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LETTER TO THE EDITOR

Unstable particles versus resonances in impurity systems; conductance in quantum wires

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Abstract
We compute the DC conductance for a homogeneous sine–Gordon model and an impurity system, which in the conformal limit can be reduced to a Luttinger liquid, by means of the thermodynamic Bethe ansatz and standard potential scattering theory. We demonstrate that unstable particles and resonances in impurity systems lead to a sharp increase of the conductance as a function of the temperature, which is characterized by the Breit–Wigner formula.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

In the context of integrable quantum field theories in 1 + 1 space-time dimensions, a large arsenal of extremely powerful non-perturbative techniques has been developed over the last two and a half decades. The original motivation of treating these theories as a testing ground for realistic theories in higher dimensions is nowadays supplemented by the possibility of direct applications, since the nanotechnology has advanced to such a degree that one-dimensional materials, i.e. quantum wires, may be realized experimentally. A quantity which can be measured directly [1] is the conductance through the quantum wire. There also already exist various proposals [2, 3] for how to obtain this quantity from general non-perturbative techniques, such as the thermodynamic Bethe ansatz (TBA) [4, 5] and the form factor approach [6] to compute the current–current two-point correlation functions in the Kubo formula [7]. Here we want to concentrate on the former approach. Whereas in [2] the emphasis was put on reproducing features of quantum Hall systems and the authors appealed extensively to massless models, we want to treat here, in contrast, systems which are purely massive. In particular, we want to investigate how the properties of unstable particles and impurity resonances are reflected in a possible conductance measurement.

2. From conductance to masses of unstable particles

The direct current I through a quantum wire can be computed simply by determining the difference of the static charge distributions at the right and left constrictions of the wire, i.e. $I = Q_R - Q_L$. This is based on the Landauer transport theory, i.e., on the assumption [2, 3] that $Q(t) \sim (Q_R - Q_L)t \sim (\rho_R - \rho_L)t$, where the ρs are the corresponding density distribution functions. For more details and a comparison with the Kubo formula, see [8]. Placing an impurity in the middle of the wire, we have to quantify the overall balance of particles of type i and anti-particles $\bar{\imath}$ carrying opposite charges $q_i = -q_{\bar{\imath}}$ at the end of the wire at different potentials. This is achieved once we know the density distribution $\rho_i^r(\theta, r, \mu_i)$ as a function of the rapidity θ, the inverse temperature r and the chemical potential μ_i. In the set-up described, half of the particles of one type are already at the same potential at one of the ends of the wire and the probability for them to reach the other is determined by the amplitude $|T_i(\theta)|$ for transmission through the impurity. Therefore

$$I = \sum_i I_i(r, \mu_i) = \sum_i \int \mathrm{d}\theta \, \frac{q_i}{2} [(\rho_i^r(\theta, r, \mu_i^R) - \rho_i^r(\theta, r, \mu_i^L))|T_i^2(\theta)|]. \tag{1}$$

By definition, the DC conductance results as

$$G(r) = \sum_i G_i(r) = \sum_i \lim_{\mu_i \to 0} I_i(r, \mu_i)/\mu_i \tag{2}$$

and is of course a property of the material itself and a function of the temperature. In general, the expressions in (1) tend to zero for vanishing chemical potential such that the limit in (2) is non-trivial.

Let us now compute the density distribution by means of the TBA. As was pointed out in [9], the TBA equations for a bulk system and a system with a purely transmitting defect are identical. This is due to the fact that in the thermodynamic limit the number of defects is kept fixed and is therefore insignificant in thermodynamic considerations. Therefore the same equations also hold when we allow the impurity to be such that transmission and reflection are simultaneously possible. We recall the main equations of the TBA analysis which are directly relevant in this context; see [4] for more details and, in particular for the introduction of the chemical potential, see [5]. For a detailed derivation of the TBA equations in this context see [8]. The main input into the entire analysis is the dynamical interaction encoded into the scattering matrix $S_{ij}(\theta)$ of two particles of masses m_i and m_j and the assumption regarding the statistical interaction, which we take to be fermionic. As usual [4, 5], by taking the logarithmic derivative of the Bethe ansatz equation and relating the density of states $\rho_i(\theta)$ for particles of type i to the density of occupied states $\rho_i^r(\theta)$, one obtains

$$\rho_i(\theta, r, \mu_i) = \frac{m_i}{2\pi} \cosh\theta + \sum_j [\varphi_{ij} * \rho_j^r](\theta). \tag{3}$$

