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LETTER TO THE EDITOR

Form-factors computation of Friedel oscillations in Luttinger liquids

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Abstract. We show how the form-factors approach can be used to compute correlators of operators with non-trivial anomalous dimension in quantum impurity problems. This is done by a series of regularizations that cure completely the infrared divergencies, without spoiling the exactness of the method. As an application, we compute for $g \leq \frac{1}{2}$ the ‘Friedel oscillations’ of charge density induced by a single impurity in a one-dimensional Luttinger liquid of spinless electrons.

The general problem of a Luttinger liquid interacting with an impurity—that may have internal degrees of freedom—has attracted constant attention. The first reason is the wealth of physical applications: they include the anisotropic Kondo model, the double well problem [1] and the washboard potential problem of dissipative quantum mechanics, scattering through an impurity in quantum wires [2], and tunnelling through a point contact in the fractional quantum Hall effect [3]. Another reason is that this general problem is integrable, and therefore the possibility of obtaining exact solutions exists. Until recently, however, such solutions had been restricted to thermodynamic properties. While of crucial experimental interest, correlation functions and related transport and dynamical properties had remained inaccessible analytically. Numerical simulations were quite difficult, and not always conclusive.

Recently, major progress has been made. Based on a new basis of massless quasiparticles suggested by integrability, together with a generalization of the Landauer Büttiker approach, DC properties have been exactly computed, in remarkable agreement with experimental results [4]. Using the form-factors approach [5, 6], the dynamical properties of currents have also been obtained exactly [7], or, more precisely, in closed forms that have an arbitrary accuracy all the way from the ultraviolet (UV) to the infrared (IR) fixed points.

The method used in [7] worked only for currents, i.e. for operators with no anomalous dimension. This was a major drawback, since many physical properties are described by more complicated operators, for which the expressions of [7] are very strongly IR divergent. We show in this letter that this problem can be cured by a series of elementary manipulations that do not spoil the exactness of the approach. As an application, we determine the $2k_F$ part of the charge density profile in a one-dimensional Luttinger liquid away from an impurity, a problem which has attracted a lot of interest recently [8, 9].

We start with the bosonized form of the model. The Hamiltonian takes the form

$$H = \int_{-\infty}^{\infty} dx \left[8\pi g \Pi^2 + \frac{1}{8\pi g} (\partial_x \phi)^2 \right] + \lambda \cos \phi(0) \quad (1)$$

where we have set $v_F = g$. Then for the Friedel oscillations, the charge density operator is just

$$\rho(x) = \rho_0 + 2\partial_x\phi + \frac{k_F}{\pi} \cos[2k_F x + \phi(x)]. \quad (2)$$

with $\rho_0 = k_F/\pi$ is the background charge. We decompose this system into even and odd bases [10] by decomposing $\phi = \phi_L + \phi_R$ and setting

$$\begin{aligned} \phi^e(x+t) &= \frac{1}{\sqrt{2}} [\phi_L(x,t) + \phi_R(-x,t)] \\ \phi^o(x+t) &= \frac{1}{\sqrt{2}} [\phi_L(x,t) - \phi_R(-x,t)]. \end{aligned} \quad (3)$$

Observe that these two field are left movers. We now fold the system by setting

$$\begin{aligned} \phi_L^e &= \sqrt{2}\phi^e(x+t) \quad x < 0 & \phi_R^e &= \sqrt{2}\phi^e(-x+t) \quad x < 0 \\ \phi_L^o &= \sqrt{2}\phi^o(x+t) \quad x < 0 & \phi_R^o &= -\sqrt{2}\phi^o(-x+t) \quad x < 0 \end{aligned} \quad (4)$$

and introduce new fields $\phi^{e,o} = \phi_L^{e,o} + \phi_R^{e,o}$. The density oscillations now read

