown in Fig. 2 together with the contribution of the bound state for some fixed values of the parameters g and ϵ_d. The values of $C^1(l)$ are found to oscillate around the exponentially decaying curve of $C^b(l)$. Since they appear with opposite signs in Eq. (16), the average value will cancel, corresponding to the screening of the impurity induced localized state by the conduction electrons.

The overall contribution is shown in the inset of the figure. A careful analysis shows that the asymptotic behavior has the form of Friedel oscillations

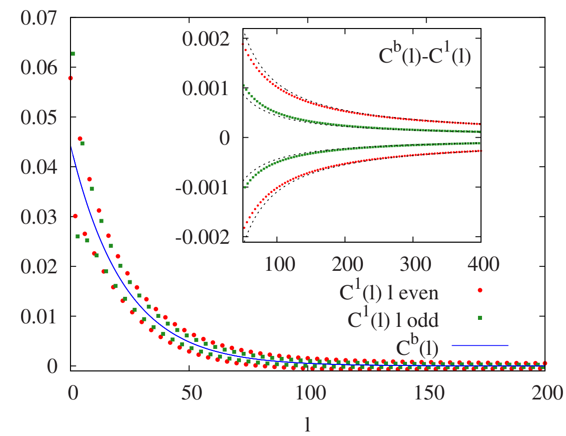

FIG. 2. (Color online) Contributions to the correlations from the bound state $C^b(l)$ and from the conduction band $C^1(l)$ for the parameter values $g=0.2$ and $\epsilon_d = -0.1$. The inset shows the difference between these two contributions, compared to the asymptotic form in Eq. (17) represented by the dashed lines.

$$C^b(l) - C^1(l) \approx C^F(l) = \frac{1}{\pi l} \sin \delta_F \cos(q_F l + \delta_F), \tag{17}$$

where only the scattering phase $\delta_F = \delta(q_F)$ at the Fermi-level enters. $C^F(l)$ is depicted by the dashed lines in the inset of Fig. 2 and shows a good agreement with the numerical data. The derivation of Eq. (17) is summarized in Appendix A. It relies on an appropriate transformation of the integrals in Eq. (14) and is valid for $l \gg l_0$ where the length scale l_0 is given in Eq. (A7).

B. Entanglement entropy

The elements of the correlation matrix Eq. (16) will be used to obtain the entanglement entropy of a block numerically as described in Sec. II. In some simple cases one can already give an answer by looking at the limiting form of the correlations. Taking $\epsilon_d \to \pm\infty$, the impurity site will either be completely empty or completely occupied and therefore it becomes decoupled from the rest of the chain. One has $\delta(q) \equiv 0$ while the contributions from the bound state also vanish $C^b(l) = 0$, hence $C_{mn} = C^0(m-n)$ and the entropy will just be that of a homogeneous hopping model given by Eq. (1) with $c=1$. Obviously, the limit of a vanishing coupling yields the same behavior.

On the other hand, one could take the limit $g \gg 1$ for very strong coupling. This corresponds to $|\delta(q)| \to \pi/2$, that is, one has resonant scattering at every wavelength. The ground state will correspond to a singlet formed by the impurity and site zero that is otherwise decoupled from the rest of the system. The bound-state correlations contribute only on site zero $C^b(l) = \delta_{l,0}/2$ while for sites $m,n > 0$ one has $C_{mn} = C^0(m-n) - C^0(m+n)$, which is the form for a semi-infinite chain. The entropy of this geometry is known to scale logarithmically with a coefficient 1/6, which is half of the value that appears in the homogeneous case.[27]

The previous analysis shows that resonant scattering tends to decrease the coefficient of the entropy scaling. However, in general, a Fano resonance is concentrated around a single

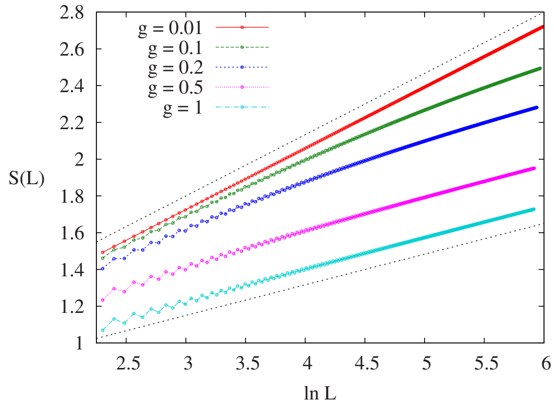

FIG. 3. (Color online) Crossover in the entropy scaling in the resonant case $\epsilon_d=0$ at half filling and for various coupling strengths g. The upper and lower-most dashed lines have slopes 1/3 and 1/6, respectively, acting as guides to the eyes.