By $(f * g)(\theta) := [1/(2\pi)] \int \mathrm{d}\theta' \, f(\theta - \theta') g(\theta')$ we denote the convolution of two functions and $\varphi_{ij}(\theta) = -\mathrm{i} \, \mathrm{d} \ln S_{ij}(\theta)/\mathrm{d}\theta$. The ratio of the densities serves as the definition of the so-called pseudo-energies $\varepsilon_i(\theta)$:

$$\frac{\rho_i^r(\theta, r, \mu_i)}{\rho_i(\theta, r, \mu_i)} = \frac{\mathrm{e}^{-\varepsilon_i(\theta, r, \mu_i)}}{1 + \mathrm{e}^{-\varepsilon_i(\theta, r, \mu_i)}}, \tag{4}$$

which have to be positive and real. At thermodynamic equilibrium one obtains then the TBA equations, which read in these variables

$$r m_i \cosh\theta = \varepsilon_i(\theta, r, \mu_i) + r\mu_i + \sum_j [\varphi_{ij} * L_j](\theta), \tag{5}$$

where $r = m/T$, $m_l \to m_l/m$, $\mu_i \to \mu_i/m$, $L_i(\theta, r, \mu_i) = \ln(1 + \mathrm{e}^{-\varepsilon_i(\theta, r, \mu_i)})$, with m being the mass of the lightest particle in the model and T the temperature. It is important to note that μ_i is restricted to being smaller than 1. This follows immediately from (5) on recalling that

$\varepsilon_i \geqslant 0$ and that for r large, $\varepsilon_i(\theta, r, \mu_i)$ tends to infinity. As pointed out already in [4], here, just with a small modification of a chemical potential, the comparison between (3) and (5) leads to the useful relation

$$\rho_i(\theta, r, \mu_i) = \frac{1}{2\pi}\left(\frac{\mathrm{d}\varepsilon_i(\theta, r, \mu_i)}{\mathrm{d}r} + \mu_i\right). \tag{6}$$

The main task is therefore to solve (5) for the pseudo-energies from which all densities can then be reconstructed. In general, due to the non-linear nature of the TBA equation, this is done numerically. However, in the large-temperature regime, one may carry out various analytical approximations. For large rapidities and small r, one [4] can approximate the density of states by

$$\rho_i(\theta, r, \mu_i) \sim \frac{m_i}{4\pi}\mathrm{e}^{|\theta|} \sim \frac{1}{2\pi r}\epsilon(\theta)\frac{\mathrm{d}\varepsilon_i(\theta, r, \mu_i)}{\mathrm{d}\theta}, \tag{7}$$

where $\epsilon(\theta)$ is the step function. To obtain this, we assume in (4) that in the large-rapidity regime $\rho_i^r(\theta, r, \mu_i)$ is dominated by (7) and in the small-rapidity regime by the Fermi distribution function; therefore,

$$\rho_i^r(\theta, r, \mu_i) \sim \frac{1}{2\pi r}\epsilon(\theta)\frac{\mathrm{d}}{\mathrm{d}\theta}\ln[1 + \exp(-\varepsilon_i(\theta, r, \mu_i))]. \tag{8}$$

Using this expression, we approximate the current in (1) and for $\mu_i^R = -\mu_i^L = V/2$ the conductance results as

$$\lim_{r\to 0} G_i(r) \sim \frac{q_i}{2\pi r}\int_{-\infty}^{\infty}\mathrm{d}\theta\,\frac{1}{1 + \exp[\varepsilon_i(\theta, r, 0)]}\left.\frac{\mathrm{d}\varepsilon_i(\theta, r, V/2)}{\mathrm{d}V}\right|_{V=0}\frac{\mathrm{d}[\epsilon(\theta)|T_i(\theta)|^2]}{\mathrm{d}\theta}. \tag{9}$$

