Friedel oscillations in a Luttinger liquid with long-range interactions

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Abstract

We introduce a path-integral approach that allows to compute charge density oscillations in a Luttinger liquid with impurities. We obtain an explicit expression for the envelope of Friedel oscillations in the presence of arbitrary electron-electron potentials. As examples, in order to illustrate the procedure, we show how to use our formula for contact and Coulomb potentials.

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In the last years there has been much activity addressed to the study of condensed matter and statistical mechanics problems through field-theoretical methods [1]. In particular the physics of one-dimensional (1d) systems of strongly correlated particles has become a very interesting subject since one can take advantage of the simplicity of the models at hand and, at the same time, expect to make contact with experiments. For instance, the recently built quantum wire [2] is a good realization of a 1d electron gas. From the theoretical side, the simplest formulation of a 1d electronic system is given by the Tomonaga-Luttinger (TL) model [3] which has been successful in describing some qualitative features of a Luttinger liquid such as spin-charge separation and non-universal exponents in the decay law of correlation functions [4]. There are, however, two crucial issues that are not considered in the original versions of this model: the presence of a non trivial interaction between electrons and impurities [5] and the effect of long-range (LR) electron-electron interactions [6] [7]. As it is well known, the former leads to the occurrence of Friedel oscillations in the charge density profile, at least for Fermi liquids [8]. On the other hand, as the dimensionality of a system decreases, charge screening effects become less important and the LR interaction between electrons is expected to play a central role in determining the properties of the system. In fact, from a theoretical point of view, the effects of LR interactions have been recently discussed in connection to several problems such as the Fermi-edge singularity [9], the insulator-metal transition [10] and the role of the lattice through umklapp scattering and size dependent effects [11]. Thus, it is quite interesting to study the interplay between impurities and LR interactions by considering Friedel oscillations in a 1d system. Some time ago, Egger and Grabert [12] analyzed this phenomenon. By combining the techniques of standard bosonization [13] with the self-consistent harmonic approximation [14] and quantum Monte Carlo simulations [15], they were able to get explicit results for both weak and strong impurity scattering regimes. Later on, the authors of Ref. [16] used bosonization and a scattering description to get some exact results for the short-range case and for a special value of the coupling constant, equivalent to the so called ”Toulouse point” in the anisotropic Kondo problem. More recently, the authors of Ref. [17] used again standard bosonization to address the same problem emphasizing the equivalence between the TL model in the presence of a single non-magnetic impurity and a boundary Sine-Gordon model.
In this work we present an alternative approach to this problem based on
a path-integral bosonization technique previously developed in the context
of non local quantum field theories [18]. This method seems to be specially
adequate to consider LR interactions. Indeed, it has recently provided a
straightforward derivation of the electronic Green’s function in the presence
of non contact potentials [19]. Then, our main purpose here is to show how
to extend this formulation to the computation of Friedel oscillations.

We start from a modified non local Thirring model [20] described by the
following (Euclidean) Lagrangian density:

\[ L = i \bar{\Psi} (\partial + \gamma_0 k_F) \Psi + \int d^2 y J_\mu(x) U(\mu)(x, y) J_\mu(y) + \bar{\Psi} \gamma_\mu \Psi - M(x) \bar{\Psi} \Psi \]  

(1)

where \( x = (\tau_x, x) = (x_0, x_1) \), and \( J_\mu = \bar{\Psi} \gamma_\mu \Psi \). The functions \( U(\mu)(x, y) \) are
forward-scattering potentials. Setting \( U(0) = U(1) = -\delta^2 (x - y) \) one gets
the covariant and local version of the Thirring model usually studied in the
context of (1+1) QFT’s.

On the other hand, the choice \( U(0)(x, y) = U(|x - y|) \delta(\tau_x - \tau_y) \)
and \( U(1)(x, y) = 0 \), yields the simplest version of the Tomonaga-Luttinger (TL) model with
an instantaneous distance dependent potential and no current-current fluc-
tuations. The last two terms in (1) correspond to forward and backward
electron-impurity scattering, respectively.