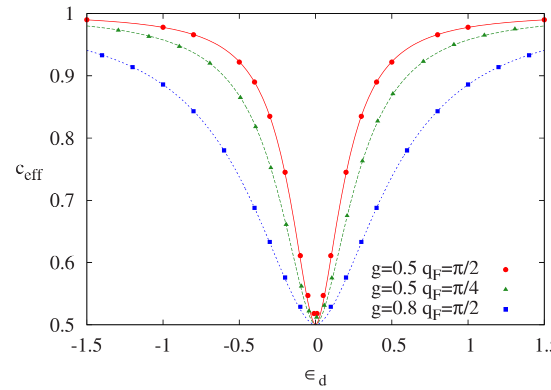

FIG. 4. (Color online) Effective central charge, obtained from fits of the numerical data, as a function of ϵ_d and for various values of g and q_F. The lines show the analytical form in Eq. (19) evaluated for the corresponding values of the parameter s.

wave number. This is expected to have the largest effect on the asymptotic behavior if the location of the resonance coincides with the Fermi-level $|\delta(q_F)| \to \pi/2$ yielding the condition $\epsilon_d \to \epsilon_{q_F}=0$. We take this value of the site energy in Fig. 3, in which we plot the entropy for a range of values for the coupling g. We see that the entropy crosses over between the two limiting behaviors, giving a slope of 1/3 for small L and 1/6 for large L when plotted against $\ln L$. Therefore, taking the block size large enough the impurity behaves like a cut in the chain.

This effect is reminiscent of the Kondo screening mechanism, where conduction electrons form a cloud around a magnetic impurity. The Kondo effect has an associated length scale[28] that being the distance beyond which the impurity appears to be screened off. In the present case a natural length scale also enters, which marks the asymptotic regime of the correlations and could be expected to appear in the entropy scaling. From Eq. (A7) one has $l_0 \sim 1/g^2$ for $\epsilon_d=0$ and $q_F=\pi/2$, which seems to be consistent with the location of the crossover moving toward larger L in Fig. 3 as the coupling g decreases. In order to reliably verify the scaling of the crossover length one would have to consider larger blocks. Unfortunately, the achievable sizes were limited to $L \approx 400$ by the increasing numerical difficulty in evaluating the oscillatory integrands for the matrix elements in Eq. (14).

For $L \gg l_0$ the screening cloud is effectively in a singlet state with the impurity electron and cuts the system in two parts. The coefficient of the entropy therefore renormalizes to the value 1/6 corresponding to a semi-infinite chain with an open boundary. Note that a similar renormalization behavior was found for *interacting* electrons in the Luttinger-liquid regime bisected by a hopping defect.[10,11]

Our further numerical analysis shows that, for arbitrary parameter values and $L \gg 1$, the entropy can be written in the form

$$S(L) = \frac{c_{\text{eff}}}{3} \ln L + k, \qquad (18)$$

where the effective central charge c_{eff} varies continuously between the values 1/2 and 1. The same behavior was found for free fermionic models with hopping defects[6,8] where the dependence of c_{eff} on the defect strength was determined by data fits. Recently, Sakai and Satoh derived the same form as Eq. (18) for the case of two conformal field theories coupled through a conformal interface. In their case they found c_{eff} in a closed form with dependence only on a single scattering amplitude.[12] These conformal interfaces describe a discontinuity in the compactification radii of two bosonic CFTs, which correspond to Luttinger liquids with unequal interaction parameters on the left- and right-hand sides.[29]

Although the result from Ref. 12 is not directly applicable, a closely related form was recently found to describe the case of free fermions with simple interface defects.[9] We therefore attempted to generalize these results to the present model. Motivated by Eq. (17), we argue that the asymptotic behavior of $S(L)$ and thus c_{eff} should depend only on the scattering phase at the Fermi level and a suitable scattering amplitude can be defined as $s=\cos \delta_F$. Hence, we propose

$$c_{\text{eff}} = \frac{1}{2} + \frac{6}{\pi^2} \int_0^\infty u[\sqrt{1+(s/\sinh u)^2} - 1] du, \qquad (19)$$

where 1/2 comes from the unmodified boundary while the integral is, up to a sign, the same as in Ref. 12 and describes the contribution of the impurity.

Figure 4 shows the resulting c_{eff} obtained by fitting Eq. (18) on different $S(L)$ data sets together with Eq. (19) evaluated as a function of ϵ_d for various fixed values of the coupling g and filling q_F. One has excellent agreement with the conjectured analytical form. The only visible deviations arise for $\epsilon_d \approx 0$ which can be understood through the crossover phenomenon shown in Fig. 3. In this parameter regime the asymptotic behavior sets in only for larger L and one has considerable finite-size corrections.