In order to evaluate (1) and (9) it remains to specify how to compute the transmission amplitude. In principle, this can be done by exploiting the factorization equations which result as a consequence of integrability. However, for systems with a diagonal bulk S-matrix these equations are not restrictive enough and we will below simply use a free field expansion and proceed in analogy with standard quantum mechanical potential scattering. Having obtained $T_j(\theta)$ and $R_j(\theta)$, one can construct the equivalent quantities for multiple defects from these functions. Here we are particularly interested in a double defect. Placing the two defects of the same type at $x_1 = 0$, $x_2 = y$, the total transmission amplitude $\hat{T}_j$ can be built up from those of a single defect as [10]

$$\hat{T}_j(\theta) = \frac{T_j^2(\theta)}{1 - R_j^2(\theta)\exp(\mathrm{i}\,2y\sinh\theta)}. \tag{10}$$

Having assembled all the ingredients for the computation of G, we turn to the question of how the properties of unstable particles are reflected in this quantity. Assuming that $S_{ij}(\theta)$ possesses a resonance pole at $\theta_R = \sigma - \mathrm{i}\bar{\sigma}$, the Breit–Wigner formula [11] allows us to determine the mass $M_{\tilde{c}}$ and the decay width $\Gamma_{\tilde{c}}$ of an unstable particle of type $\tilde{c}$:

$$2M_{\tilde{c}}^2 = \sqrt{\gamma^2 + \tilde{\gamma}^2} + \gamma \geqslant 2(m_i + m_j)^2 \tag{11}$$

$$\Gamma_{\tilde{c}}^2/2 = \sqrt{\gamma^2 + \tilde{\gamma}^2} - \gamma \geqslant 4m_i m_j(1 - \cosh\sigma\cos\bar{\sigma}), \tag{12}$$

where $\gamma = m_i^2 + m_j^2 + 2m_i m_j\cosh\sigma\cos\bar{\sigma}$ and $\tilde{\gamma} = 2m_i m_j\sinh|\sigma|\sin\bar{\sigma}$. The thresholds in (11) and (12) result from energetic factors [12]. We will now demonstrate that besides unstable particles, resonances in impurity systems can also be described by means of the Breit–Wigner formula. An important consequence of (11) is that we can approximate the mass therein by $M_{\tilde{c}}^2 \approx (1/2)m_i m_j(1 + \cos\bar{\sigma})\exp|\sigma|$ for large σ. Then, under a renormalization group flow $M_{\tilde{c}} \to r_C M_{\tilde{c}}$, the quantity $M_{\tilde{c}} \sim r_C^1\mathrm{e}^{\sigma_1/2} = r_C^2\mathrm{e}^{\sigma_2/2}$ remains invariant. Once the unstable

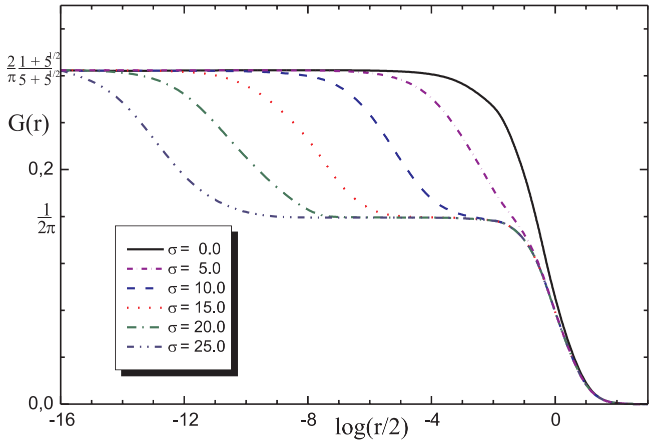

Figure 1. Conductance G for the $SU(3)_2$ HSG model as a function of $\log(r/2) = \log(m/2T)$ for various values of the resonance parameter σ.

particle can be created, it can participate in the overall conductance and one should observe an increase at T_C in G related to this process. For this interpretation to hold, we should observe the following scaling behaviour of the conductance:

$$G(r_C^1, \sigma_1) = G(r_C^2, \sigma_2) \qquad \text{for } r_C^1 e^{\sigma_1/2} = r_C^2 e^{\sigma_2/2}. \tag{13}$$

r_C is certainly not sharply defined, but taking for instance the mid-point between the beginning and the end of the onset seems reasonably reliable. Here r_C is the inverse of the critical temperature $r_C = m/T_C$ at which the unstable particle for fixed σ is formed. This means that the identification of the onset in a conductance measurement will provide r_C such that, for given σ, the mass of the unstable particle can be deduced.