The main purpose of the present paper is to evaluate the v.e.v. of the charge-
density:

\[ \langle \rho(x) \rangle = \langle \bar{\Psi} \Psi + e^{-2ik_F x} \bar{\Psi}_R \Psi_L + e^{2ik_F x} \bar{\Psi}_L \Psi_R \rangle, \]  

(2)

for an arbitrary electron-electron potential \( U(\mu)(x, y) \). Also we will be spe-
cially interested in case that the impurity terms are \( C_0(x) = V \delta(x - d) = M(x) \)
and \( C_1(x) = 0 \), where \( V \) is a constant proportional to the impurity
tunneling barrier situated at \( x = d \). Using a suitable representation of the
functional delta and introducing an auxiliary vector field \( A_\mu \) (see Ref. [18]
for details), the partition function of the model under consideration reads

\[ Z = N \int \mathcal{D} A_\mu e^{-S[A]} det \left( i \partial + \sqrt{2} A + C + \gamma_0 k_F - M(x) + s_\mu \epsilon_{\mu\nu} e^{2ik_F x} \Gamma_\nu \right) \]

(3)
where $S[A]$ is the free quadratic action for $A_\mu$, $\Gamma_0 = \Gamma$ and $\Gamma_1 = \gamma_5$. Equation (3) can be obtained by functional derivation of Eq. (3) with respect to the source $s_0$.

As it is known, the massive-like determinant in equation (3) cannot be exactly solved, even in the local case. However, we can take advantage of the fact that the vacuum to vacuum functional can be written in such a way that non local terms are not present in the determinant. Therefore the terms $\sqrt{2}A + \mathcal{C} + \mathcal{J} + i\gamma_0 k_F$ can be decoupled from fermions by performing chiral and gauge transformations in the fermionic path-integral measure. Indeed, decomposing $A_\mu(x)$ in longitudinal and transverse pieces

$$A_\mu(x) = \epsilon_{\mu\nu}\partial_\nu \left( \Phi(x) - \frac{ik_F x}{\sqrt{2}} + \partial_\mu \eta(x) - \frac{1}{\sqrt{2}}(C_\mu(x) + s_\mu(x)) \right), \quad (4)$$

where $\Phi$ and $\eta$ are boson fields (to be associated to the normal modes of the system) and applying, as anticipated, functional bosonization techniques [18] to express the fermionic determinant in terms of $\Phi$ and $\eta$, one finally obtains

$$Z = N \int \mathcal{D}\bar{\chi}\mathcal{D}\chi\mathcal{D}\Phi\mathcal{D}\eta \exp(-S_{bos}) \exp(-S_{fer}) \exp(-S[M,s_\mu]), \quad (5)$$

where $S_{fer}$ corresponds to free massless fermions ($\chi$ and $\bar{\chi}$) and

$$S[M,s_\mu] = \int d^2x \bar{\chi}(s_\mu(x)\epsilon_{\mu\nu}e^{2ik_F x_\nu} - M(x))e^{-2\gamma_5 \Phi} \chi. \quad (6)$$

Concerning $S_{bos}$, it can be more briefly described in momentum space:

$$S_{bos} = \int \frac{d^2p}{(2\pi)^2} \left( \hat{\Phi}(p) \quad \hat{\eta}(p) \quad \hat{C}'(p) \right) \left( \begin{array}{ccc} A(p) & C(p) & E(p) \\ \frac{C(p)}{2} & B(p) & F(p) \\ \frac{E(p)}{2} & \frac{F(p)}{2} & D(p) \end{array} \right) \left( \begin{array}{c} \hat{\Phi}(-p) \\ \hat{\eta}(-p) \\ \hat{C}'(-p) \end{array} \right) + \frac{ik_F}{2} \int \frac{d^2p}{(2\pi)^2} \hat{U}^{-1}_{(0)}(p)\hat{C}'_{(0)}(p)\delta^2(p), \quad (7)$$

where we have defined $C'_\mu = C_\mu + s_\mu$ and $A(p), B(p), C(p), D(p), E(p)$ and $F(p)$ are potential dependent functions (See [20] for more details).

