Friedel Oscillations for Interacting Fermions in One Dimension

Reinhold Egger and Hermann Grabert
Fakultät für Physik, Albert-Ludwigs-Universität, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany
(Received 25 April 1995)

We study Friedel oscillations in one-dimensional electron liquids for arbitrary electron-electron interaction and arbitrary impurity strength. Explicit results for spinless as well as spin-$\frac{1}{2}$ electrons are given. In the case of Luttinger-liquid leads, the Friedel oscillations decay as x^{-g} far away from the impurity where g is the interaction constant. For a weak scatterer, a slower decay is found at small-to-intermediate distances from the impurity, with a crossover to the asymptotic x^{-g} decay.

PACS numbers: 72.10.–d, 73.40.Gk

Quasi-one-dimensional (1D) interacting fermion systems have attracted renewed attention recently, partly due to the technological relevance of such systems. They are also appealing because of the existence of exact solutions for simple models [1–9]. The striking non-Fermi-liquid behavior of 1D electrons is most clearly exhibited in transport properties, especially in the presence of impurities or barriers [6]. Usually, the case of either a very weak or an almost insulating barrier has been studied explicitly. The crossover between these two regimes, however, has rarely been looked at despite its importance for several fundamental issues, e.g., pinning of a Wigner crystal [10] or charge density waves [11], breakdown of charging effects with increasing tunnel conductance [12], or transport in 1D quantum wires or heterostructure channels [13]. In this Letter, we discuss several aspects of this crossover, in particular, properties of the screening cloud around the impurity.

The presence of an impurity in a metal is known to cause Friedel oscillations in the density profile due to the sharp Fermi surface [14,15],

$$\rho(r) \sim \cos(2k_F r + \delta)/r^d,$$

where k_F is the Fermi vector, d the dimensionality, r the distance from the impurity, and δ a phase shift. This result holds far away from the impurity and for a Fermi liquid only, and in 1D the question arises of how Friedel oscillations are affected by the presence of strong electron correlations. As pointed out by Matveev, Yue, and Glazman [7], for weakly interacting electrons in 1D, one can understand the zero-voltage anomaly and power-law temperature dependence of the nonlinear conductance [6] in terms of electron backscattering by Friedel oscillations. It is thus surprising how little attention has been devoted to the modification of Friedel oscillations by strong interactions.

We treat the 1D interacting electron liquid in the framework of standard bosonization [3–6]. This approach is appropriate for low temperatures where only excitations near the Fermi surface are relevant. The electron creation operator for spin $s = \pm$ at position x is expressed in terms of the boson fields $\theta_\mu(x)$ and $\phi_\mu(x)$ ($\mu = \rho, \sigma$), which arise as linear combinations of spin-up and spin-down fields,

$$\psi_s^\dagger(x) \sim \sum_{n=\pm 1} \exp\left(in\{k_F x + \sqrt{\pi/2}[\theta_\rho(x) + s\theta_\sigma(x)]\}\right) \times \exp\{i\sqrt{\pi/2}[\phi_\rho(x) + s\phi_\sigma(x)]\}. \quad (1)$$

The boson fields obey equal-time commutation relations

$$[\phi_\mu(x), \theta_\nu(x')] = -(i/2)\delta_{\mu\nu}\mathrm{sgn}(x - x'),$$

and the canonical momentum for the θ_μ field is $\Pi_\mu = \partial_x \phi_\mu$.

We are concerned with density distributions in the presence of impurities or barriers. The bosonized form of the density operator is [8]

$$\hat\rho(x) = \sqrt{2/\pi}\,\partial_x\theta_\rho(x) + \frac{2k_F}{\pi}\cos[2k_F x + \sqrt{2\pi}\,\theta_\rho(x)] \times \cos[\sqrt{2\pi}\,\theta_\sigma(x)] + \mathrm{const} \times \cos[4k_F x + \sqrt{8\pi}\,\theta_\rho(x)], \quad (2)$$

where the background charge $\rho_0 = 2k_F/\pi$ has been omitted. The three terms in Eq. (2) are (1) the long-wavelength contribution, (2) the $2k_F$ charge density wave part, and (3) the $4k_F$ Wigner component [4,8]. The Wigner component is not present in the spinless case, since two rightmovers have to be flipped into leftmovers simultaneously for this term to arise.