3. The homogeneous sine–Gordon model

The $SU(3)_2$ homogeneous sine–Gordon (HSG) model is the simplest of its kind and contains only two self-conjugate solitons, which we denote by '+', '−', and one unstable particle, which we call $\tilde{c}$. The corresponding scattering matrix was found [13] to be $S_{\pm\pm} = -1$, $S_{\pm\mp}(\theta) = \pm\tanh(\theta \pm \sigma - i\pi/2)/2$, which means that the resonance pole is situated at $\theta_R = \mp\sigma - i\pi/2$. Stable bound states may not be formed. It is known [10] that integrable parity-invariant impurity systems with a diagonal bulk S-matrix, apart from $S = \pm 1$, do not allow simultaneously non-trivial reflection and transmission amplitudes. This statement can be extended to the parity-violating case [15]. We therefore treat (1) for a transparent defect, i.e. $|T| = 1$. The results for the conductance obtained after solving the TBA equations for $\mu_R = -\mu_L = 0.25$ numerically are depicted in figure 1.

Taking the limit $\mu \to 0$ is rather complicated when one does not have an explicit analytic expression to hand, as in our case. However, we can take the result for finite μ as a very good approximation, since we observe that $G(r)/\mu \sim$ constant for small r. We observe the onset of the unstable particle in the form of a relatively sharp increase in G and in particular the validity of (13). The interpretation is clear: only when we reach an energy scale at which the unstable particle can be formed can it participate in the conducting process. All this information is encoded in the density $\rho_i^r(\theta, r, \mu_i)$. Also, the bound in (11) is respected. Computing $\varepsilon_i(\theta, 0, 0)$ now in a standard TBA fashion (see, e.g., [16]), we predict analytically the plateaus from (9) at $2(1+\sqrt{5})/(5+\sqrt{5})\pi$ and at $1/2\pi$. The latter value is obtained from the fact that in the region in which $\sigma \gg -2\log(r/2)$, the system can be viewed as consisting of two free fermions such that (9) gives the quoted value.

4. The free fermion with impurities

The continuous version of the (1 + 1)-dimensional Ising model with a line defect was first treated in [17]. Thereafter it was also considered in [10, 18] and [19] from a different point of view. In [10, 17, 18] the impurity was taken to be of the form of the energy operator and in [19] a perturbation in the form of a single fermion has also been considered. Here we also include a further type of defect.

Let us consider the Lagrangian density for a complex free fermion ψ with ℓ defects:

$$\mathcal{L} = \bar{\psi}(\mathrm{i}\gamma^{\mu}\partial_{\mu} - m)\psi + \sum_{n=1}^{\ell}\delta(x - x_n)\mathcal{D}_n(\bar{\psi}, \psi), \tag{14}$$

where we describe the defect by the functions $\mathcal{D}_n(\bar{\psi}, \psi)$, which we assume to be linear in the Fermi fields. In the following we will restrict ourselves to the case $\ell = 2$ with $x_n = ny$ and $\mathcal{D}_n(\bar{\psi}, \psi) = \mathcal{D}(\bar{\psi}, \psi)$. We compute the transmission amplitude as indicated in [10, 18, 19], namely by decomposing the solution to these equations as $\psi(x) = \Theta(x)\psi_+(x) + \Theta(-x)\psi_-(x)$ and substituting them into the equations of motion. In this way we obtain the constraints

$$\mathrm{i}\gamma^1(\psi_+(x) - \psi_-(x))|_{x=x_n} = \left.\frac{\partial\mathcal{D}_n(\bar{\psi}, \psi)}{\partial\bar{\psi}}\right|_{x=x_n}. \tag{15}$$

Using now the standard Fourier expansion for a complex free Fermi field, the transmission and reflection amplitudes can be read off componentwise from (15) as the coefficients of $a^{\dagger}_{j,-}(\theta) = R_{\bar{j}}(\theta)a^{\dagger}_{\bar{j},-}(-\theta)$, $a^{\dagger}_{j,-}(\theta) = T_{\bar{j}}(\theta)a^{\dagger}_{j,+}(\theta)$ etc.