At this point we see that the generating functional can be formally expanded in powers of $(M - s_\mu\epsilon_{\mu\nu}e^{2ik_F x_\nu})$, in complete analogy with the usual procedure employed in the path-integral bosonization of $(1+1)$ massive QFT’s [21] [22]. In fact, the $x$ dependence of this perturbative parameter, together with
the appearance of $C'_\mu(x)$ in the bosonic action are two of the new features of the present computation. As far as these functions are well-behaved one can assume the existence of every term in the corresponding series.

From now on we will specialize the computation to the case $s_1 = 0$. This allows to define $M_\pm(x) = M(x) - s_0(x)e^{\pm 2ik_Fx}$ and one can then perform the above mentioned expansion of $Z$ taking $M_\pm(x)$ as perturbative parameters. As explained in Ref. [20] one can show that the same expansion can be obtained by starting from a purely bosonic non local extension of the sine-Gordon model given by

$$L' = \frac{1}{2}(\partial_\mu \varphi)^2 + \frac{1}{2} \int d^2 y \partial_\mu \varphi(x) d(\mu)(x,y) \partial_\mu \varphi(y) +$$
$$+ F_\mu \partial_\mu \varphi - \frac{1}{2\beta^2} \left( \alpha_+(x) e^{i\beta \varphi(x)} + \alpha_-(x) e^{-i\beta \varphi(x)} \right)$$  \hspace{1cm} (8)

where $F_\mu(x)$ represents a couple of classical functions to be related to the $C'_\mu$’s and $d(\mu)(x,y)$ are two bilocal functions that will be associated to the electron-electron potentials (a similar non locality in the kinetic term was considered in the study of the influence of LR correlations in the metal-insulator transition [23]). \(\beta\) is a constant and \(\alpha_\pm(x)\) are functions that can be considered as extensions of the parameter \(\alpha_0\) used by Coleman [24]. Indeed, for $d(\mu) = 0 = F_\mu$ and $\alpha_+ = \alpha_- = \alpha_0 = constant$, the model above coincides with the usual sine-Gordon model. In the present approach the quantities $\alpha_\pm(x)$ are related to $M_\pm(x)$, which are in turn connected to the strength of the scatterer. Let us stress that in our formulation it is straightforward to consider a non point-like impurity ($\alpha_\pm(x) \neq V \delta(x - d)$). However, in order to illustrate our method, in this paper we will consider the usual case of a completely localized impurity. For this particular case Eq. (8) contains the same terms that can be derived from standard bosonization (See for instance [12]).

Now, going to momentum space and employing standard procedures to evaluate each v.e.v., the partition function $Z'$ corresponding to this generalized sine-Gordon model coincides with $Z$ provided that the following three relations hold:

$$\frac{2\pi}{\pi [p_0^2 \hat{U}(1)(p) + p_1^2 \hat{U}(0)(p)] + p^2} = \frac{\beta^2}{2[p^2 + \hat{d}(0)(p)p_0^2 + \hat{d}(1)(p)p_1^2]},\hspace{1cm} (9)$$
\[
\frac{\alpha_\pm(x)}{\beta^2} = M_\pm(x) = M(x) - s_0(x)e^{\mp 2ik_F x} \tag{10}
\]

\[
\frac{2i\dot{C}_\mu(-p)\epsilon_{\mu\nu}p_\nu}{\pi [p_0^2 U(1)(p) + p_1^2 U(0)(p)] + p^2} = \frac{\beta \dot{F}_\mu(-p)p_\mu}{p^2 + d_0 p_0^2 + d_1 p_1^2}. \tag{11}
\]

Therefore, we have obtained an equivalence between the partition functions \(Z\) and \(Z'\) corresponding to the non local Thirring and sine-Gordon models with extra interactions defined above. This means that we can use \(Z'\) together with the above conditions in order to compute the charge-density in the Luttinger liquid in the presence of impurities. Indeed, as a result of this bosonization technique we can evaluate \(<\rho(x)\>\) through functional derivation of \(Z'\) instead of \(Z\). In so doing we obtain

\[
\langle \rho(x) \rangle = \langle \frac{i}{\sqrt{\pi}} \partial_x \varphi(x) + \cos(2\sqrt{\pi} \varphi(x) - 2k_F x) \rangle \tag{12}
\]

where the v.e.v. is taken with respect to the Lagrangian density \(\mathcal{L}'[s_0 = 0]\) obtained from (8) after using equations (9), (10) and (11) and setting \(s_0 = 0\). Note that we have also set \(\beta = 2\sqrt{\pi}\).