$$\frac{\langle \rho(x) - \rho_0 \rangle}{\rho_0} = \cos(2k_F x + \eta_F) \left\langle \cos \frac{\phi^o(x)}{2} \right\rangle \left\langle \cos \frac{\phi^e(x)}{2} \right\rangle \quad (5)$$

with η_F the additional phase shift coming from the unitary transformation to eliminate the forward scattering term. ϕ^o is the odd field with Dirichlet boundary conditions at the origin $\phi^o(0) = 0$ leading to [11]

$$\left\langle \cos \frac{\phi^o}{2} \right\rangle \propto \left(\frac{1}{x} \right)^{g/2} \quad (6)$$

and the ϕ^e part is computed with the Hamiltonian

$$H^e = \frac{1}{2} \int_{-\infty}^0 dx \left[8\pi g \Pi^{e2} + \frac{1}{8\pi g} (\partial_x \phi^e)^2 \right] + \lambda \cos \frac{\phi^e(0)}{2}. \quad (7)$$

On general grounds, we expect the scaling form

$$\left\langle \cos \frac{\phi^o}{2} \right\rangle \propto \left(\frac{1}{x} \right)^{g/2} F(\lambda x^{1-g}) \quad (8)$$

where F is a scaling function to be determined. Note that even the small x behaviour of this function is not known in general.

Our approach is based on the fact that both systems are integrable. By considering the free boson as a limit of the sine-Gordon model [12], we describe it using a basis of quasiparticle states, the quasiparticles being massless solitons/antisolitons and breathers, with factorized scattering. The boundary interaction is then described by a scattering matrix, which is elastic [13, 14].

To compute the correlation functions, it is convenient to represent the boundary interaction through a boundary state [13] $|B\rangle$:

$$|B\rangle = \exp \left[\sum_{\epsilon_1, \epsilon_2} \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} Z_{\epsilon_1}^{*(L)}(\theta) Z_{\epsilon_2}^{*(R)}(\theta) K^{\epsilon_1 \epsilon_2}(\theta_B - \theta) \right] \quad (9)$$

where ϵ_i denote the type of particles (solitons/antisolitons or breathers) and the superscript denotes whether they are left or right movers since they are massless particles. Here θ_B is a scale related to λ encoding the boundary interaction, $\lambda \rightarrow 0$ corresponds to $\theta_B \rightarrow -\infty$ and $\lambda \rightarrow \infty$ to $\theta_B \rightarrow \infty$. $K_{\epsilon\epsilon'}$ is related to the reflection matrices [13]. As usual we have

used rapidity variables θ to encode energy and momentum. For solitons and antisolitons for instance, $e = \pm p = \mu e^\theta$, μ an arbitrary energy scale.

The one point function of interest then reads $\langle 0 | \cos \frac{1}{2} \phi | B \rangle$. To use (9), we first need the matrix elements of the operator $\cos \frac{1}{2} \phi$ in the quasiparticle basis: these follow easily from the massive sine-Gordon form factors [5]. Unfortunately, as discussed briefly in [7], the resulting integrals are all IR divergent! This was not the case for the current operator, whose form factor has the naive engineering dimension of energy, leading to convergent integrals. Some sort of regularization is needed, and the correlations of $\cos \frac{1}{2} \phi$ with a boundary have so far remained inaccessible. Our purpose is to show how to cure this problem.

To explain our strategy, we first consider the case $g = 1/2$. Here, the Friedel oscillations are simply [10] related to the spin-one point function in an Ising model with boundary magnetic field. By using the same approach as that outlined before, one finds the following form-factors expansion

$$\langle \sigma(x) \rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_{-\infty}^{\infty} \prod_{i=1}^n \left\{ \frac{d\theta_i}{2\pi} \tanh \frac{\theta_B - \theta_i}{2} e^{-2\mu x e^{\theta_i}} \right\} \prod_{i < j} \left(\tanh \frac{\theta_i - \theta_j}{2} \right)^2. \quad (10)$$