Recalling now that for the free fermion the TBA equations are simply solved by $\varepsilon_i(\theta, r, \mu_i) = rm_i\cosh\theta - r\mu_i$, we compute

$$G(r) = \frac{r}{2\pi}\int_0^{\infty}\mathrm{d}\theta\,\frac{\cosh\theta|T_i(\theta)|^2}{1+\cosh(r\cosh\theta)}. \tag{16}$$

To proceed further we have to specify the impurity.

4.1. The energy operator defect, $\mathcal{D}(\bar{\psi}, \psi) = g\bar{\psi}\psi$

From (15) we compute

$$R_j(\theta, B) = R_{\bar{j}}(\theta, B) = -\frac{\mathrm{i}\sin B\cosh\theta}{\sinh\theta + \mathrm{i}\sin B}, \tag{17}$$

$$T_j(\theta, B) = T_{\bar{j}}(\theta, B) = \frac{\cos B\sinh\theta}{\sinh\theta + \mathrm{i}\sin B}, \tag{18}$$

where we used a common parametrization in this context, $\sin B = -4g/(4+g^2)$. The expressions $R_{\bar{j}}(\theta, B)$ and $T_{\bar{j}}(\theta, B)$ coincide with the solutions found in [10], which, however, in general does not correspond to taking our particles simply to be self-conjugate, since we use Dirac fermions. Using (17) and (18) we compute using (10) the conductance for a double defect with varying distance y. The results of our numerical computations for the conductance are depicted in figure 2.

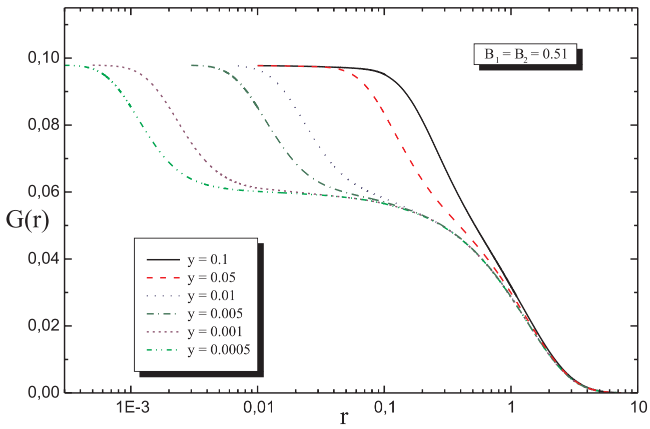

Figure 2. Conductance G for the free fermion with a double energy defect at distance y as a function of the inverse temperature $r = m/T$.

In the high-temperature regime we can confirm these data once more by making some analytical computations. From (9) we obtain

$$\frac{1}{2\pi}\left(\frac{\cos^2 B}{1+\sin^2 B}\right)^2 \leqslant G(r, y) < \frac{1}{2\pi}. \tag{19}$$

The lower bound becomes exact for $y/r < 1$. For $B = 0.51$ the values 0.0602 are well reproduced in figure 2.