The integral Eq. (19) depends on the model parameters only through the variable

$$s^2 = \frac{\epsilon_d^2 \sin^2 q_F}{\epsilon_d^2 \sin^2 q_F + g^4}. \qquad (20)$$

Interestingly, the above formula *exactly* coincides with the

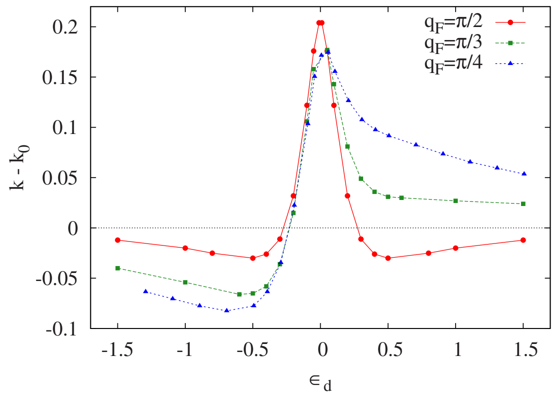

FIG. 5. (Color online) Subleading term k of the entropy as a function of ϵ_d for different fillings and $g=0.5$. The homogeneous value k_0 has been subtracted for better comparison.

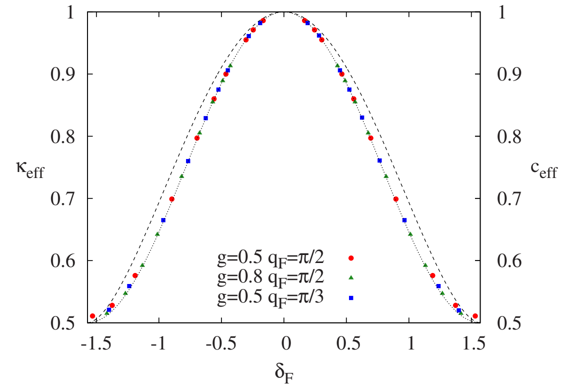

FIG. 6. (Color online) Fitted coefficients κ_{eff} of the logarithmic term in the particle-number fluctuation for various values of g and q_F, plotted against the scaling variable δ_F. The dotted line is the function $(1+\cos^2\,\delta_F)/2$. The dashed line shows c_{eff} as a function of δ_F for better comparison.

transmission coefficient of the Fano-Anderson model[30] with the Fermi-energy set equal to zero. Therefore, the effective central charge is directly linked to a simple physical quantity that, in experimental realizations, is obtainable via conductance measurements at very low temperatures. Although the description of Fano resonances measured in various nanostructure experiments[22] typically require more detailed impurity models, the simple relation between c_{eff} and the transmission coefficient might still survive in some parameter regime. This could open up the possibility of an indirect measurement of the leading term in the entropy.

It should be pointed out that the impurity integral in c_{eff} has been obtained *analytically* for a transverse Ising chain in a DMRG geometry.[9] The calculation relies on a correspondence between transfer-matrix spectra of classical two-dimensional (2D) Ising models and the single-particle eigenvalues of $\mathcal{H}$ in the reduced density matrix $\rho\sim e^{-\mathcal{H}}$ of the quantum chain. This analogy is well known in the homogeneous case[24,31] and can be extended by considering the transfer matrix of a 2D strip with a defect line. In turn, an alternative representation of the integral in Eq. (19) via dilogarithm functions was obtained. In our present model, however, a direct calculation of c_{eff} through the single-particle eigenvalues seems to be a far more challenging problem.

We also extracted the subleading contribution k in Eq. (18) from our data as shown in Fig. 5 for different values of the filling. Its value k_0 without the impurity also depends on q_F (see Ref. 32) and was subtracted in the figure. One has a peaked structure around $\epsilon_d=0$, however, unlike c_{eff} the constant k is, in general, not symmetric with respect to ϵ_d. Instead, one has the relation

$$S(g,\epsilon_d,q_F) = S(g,-\epsilon_d,\pi-q_F) \tag{21}$$

which is a direct consequence of the symmetry property Eq. (A8) of the correlations proven in Appendix A.

C. Particle-number fluctuation

In the last part of this section we will investigate the fluctuations in the number of electrons $\hat{N}=\sum_{n=1}^{L}c_n^\dagger c_n$ contained in the block next to the impurity. Although being a simpler physical quantity, its scaling properties were shown to be similar to that of the entanglement entropy in a variety of 1D quantum systems[33] and, in the case of free fermions, also in arbitrary dimensions.[34,35] Therefore it is an interesting question whether this connection persists for the present impurity problem.