The integrals are all divergent at low energies, when $\theta_i \rightarrow -\infty$ and the integrand tends to a constant. Let us then introduce an IR cut-off (we chose $\theta \geq \theta_{\min}$ and set $\Lambda \equiv e^{\theta_{\min}}$) and take the log of the previous expressions (a similar method has been used in [5] to study the UV limit of massive correlators, see also [15, 16]). Ordering this log by increasing number of integrations, one can show that each term diverges as $\ln \Lambda$. Moreover, since the divergence occurs at very low energy, where the tanh goes to unity, the amplitudes of these $\ln \Lambda$ do *not* depend on θ_B (for $\theta_B \neq -\infty$), i.e. on the boundary coupling. It is then easy to get rid of the cut-off: we simply subtract the log of the IR spin function, i.e. we subtract the same formal expression with $\theta_B = \infty$. The first two terms of the resulting expression read

$$\ln \frac{\langle \sigma(x) \rangle_{T_B}}{\langle \sigma(x) \rangle_{\text{IR}}} = \int_{\Lambda}^{\infty} \frac{du}{2\pi u} e^{-2ux} \left(\frac{T_B - u}{T_B + u} - 1 \right) + \frac{1}{2} \int_{\Lambda}^{\infty} \prod_{i=1}^2 \frac{du_i}{2\pi u_i} e^{-2\mu u_i x} \left(\prod_{i=1}^2 \frac{T_B - u_i}{T_B + u_i} - 1 \right) \times \left[\left(\frac{u_1 - u_2}{u_1 + u_2} \right)^2 - 1 \right] + \dots \quad (11)$$

where we have set $\mu = 1$, $u_i = e^{\theta_i}$, $T_B = e^{\theta_B} \propto \lambda^{1/(1-g)}$.

Clearly, the integrals are now convergent at low energies, and we can send Λ to zero. Since the IR value of the one point function is easily determined by other means, $\langle \sigma(x) \rangle_{\text{IR}} \propto x^{-1/8}$ [17], we can now obtain $\langle \sigma(x) \rangle_{T_B}$ from (11). Hence the procedure involves a *double* regularization. Of course, there remains an infinity of terms to sum over. However, as in the case of current operators, the convergence of the form-factors expansion is very quick, and the first few terms are sufficient to obtain excellent accuracy all the way from UV to IR. To illustrate this more precisely, we recall that for $g = 1/2$ (11) can be resummed in closed form, giving rise to

$$R_{\text{exact}} = \frac{\langle \sigma(x) \rangle_{T_B}}{\langle \sigma(x) \rangle_{\text{IR}}} = \frac{1}{\sqrt{\pi}} \sqrt{2x T_B} e^{x T_B} K_0(x T_B). \quad (12)$$

By re-exponentiating the two first terms in (11), one obtains a ratio differing from (12) by at most 1/100 for $x T_B \in [0, \infty)$ (see figure 1).

By re-exponentiating the first three terms, accuracy is improved to more than 1/1000. Clearly, the form-factors approach thus provides analytical expressions that can be considered as exact for most reasonable purposes.

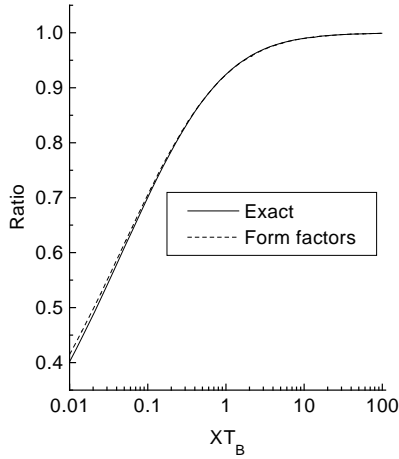


Figure 1. Accuracy of finite T_B over the IR part of the envelope of $\rho(x)$ for $g = 1/2$.