We observe a type of behaviour like that in the preceding section and again denote the point of onset in the conductance by r_C. Then, we deduce from our data the following scaling relations:

$$G(r_C^1, y_1) = G(r_C^2, y_2) \qquad \text{for } r_C^2 y_1 = r_C^1 y_2. \tag{20}$$

Comparison with (13) suggests that we can relate the distance between the two defects to the resonance parameter as $\sigma = 2\ln(\text{constant}/y)$. However, despite the fact that the net result with regard to the conductance is the same, the origin of the onset is different. Whereas in the previous section it resulted from a change in the density distribution function, it is now triggered by the structure of $|\hat{T}(\theta)|$. Since ρ^r keeps its overall shape and just moves its peak with varying temperature, the onset has to occur when $|\hat{T}(\theta)|$ reaches its maximum. Using (17), (18) and (10), it is easy to verify that $|\hat{T}(\theta = \ln[(2n+1)\pi/y])| \approx 1$. Drawing now an analogy to the scattering matrix, this value plays the same role as θ_R and we therefore make the identification

$$\sigma_n = \ln[(2n+1)\pi/y]. \tag{21}$$

Having fixed the resonance parameter σ we may, in view of (20), relate the temperature to the mass scale of the unstable particle, associated now with the resonance, analogously to in the discussion after (13). However, there are some differences. Whereas in the HSG model the onset is attributed to a single particle, the effect for the double-defect system is attributed to several resonances. We make the identification $\sigma \approx \sigma_0 + \sigma_1$. The other difference is that y is now a measurable quantity, such that σ in (21) can be experimentally determined. On the other hand, the sigma in (13) is usually a free parameter in the HSG-type models. Let us now verify our observations for a different type of defect.

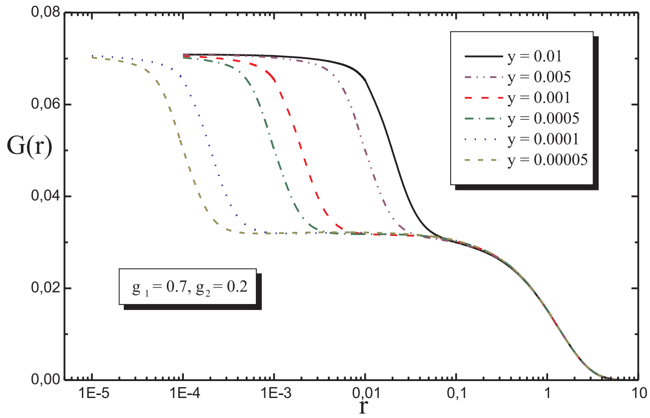

Figure 3. Conductance G for the free fermion with two defects $D_n(\bar{\psi}, \psi) = \bar{\psi}(g_1 + g_2\gamma^0)\psi$ at distance y as a function of the inverse temperature m/T.

4.2. *Luttinger-type liquid,* $\mathcal{D}(\bar{\psi}, \psi) = \bar{\psi}(g_1 + g_2\gamma^0)\psi$

There exist various ways to realize Luttinger-type liquids [20]. Taking the conformal limit of the defect $\mathcal{D}(\bar{\psi}, \psi) = \bar{\psi}(g_1 + g_2\gamma^0)\psi$, we obtain an impurity which played a role in this context [21] when setting the bosonic number counting in there to one. In analogy with the previous sections, we compute the related transmission and reflection amplitudes

$$R_j(\theta, g_1, g_2) = \frac{4\mathrm{i}(g_2 - g_1 \cosh\theta)}{4\mathrm{i}(g_1 - g_2\cosh\theta) + (4 + g_1^2 - g_2^2)\sinh\theta},$$

$$T_j(\theta, g_1, g_2) = \frac{(4 + g_2^2 - g_1^2)\sinh\theta}{4\mathrm{i}(g_1 - g_2\cosh\theta) + (4 + g_1^2 - g_2^2)\sinh\theta}.$$

The expressions for the particle $\bar{\jmath}$ are obtained by making the replacement $g_1 \to -g_1$. The results of our numerical computation for $g_1 = 0.7$ and $g_2 = 0.2$ depicted in figure 3 confirm the same physical picture as that outlined in the previous subsection. Our analytical prediction for the lowest plateau from (9) is 0.0324.

5. Conclusions

By using the TBA to compute the density distribution function and relativistic potential scattering theory to determine the transmission amplitude, we evaluated the DC conductance by means of equation (1). We demonstrated that the sharp increase of the conductance as a function of the temperature can be attributed to the presence of unstable particles in the HSG models or likewise to a resonance of a double-defect system.

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