The particle-number fluctuation is a simple quadratic function of the correlation matrix and without the impurity is readily evaluated as[36]

$$\langle\Delta\hat{N}^2\rangle_0 = \operatorname{tr}\,\mathbf{C}^0(\mathbf{1}-\mathbf{C}^0) \approx \frac{1}{\pi^2}\ln L + k_0' \tag{22}$$

with $k_0'=(\ln 2+\gamma+1)/\pi^2$. Note that here the leading-order logarithmic behavior was seen to emerge from the large distance decay properties of the correlations. Therefore, we will use the approximation in Eq. (17) to write $\mathbf{C}\approx\mathbf{C}^0+\mathbf{C}^F$. Carrying out the traces, one finds that the additional term $\operatorname{tr}(\mathbf{C}^F)^2$ has a logarithmic contribution while $\operatorname{tr}\,\mathbf{C}^F(\mathbf{1}-2\mathbf{C}^0)$ evaluates to a constant. The fluctuations then read

$$\langle\Delta\hat{N}^2\rangle = \frac{\kappa_{\text{eff}}}{\pi^2}\ln L + k' \tag{23}$$

with the prefactor given by $\kappa_{\text{eff}}=(1+\cos^2\,\delta_F)/2$.

The result is tested by comparing with the fitted values of κ_{eff} as shown in Fig. 6. The agreement is very good with the only sizeable deviations appearing in the region $|\delta_F|\approx\pi/2$ where the Fano resonance is close to the Fermi level and the approximation Eq. (17) breaks down for the numerically attainable block sizes. Note however that, in general, the small distance deviations from the asymptotic form lead only to a different numerical value of k' as compared with the one obtained by evaluating the subleading terms in the traces. Finally, one has to point out that, apart from the similar logarithmic scaling, the prefactor κ_{eff} of the fluctuations is given by a much simpler function of the scattering amplitude than that governing the entropy.

IV. SEMI-INFINITE GEOMETRY

We now turn to the investigation of the semi-infinite model. Our motivation behind studying a system with an open boundary is twofold. On one hand, we would like to cross-check our argument used for explaining Eq. (19) and show that the contributions in $c_{\rm eff}$ are additive. In other words, we want to test our expectation $\tilde{c}_{\rm eff}=c_{\rm eff}-1/2$ for the semi-infinite effective central charge $\tilde{c}_{\rm eff}$ of a subsystem with an open end. On the other hand, boundaries were shown to induce interesting subleading behavior of the entropy for pure chains,[37] therefore it is interesting to extend these investigations to the present impurity problem.

A. Correlation functions

The main difference from the infinite case is that the couplings t_q are now dependent on the wave number. In principle, the calculations are very similar, leading to slightly more lengthy expressions that are therefore summarized in Appendix B. However, there is an additional feature which leads to the emergence of bound states in the continuum (BIC) which were studied before.[38,39] We will show how these BIC naturally enter the problem at the correlation function level.

Our main interest is to determine the entropy of a block with $L=n_0-1$ sites located on the left-hand side of the impurity. Apart from the usual bound-state contribution, the correlations from the conduction band now include

$$\tilde{C}_{mn}=2\int_0^{q_F}\frac{dq}{\pi}\mathcal{R}(q)\sin qm\,\sin qn \tag{24}$$

with $m,n<n_0$ and we have defined the function

$$\mathcal{R}(q)=\frac{(\epsilon_q-\epsilon_d)^2}{(\epsilon_q-\epsilon_d-\Delta_q)^2+\Gamma_q^2}, \tag{25}$$

where Δ_q and Γ_q are the real and imaginary parts of the self-energy Eq. (B5), respectively, and are related to the parameter $\Sigma_q=\text{Im}\,\Sigma(\epsilon_q+i\delta)$ of the infinite system as

$$\Delta_q=\Sigma_q\sin 2n_0q,\quad \Gamma_q=\Sigma_q 2\sin^2 n_0q. \tag{26}$$

Note that the term C^0_{mn} does not now appear in the correlations.

It is instructive to analyze the main features of the integral in Eq. (24). Taking $|\epsilon_d|\to\infty$ one has $\mathcal{R}(q)\equiv 1$ and the integral reproduces the correlations of a pure semi-infinite chain. For very strong coupling $g\to\infty$ one has $\Sigma_q\to\infty$ and therefore both of the parameters in Eq. (26) take very large values apart from a discrete set defined by the condition $\tilde{q}_n=n\pi/n_0$, $n=1,\ldots,n_0$, where $\Delta_q=\Gamma_q=0$. Therefore, the function $\mathcal{R}(q)$ will become sharply peaked around these $\tilde{q}_n$ values and formally one can substitute

$$\int\frac{dq}{\pi}\mathcal{R}(q)\to\frac{1}{n_0}\sum_{\tilde{q}_n} \tag{27}$$

where the factor $1/n_0$ is needed for proper normalization. Setting $n_0=L+1$, the $\tilde{q}_n$ correspond exactly to the allowed wave numbers in a *finite* chain of length L. Therefore the block is effectively decoupled by the impurity and $\tilde{C}_{mn}$ reproduces the correlations in a finite segment.