It is fair to mention, however, that, at any given order in (11) the exponent controlling the $x \rightarrow 0$ behaviour is not exactly reproduced, as can be seen on a log–log plot. For instance, the first term is immediately found to produce a behaviour $R(x) \propto x^{1/\pi}$, to be compared with the result $R_{\text{exact}}(x) \propto x^{1/2} \ln x$. The comparison of the exact result (12) and of (11) show that the form-factors expression has, term by term, the correct asymptotic expansion, i.e. the IR expansion in powers of $1/xT_B$. Adding terms with more form factors simply gives a more accurate determination of the coefficients. This is to be compared with the results of [7], for example, the frequency-dependent conductance, where the form-factors expression has the correct functional dependence both in the UV and in the IR. This is not to say that our method is inefficient in the UV, because we know, at least formally, all the terms. In fact, we will show in what follows how (11) can always be resummed in the UV, and that the exponent can also be exactly obtained from our approach.

The regularization is the same for other values of g . Here, we discuss $g = 1/t$ with t an integer. For these values, the scattering is diagonal and the form factors are rather simple. To obtain them, we take the massless limit of the results in [5] and impose that half of the quasiparticles become right movers and half become left movers, since the boundary state always involve pairs of right and left moving particles. It is in fact easier to take that limit if we change basis from the solitons and antisolitons to $(1/\sqrt{2})(|S\rangle \pm |A\rangle)$. In that case, the boundary scattering matrix becomes diagonal and the isotopic indices always come in pairs. The reflection matrices in this new basis are given by

$$\begin{aligned} K_-(\theta) &= -e^{i(\pi/4)(2-t)} \tanh\left(\frac{(t-1)\theta}{2} + i\frac{\pi(t-2)}{4}\right) R\left(i\frac{\pi}{2} - \theta\right) \\ K_+(\theta) &= e^{i(\pi/4)(2-t)} R\left(i\frac{\pi}{2} - \theta\right) \end{aligned} \quad (13)$$

with

$$R(\theta) = \exp\left(i \int_{-\infty}^{\infty} \frac{dy}{2y} \frac{\sin(2(t-1)y\theta/\pi) \sinh((t-2)y)}{\sinh(2y) \cosh((t-1)y)}\right). \quad (14)$$

The breathers reflection matrices are given in [18].

The case $g = 1/2$ has already been worked out, so let us concentrate on $g = 1/3$ as an example. Then, in addition to the soliton and antisoliton, there is also one breather. The first contribution to the one point function comes from the two-breather form factor, with one right moving and one left moving breather. It is given by a constant,

$$f(\theta, \theta)_{11}^{\text{LR}} = c_1 \quad (15)$$

and this obviously leads to IR divergences. Other contributions come from $2n$ -breather form factors, and $4n$ -soliton form factors. The whole expression can be controlled, as for $g = 1/2$, by taking the log and factoring out the IR part. Setting $c(x) = \cos \frac{1}{2}\phi(x)$, we organize the sum as follows:

$$\ln \frac{\langle c(x) \rangle_{T_B}}{\langle c(x) \rangle_{\text{IR}}} = \ln R^{(2)} + \ln R^{(4)} + \dots \quad (16)$$

with the subscript denoting the number of intermediate excitations.

Then, using the explicit expressions for $g = 1/3$ we find

$$\ln R^{(2)} = 2c_1 e^{2\sqrt{2}T_B x} \text{Ei}(-2\sqrt{2}T_B x) \quad (17)$$

where Ei is the standard exponential integral. The next term $\ln R^{(4)}$ is a bit bulky to be written here, but is very easy to obtain—similar expressions have been explicitly given in [7]. This is all that is needed for an accuracy better than 1%. In figure 2 we present the results of the ratio at $g = 1/2, 1/3, 1/4$ for the Friedel oscillations. It should be noted that this ratio is just the pinning function of [8] and our results agree well qualitatively with the results found there.