Let us remark that there is an additional contribution to Eq. (12), coming from the functional derivative of the normalization constant \(N'[\mathcal{C}']\) with respect to \(s_\mu\). Since this quantity is a constant, its only effect is to shift the background value of the charge density. For this reason we have just disregarded it.

Now we return to our main goal, that is to use the path-integral framework depicted above in order to obtain an explicit formula for the charge-density in a Luttinger liquid with an arbitrary electron-electron and electron-impurity interactions. When one imposes these conditions in \(\mathcal{L}'[s_0 = 0]\) one gets a Lagrangian density which has an undefined parity as functional of \(\varphi\). However it is much simpler to work with an even Lagrangian since in this case all v.e.v.’s of odd functions of \(\varphi\) will vanish. It is easy to see that the translation \(\varphi(x) \rightarrow \varphi(x) + f(x)\) yields an even Lagrangian \(\mathcal{L}'_{even}\) provided that the classical function \(f(x)\) is \(\tau_x\)-independent and its gradient satisfies:

\[
\partial_x f(x) + \frac{2}{\pi} \int dy U(x - y) \partial_y f(\tau_x y) + \frac{i}{\sqrt{\pi}} V \delta(x - d) = 0. \tag{13}
\]
We then get
\[ \langle \rho(x) \rangle = \frac{i}{\sqrt{\pi}} \text{\partial}_x f + \cos(\sqrt{4\pi} f(x) - 2k_F x) \langle \cos(\sqrt{4\pi} \varphi(x)) \rangle \mathcal{L}^\prime_{\text{even}}, \]  
(14)

where \( \cos(\sqrt{4\pi} f(x) - 2k_F x) \) is called the Friedel oscillation and \( A(x) = \langle \cos(\sqrt{4\pi} \varphi(x)) \rangle \mathcal{L}^\prime_{\text{even}} \) is the corresponding envelope.

Let us point out that Eq. (13) has been previously found in Ref. [17]. As shown by these authors, in the short-range case it has the solution \( f = \text{constant} \propto U \) whose only effect is to add a constant phase in the cosine term associated to the Friedel oscillation. A non trivial phenomenon takes place for LR potentials, since the cosine ceases to be a periodic function. This nonperiodicity effect, although weak at large distances, could eventually be observed in carbon nanotubes [25].

From now on we shall focus our attention on the computation of the envelope of the oscillation. Since \( \mathcal{L}^\prime_{\text{even}} \) is not exactly solvable, we shall employ the well-known self-consistent harmonic approximation [14], which amounts to replacing \( \mathcal{L}^\prime_{\text{even}} \) by
\[ \mathcal{L}_{\text{SCHA}} = \frac{1}{2} (\partial_\mu \varphi)^2 + \frac{1}{\pi} \int dy \partial_x \varphi(\tau_x, x) U(x-y) \partial_x \varphi(\tau_x, y) + \frac{m(V)}{2} \delta(x-d) \varphi^2 \]  
(15)

where \( m(V) \) is a constant, related to the impurity strength, to be variationally determined. The precise relationship between \( m(V) \) and \( V \) was obtained in Ref. [12]. For instance, in the strong-scattering limit, when \( V \) is much larger than a certain bandwidth, one has simply \( m = V \) (See also Ref. [17]).

Let us now consider the computation of \( A(x) \) using this approximation. Performing a translation in the field \( \varphi(x) \rightarrow \varphi(x) + a(x) \), with \( a(x) \) a classical function, we find \( A(x) = \exp i \sqrt{\pi} a(x) \).