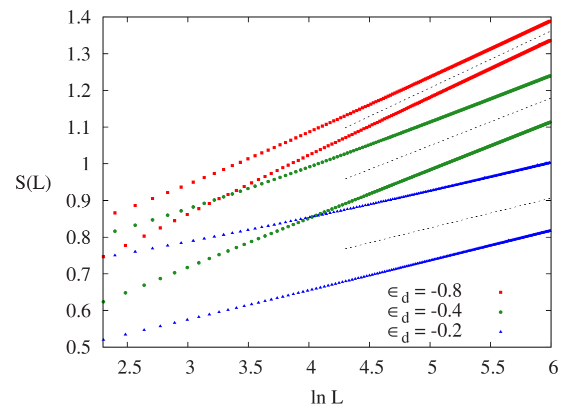

FIG. 7. (Color online) Entropy scaling for a segment with an open boundary for different values of ϵ_d at half filling and $g=0.5$. The dashed lines have corresponding slopes $\tilde{c}_{\rm eff}=c_{\rm eff}-1/2$ and are shown for comparison.

The above argument breaks down for special $\tilde{q}_n$ values fulfilling $\epsilon_{\tilde{q}_n}=\epsilon_d$, where $\mathcal{R}(q)$ becomes zero and the corresponding peak is missing. However, this is exactly the condition for the existence of the BIC. It has been shown that these states have nonvanishing amplitude only at the impurity site and inside the segment where they reproduce, up to normalization, the eigenstates of a chain of length $L=n_0-1$.[38] For $g\to\infty$ even the normalization becomes exact and the contribution of the missing peak is therefore reincluded this way.

While for these special values of ϵ_d the BIC are exactly located at $\tilde{q}_n$, the resonances of $\mathcal{R}(q)$ gradually shift toward the wave numbers of the decoupled block as the coupling to the impurity becomes larger. Hence, their contribution to the entropy is expected to diminish.

B. Entanglement entropy

The numerical study of the entropy is now carried out using the exact form of the correlations $\tilde{C}_{mn}+\tilde{C}^b_{mn}$. The scaling of the entropy at half filling is shown in Fig. 7 for various ϵ_d values. In agreement with our expectations, the slope of the curves coincides well with $\tilde{c}_{\rm eff}=c_{\rm eff}-1/2$ as illustrated by the dashed lines. Additionally, one observes large amplitude oscillations in the data which seem to persist for large values of L. Although such oscillations were already pointed out in case of quantum chains with a boundary, they were found to decay according to a power law and therefore vanish in the limit $L\to\infty$.[37]

A qualitative argument for this alternation can be given by considering the main parameters in Eq. (26) entering the integrals. They contain oscillatory functions of q that, for large n_0, are expected to average out upon integration, yielding $\bar{\Delta}_q=0$ and $\bar{\Gamma}_q=\Sigma_q$. These are just the values for the infinite case, explaining the average behavior of the entropy. However, as seen before the Fermi level plays an important role in the asymptotics and at $q=q_F$ the parameters assume values which differ from the average. For half filling one has $\Delta_{\pi/2}$

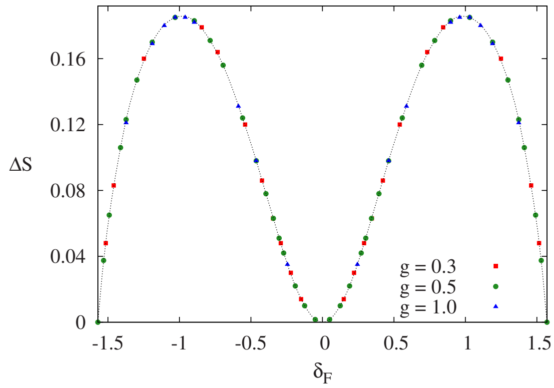

FIG. 8. (Color online) Alternating term ΔS in the entanglement entropy at half filling, as obtained from data fits. The symbols correspond to different values of ϵ_d and g and show a nice collapse when plotted against the scaling variable δ_F of the infinite geometry.

$=0$ while $\Gamma_{\pi/2}=0$ for n_0 even and $\Gamma_{\pi/2}=2\Sigma_{\pi/2}$ for n_0 odd, and thus oscillates around the average $\Sigma_{\pi/2}$. This effect could result in subleading corrections to the entropy that survive the $n_0\to\infty$ limit.

To extract this term, we have fitted our data according to $S(L+1)-S(L)=\Delta S+a/L$. This form, in general, gives a good description of the alternating part. The results on ΔS are plotted in Fig. 8 against the variable δ_F. This choice is justified through our previous argument, where the only nonvanishing parameter is given by $2\Sigma_{\pi/2}$ and thus the scattering phase of the infinite case is still expected to be a relevant scaling variable. The data show indeed a nice collapse to an interpolated scaling function which is shown by the dotted line. It has a zero at $\delta_F=0$ corresponding to the pure semi-infinite chain where the alternating term is known to vanish asymptotically.[37] Note that the symmetry under the exchange $\delta_F\to-\delta_F$ is valid also for $S(L)$ itself.