As mentioned before, the deep UV behaviour is a little more difficult to obtain: the accuracy is good because the ratio goes to zero anyway, but the numerical evaluation of the power law is not very accurate with the number of terms we consider. Fortunately, the full form-factors expansion allows the analytic determination of this exponent. First, observe for instance that in (11) the integrals converge for all $T_B \neq 0$, but strictly at $T_B = 0$ they do not. To find the dependence of $\langle c(x) \rangle$ as $T_B \rightarrow 0$, we will consider the logarithm of another ratio, $\ln(\langle c(x) \rangle_{T_B} / \langle c(x') \rangle_{T_B})$, where x and x' are two arbitrary coordinates. For this ratio, even at $T_B = 0$, the integrals are convergent. But $T_B = 0$ is the UV fixed point, with Neumann boundary conditions. While the one point function $\langle c(x) \rangle_{\text{UV}}$ vanishes, the ratio of two such one point functions is well defined, and can be computed by adding an IR cut-off (a finite system). One finds that it goes as $(x/x')^{g/2}$. By regularity, as $T_B \rightarrow 0$, the same is true for the ratio close to $T_B = 0$, and thus one has

$$\langle c(x) \rangle \propto (xT_B)^{g/2} \quad x(T_B) \rightarrow 0. \quad (18)$$

This shows that the universal scaling function in (8) behaves as $F(y) \propto y^{g/(1-g)}$ for $g < 1/2$. This exponent can actually be obtained by perturbation theory. Indeed, the first term in the perturbative expansion of $\langle c(x) \rangle$ is

$$\lambda x^{g/2} \int_{-\infty}^{\infty} \frac{dy}{(x^2 + y^2)^g}. \quad (19)$$

For $g < 1/2$, this integral diverges in the IR. To regulate it, we need to put a new cut-off: since there is no other length scale in the problem, this can be nothing but $1/T_B$. Changing variables, the leading behaviour is $x^{g/2} T_B^g \propto x^{g/2} \lambda^{g/1-g}$, in agreement with the previous discussion.

The leading behaviour was studied numerically in [8]; the resulting estimates of the exponent (called δ_g there) are considerably smaller than the exact result ($\delta_g = g$) following

from the foregoing discussion: presumably, the short distance behaviour is more difficult to control numerically than the error bars of [8] indicate.

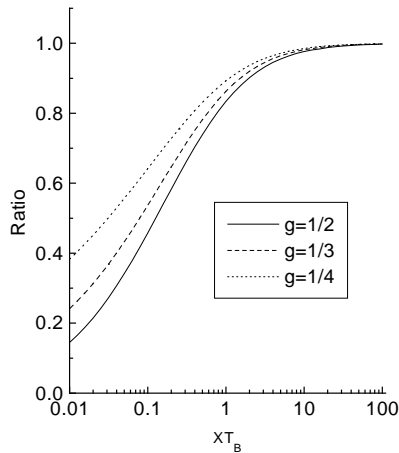


Figure 2. Ratio of finite T_B over the IR part of the envelope of $\rho(x)$.

The function $F(y)$ behaves as $y \ln y$ for $g = 1/2$. For $g > 1/2$, its behaviour is simply $F(y) \propto y$, as can be easily shown since the perturbative approach is now convergent.

The method presented here is very successful in obtaining analytical results for $g \leq 1/2$ —although we have limited ourselves to $g = 1/t$ with t an integer, all values of $g < 1/2$ are accessible, but computations are more complicated since the bulk scattering is non-diagonal. The method should be generalizable to other problems, in particular the determination of the screening cloud in the anisotropic Kondo model [19], as will be reported elsewhere. The region $g > 1/2$ presents additional difficulties, unresolved for the moment—in particular, the massless limit of the form factors does not seem to be meaningful. Of course the case $g = 1$ can be solved by fermionization. In our approach, this point is non-trivial because of the folding. This folding, however, is necessary for any value $g \neq 1$: except at $g = 1$, the problem on the whole line would not be integrable otherwise.

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