Going to momentum space we see that the Fourier transform of \( a(x) \) satisfies an integral equation whose solution is
\[ \hat{a}(p) = \frac{2i \sqrt{\pi}}{p^2 + p^2_{1} 2U(p_1)} e^{-ip_\mu x_\mu} \left( 1 - \frac{me^{ip_1r} I(p_0, r)}{\pi + mI(p_0, 0)} \right) \]  
(16)

with
\[ I(p_0, r) = \int_0^\infty dq_1 \frac{\cos(q_1 r)}{p_0^2 + q_1^2 (1 + \frac{2U(q_1)}{\pi})}, \]  
(17)

\[ \text{with} \]
where we defined \( r = |x - d| \).

The envelope of the Friedel oscillation then reads

\[
A(r) = \exp \left( -\frac{1}{\pi} \int_{-\infty}^{\infty} dp_0 \left( I(p_0, 0) - \frac{m I^2(p_0, r)}{\pi + m I(p_0, 0)} \right) \right),
\]

which is our main formal result. Indeed, formulae (17) and (18) give an analytical expression (exact within the gaussian approximation) for \( A(r) \) as functional of both the electron-electron potential and the variational parameter \( m(V) \). Since the self-consistent harmonic approximation seems to fail for weak impurity strength, due to the neglect of interwell tunneling \[12\], we restrict our analysis to the strong impurity regime. We also consider a large distance approximation of Eq. (17) which consists of inserting \( 1/r \) as infrared cutoff. Let us call \( I_r(p_0, r) \) the integral (17) regulated in this way.

We will examine, as examples, two specific short range and Coulomb potentials. This, in turn will allow us to illustrate how to use our general formula (18) for other cases. Moreover, since these problems were previously considered in Refs. \[12\] and \[17\] by using standard (operational) bosonization, our computation will give an independent confirmation by means of a different approach. First of all we note that it is convenient to split out the two terms of the exponential factor on Eq. (18), such that

\[
A(r) = \exp \left( T(r) + W(r) \right).
\]

For the simple contact potential \( U(q_1) = U = \text{constant} \), we get

\[
T(r) = \ln(\Lambda r)^{-g}
\]

and

\[
W(r) = g \exp(mg^2 r) E_i(-mg^2 r) - g \exp(2g) E_i(-2g)
\]

where \( \Lambda \) is an ultraviolet cutoff. We have also introduced the interaction constant \( g = (1 + \frac{2U}{\pi})^{-\frac{1}{2}} \). Taking into account the asymptotic behaviour of the exponential integral function \( E_i \) for \( mg^2 r >> 1 \), one obtains

\[
A(r) = \mathcal{C}(g, \Lambda) (2g r)^{-g} \exp\left(-\frac{1}{mg r}\right)
\]

which coincides with Refs. \[12\] and \[17\] under the same regime.

In the Coulombian case, one has \( U(|x|) = U/\sqrt{|x|^2 + b^2} \), whose Fourier transform is \( U(q_1) = 2UK_0(bq_1) \), where \( b \) plays the role of a lattice spacing.
Inserting this expression in $T$ and $W$, and considering the same regime as before we find that $W$ vanishes and

$$T(r) = -\frac{\pi}{2U} \left( \sqrt{1 - \frac{4U}{\pi} \ln \frac{b}{2r}} - \sqrt{1 - \frac{4U}{\pi} \ln \frac{b\Lambda}{2}} \right) \quad (22)$$

which yields

$$A(r) = C'(g, b, \Lambda) \exp \left( -\sqrt{\frac{\pi}{U}} \ln \frac{r}{b} \right). \quad (23)$$

Again, this behaviour is equal to the one previously found in Refs. [12] and [17].

In summary, we have described an alternative bosonization approach to the computation of charge-density fluctuations. This technique, previously originated in the context of QFT’s, parallels, in the path-integral framework, the operational schemes usually employed in condensed matter applications. In particular, we have computed the envelope of Friedel oscillations in a simple version of the TL model with a non-magnetic impurity. By combining that bosonization procedure and the self-consistent harmonic approximation we were able to express the envelope of the oscillations as a functional of the electron-electron interaction (see Eqs. (17) and (18)). Finally, as a consistency check of this formal result, and in order to illustrate our method, we considered the long-distance regime for contact interactions and Coulomb potentials. Our results are in agreement with Refs. [12] and [17].

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