The behavior of the entropy becomes more complicated when we choose another value of the filling. This is illustrated in Fig. 9 where we have compared $q_F=\pi/3$, corresponding to one-third filling, with $q_F=1$ which gives an *incommensurate* value for the filling. In the former case the entropy curve splits into three parts, shifted from each other

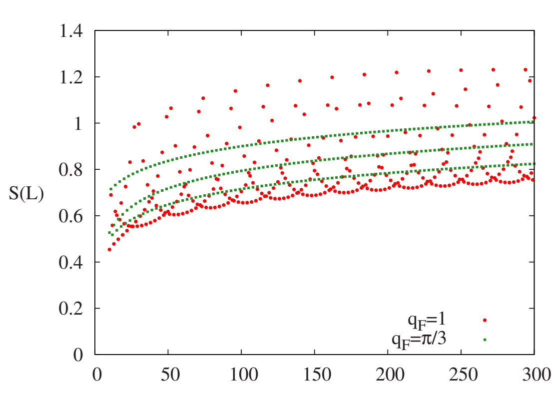

FIG. 9. (Color online) Oscillating behavior of the entropy for a commensurate $q_F=\pi/3$ and an incommensurate $q_F=1$ value of the filling. The parameters are $g=0.5$ and $\epsilon_d=-0.8$.

in a similar way as was observed for half filling in Fig. 7. This corresponds to the three possible values $\Delta_{\pi/3}$ and $\Gamma_{\pi/3}$ can take. However, in the incommensurate case the number of distinct values is infinite, resulting in a highly irregular entropy behavior. Since $\pi/3\approx1.05$, the effective central charges for the two cases are almost equal which explains why the averaged slope of the curves is very similar. Nevertheless, for the small block sizes numerically achievable, the amplitude of the oscillations has the same magnitude as the average entropy. Therefore, a quantitative understanding of the subleading term would be clearly desirable and requires further investigation.

V. CONCLUSIONS

We have studied the entanglement in the ground state of a single-impurity problem described by the Fano-Anderson model, focusing on the analysis of the effective central charge that appears in the entropy scaling. We provided strong numerical evidence for the validity of a formula which gives the functional form of c_{eff} for arbitrary parameter values of the model. In particular, this formula depends only on a single parameter, given by Eq. (20), that has a simple physical interpretation, namely, it is the transmission coefficient of the impurity. This, in turn, establishes a connection between the entanglement entropy and the low-temperature conductance of the quantum chain that can be measured in experiments with quantum-dot nanostructures.[22] Therefore, it would be interesting to generalize the study of the block entropy for Anderson-type impurities, including on-site Coulomb interaction between electrons of different spin, that give a more realistic model of the quantum dots in experiments and yet are still tractable with DMRG techniques.

On the other hand, an exact analytical treatment of the present problem is still lacking. One could follow the lines of Ref. 9 and try to relate the reduced density matrix to the transfer matrix of an appropriate 2D classical system. Another possible approach would be the direct calculation of the entropy from the correlation matrix, which, in the pure case, requires knowledge of the eigenvalues of a Toeplitz matrix.[32] With an impurity one has a sum of Toeplitz and Hankel matrices, which poses a much more difficult problem. However, the analysis of the correlations has led to a simple asymptotic form, enabling us to calculate the particle-number fluctuation that involves, instead of diagonalization, only the traces of the correlation matrix.

The investigation of the semi-infinite geometry has, on one hand, supported our general belief that the leading contributions from both of the interfaces bordering the segment simply add up in the entropy. On the other hand, we found a subleading term which shows an interesting oscillatory behavior. The amplitude of the oscillations remains finite even asymptotically, an effect that has not been observed for pure chains. Although some arguments were given to describe its main features, a proper understanding could only be achieved through, analogous to the infinite case, a careful investigation of the asymptotic correlations.

Finally, it would be worth extending this study to the case where the impurity is located further apart from the boundary

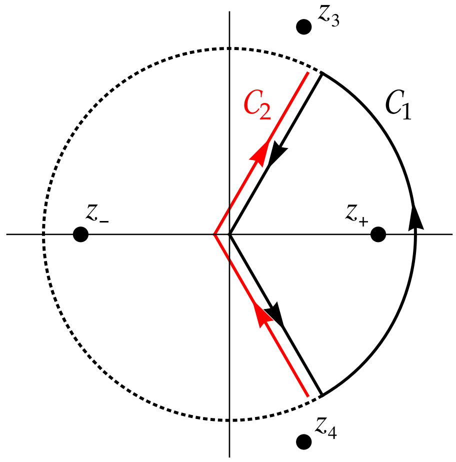

FIG. 10. (Color online) Integration contours and poles of the integrand appearing in Eq. (A3). The dashed line shows the boundary of the complex unit disk.

of the subsystem. If this distance grows large, the effective central charge must return to the value of a pure system and an interesting crossover behavior might emerge.

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APPENDIX A: ASYMPTOTIC FORM OF THE CORRELATIONS

The expression for the correlation functions involves the integrals in Eq. (14) containing an oscillatory integrand. In the limit $l \gg 1$ one could approximate it by considering the scattering phase to be a constant. However, this method only works for slowly varying $\delta(q)$ functions which is not fulfilled by Eq. (15) for $q \approx 0$ and $\epsilon_q \approx \epsilon_d$. It will be shown that with a suitable transformation of the integral one can extract the resonant contributions which exactly reproduce the term $C^b(l)$ associated with the bound state. To show this, we first rewrite Eq. (14) in the form

$$C^1(l) = \int_{-q_F}^{q_F} \frac{dq}{2\pi} \frac{\Sigma_q^2 \cos ql + \Sigma_q(\epsilon_q - \epsilon_d)\sin ql}{(\epsilon_q - \epsilon_d)^2 + \Sigma_q^2}, \tag{A1}$$

where we defined

$$\Sigma_q = -\frac{g^2}{\sin q} = \begin{cases} \mathrm{Im}\,\Sigma(\epsilon_q + i\delta) & \text{if } q > 0 \\ \mathrm{Im}\,\Sigma(\epsilon_q - i\delta) & \text{if } q < 0. \end{cases} \tag{A2}$$

Note, that the denominator is just the product $\eta_+(\epsilon_q)\eta_-(\epsilon_q)$ which is strictly positive along the integration path in Eq. (A1) but, in general, has four roots on the complex plane.[26] Introducing the variable $z = e^{iq}$ the integration is now taken along an arc of the complex unit circle which can be written as the sum of the two contours shown in Fig. 10. After changing variables and using the symmetry under $z \to z^{-1}$ it takes the following form:

$$C^1(l) = \int_{\mathcal{C}_1+\mathcal{C}_2} \frac{dz}{2\pi i} \frac{4g^2 z}{\Theta(z)} z^l \tag{A3}$$

with the fourth-order polynomial

$$\Theta(z) = z^4 + 2z(z^2 - 1)(\epsilon_d - \epsilon_0) + 4g^2 z^2 - 1. \tag{A4}$$

It is easy to show that the polynomial has two real solutions $z_\pm = \pm e^{-1/\xi_\mp}$ which lie inside the unit disk and z_+ (z_-) is related to the lower (upper) bound-state solutions as $\epsilon_\mp = -(z_\pm + z_\pm^{-1})/2 = \mp \cosh \xi_\mp^{-1}$. The remaining solutions form a complex-conjugate pair $z_3 = z_4^*$ and lie outside the unit disk. The closed contour $\mathcal{C}_1$ therefore only encircles the pole at z_+ and the residue is evaluated as

$$\operatorname*{Res}_{z=z_+} \frac{4g^2 z}{\Theta(z)} z^l = C^b(l), \tag{A5}$$

where $C^b(l)$ is defined under Eq. (12). The remaining integral is taken along the contour $\mathcal{C}_2$ which is parametrized as $z = e^{\pm iq_F} e^{-q'}$ and using the analytic continuation of the scattering phase it reads

$$-\mathrm{Re} \int_0^\infty \frac{dq'}{\pi} \sin \delta(q_F + iq') e^{i(q_F+iq')l} e^{i\delta(q_F+iq')}. \tag{A6}$$

Note, that $\delta(q_F + iq')$ varies smoothly and vanishes for $q' \to \infty$. For $l \gg 1$ the integrand is rapidly decaying, thus one can approximate the phase around $q'=0$ as $\delta(q_F + iq') \approx \delta_F + iq' \frac{d\delta(q)}{dq}\big|_{q_F}$. If the derivative is small, that is we are far away from the Fano resonance, one can set $\delta(q_F + iq') = \delta_F$ and the integral Eq. (A6) can be trivially carried out to yield the result in Eq. (17). The derivative term is then used to define a length scale

$$l_0 \sim \left.\frac{d\delta(q)}{dq}\right|_{q_F} = \frac{g^2(\sin^2 q_F - \epsilon_d \cos q_F)}{\epsilon_d^2 \sin^2 q_F + g^4} \tag{A7}$$

which marks the regime $l \gg l_0$ where the approximation is valid. Note that l_0 can only grow large if the conditions $\epsilon_d^2 \ll g^2 \ll 1$ are satisfied.

The contour integral can also be used to prove an exact symmetry property of the correlations. We define the particle-hole transformed functions $\bar{C}^b(l)$ and $\bar{C}^1(l)$ by performing the changes $\epsilon_d \to -\epsilon_d$ and $q_F \to \pi - q_F$. Now, one can show that the sum $C^1(l) + (-1)^l \bar{C}^1(l)$ can be written as the integral Eq. (A3) over the *complete* unit circle which is exactly evaluated as the sum of the residues at z_+ and z_-. Using the symmetry property $\epsilon_+ = -\bar{\epsilon}_-$, the latter pole contributes $(-1)^l \bar{C}^b(l)$ which, after reordering, yields the relation

$$\bar{C}^b(l) - \bar{C}^1(l) = (-1)^l [C^b(l) - C^1(l)]. \tag{A8}$$

APPENDIX B: SEMI-INFINITE FORMULAS

We present here some of the formulas which are necessary for the calculations in the semi-infinite geometry. First, the self-energy function outside the band reads

$$\tilde{\Sigma}(\epsilon_\pm) = \pm \frac{g^2}{\sqrt{\epsilon_\pm^2 - 1}}[1 - (|\epsilon_\pm| - \sqrt{\epsilon_\pm^2 - 1})^{2n_0}] \quad \text{(B1)}$$

and the bound-state energies $\epsilon_+ > 1$ and $\epsilon_- < -1$ are obtained numerically as the roots of

$$\epsilon_\pm - \epsilon_d - \tilde{\Sigma}(\epsilon_\pm) = 0. \quad \text{(B2)}$$

Note that ϵ_+ (ϵ_-) exists only for parameter values fulfilling $\epsilon_d > 1 - 2g^2 n_0$ ($\epsilon_d < -1 + 2g^2 n_0$). On the other hand, using the definition of the inverse correlation length $\epsilon_\pm = \pm \cosh \xi_\pm^{-1}$ the second term in the parentheses in Eq. (B1) can be written as $e^{-2n_0/\xi_\pm}$. Therefore, if the impurity lies deep in the bulk of the chain with $n_0 \to \infty$ one has $\tilde{\Sigma}(\epsilon_\pm) = \Sigma(\epsilon_\pm)$ and consequently the same solutions for $\epsilon_\pm$ as in the infinite case.

The contribution $\tilde{C}^b_{mn}$ from the lower bound state can be evaluated as

$$\frac{g^2 \tilde{N}_-}{\epsilon_-^2 - 1} \begin{cases} 4 \sinh^2 \frac{n_0}{\xi_-} e^{-(m+n)/\xi_-} & \text{if } m,n \geq n_0 \\ 4 \sinh \frac{m}{\xi_-} \sinh \frac{n}{\xi_-} e^{-2n_0/\xi_-} & \text{if } m,n < n_0 \end{cases} \quad \text{(B3)}$$

with the normalization factor

$$\tilde{N}_- = \frac{\epsilon_-^2 - 1}{2\epsilon_-^2 - \epsilon_- \epsilon_d - 1 - 2n_0 g^2 e^{-2n_0/\xi_-}}. \quad \text{(B4)}$$

The limit $n_0 \to \infty$ gives $\tilde{N}_- = N_-$ and the right-hand side of Eq. (B3) becomes $e^{-(m'+n')/\xi_-}$ with the shifted indices $m' = |m - n_0|$ and $n' = |n - n_0|$, thus recovering again the result in Eq. (12) for the infinite case.

Finally, one needs the expression for the retarded self-energy inside the band

$$\tilde{\Sigma}(\epsilon_q + i\delta) = -2g^2 \frac{\sin n_0 q}{\sin q} e^{i n_0 q} \quad \text{(B5)}$$

which is an oscillatory function of the position n_0. This eventually leads to the emergence of bound states in the continuum, as described in the text. The scattering phases are defined as

$$\tan \tilde{\delta}(q) = \frac{\Gamma_q}{\epsilon_q - \epsilon_d - \Delta_q} \quad \text{(B6)}$$

with $\Delta_q = \mathrm{Re}\, \tilde{\Sigma}(\epsilon_q + i\delta)$ and $\Gamma_q = \mathrm{Im}\, \tilde{\Sigma}(\epsilon_q + i\delta)$.

The band contributions also have to be treated separately on either sides of the impurity. On the right-hand side, analogously to the infinite case, it can be expressed in the form $\tilde{C}^0(m-n) - \tilde{C}^1(m+n)$ with

$$\tilde{C}^1(l) = \int_0^{q_F} \frac{dq}{\pi} \cos[ql + 2\tilde{\delta}(q)] \quad \text{(B7)}$$

while the translationally invariant term $\tilde{C}^0(m-n) = C^0(m-n)$ is unmodified. The correlations on the left-hand side cannot be given in that simple form and are analyzed in the text.

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