Assuming to be away from lattice or spin density wave instabilities, and neglecting electron-electron backscattering for the moment, the clean system is described by $H_0 = H_\sigma + H_\rho$ with

$$H_\rho = \frac{v_F}{2}\int dx\{\Pi_\rho^2(x) + [\partial_x\theta_\rho(x)]^2\} + \frac{1}{\pi}\int dx\,dx'\,U(x - x')\,\partial_x\theta_\rho(x)\,\partial_{x'}\theta_\rho(x'), \quad (3)$$

where v_F is the Fermi velocity and $\hbar = 1$. The spin part H_σ is identical to the charge part H_ρ with no interaction

0031-9007/95/75(19)/3505(4)$06.00

potential U and the ρ fields replaced by the σ fields. Here, $U(x)$ is a (screened) Coulomb interaction, and we will explicitly study a short-ranged potential (Luttinger liquid) [5] and a $1/r$ long-ranged potential [8,9].

Let us now consider a scattering potential. Assuming an essentially pointlike scatterer at $x = 0$, one finds

$$H_{\text{imp}} = V \cos[\sqrt{2\pi}\, \theta_\rho(0)] \cos[\sqrt{2\pi}\, \theta_\sigma(0)]. \quad (4)$$

Spin and charge parts are now coupled through this term [6]. Actual computations using the bosonized model $H_{\text{bos}} = H_0 + H_{\text{imp}}$ necessitate introduction of a cutoff parameter ω_c [16]. Increasing V/ω_c from zero to infinity corresponds to tuning the barrier from transmittance one down to zero. Near zero transmittance, the weak-link model used in Ref. [6] is reproduced by the instanton treatment of H_{bos}. One may also show [17] by direct comparison with the exactly solvable Fano-Anderson model that H_{bos} can reproduce the full crossover *quantitatively*, thus validating Eq. (4) for arbitrary V/ω_c. Although this comparison can be carried out only in the absence of Coulomb interactions, it implies that a complete description of the crossover is indeed possible using H_{bos}.

Friedel oscillations can be extracted from the generating functional

$$Z(x, \lambda_\mu) = \left\langle \exp\left[\sqrt{2\pi}\, i \sum_{\mu=\rho,\sigma} \lambda_\mu \theta_\mu(x) \right] \right\rangle, \quad (5)$$

where the average is taken over H_{bos}. Since the impurity influences θ_μ only at $x = 0$, we constrain $\theta_\mu(x = 0)$ to be equal to new fields, say, $q_\mu = \sqrt{2\pi}\, \theta_\mu(0)$. Representing these constraints by a Fourier functional integral, one can integrate out all $\theta_\mu(x)$ modes due to their Gaussian nature. In contrast to previous treatments of this problem, we keep explicit information about the electron liquid away from the barrier. The remaining auxiliary field integrations coming from the above constraints are Gaussian and hence also performed easily. In the end, one is left with the nontrivial average over the q_μ fields alone, which are coupled to each other through H_{imp}.

Collecting together all terms, we obtain

$$Z = \mathcal{B}(x, \lambda_\mu, V) \prod_{\mu=\rho,\sigma} W_\mu^{\lambda_\mu^2}(x). \quad (6)$$

The functions $W_\mu(x)$ are independent of the barrier height, since they do not participate in the q average,

$$W_\mu(x) = \exp\left(\frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{F_n^{(\mu)2}(x) - F_n^{(\mu)2}(0)}{F_n^{(\mu)}(0)} \right), \quad (7)$$

where $\beta = 1/k_B T$ and

$$F_n^{(\mu)}(x) = v_F \int_{-\infty}^{\infty} dk\, \frac{\cos(kx)}{\omega_n^2 + v_F^2 k^2 (1 + 2U_k \delta_{\mu\rho}/\pi v_F)}. \quad (8)$$

Here, $\omega_n = 2\pi n/\beta$ are the Matsubara frequencies and U_k is the Fourier transformed electron-electron interaction [18]. A Luttinger liquid is governed by the interaction constants $g_\sigma = 1$ and $g_\rho = g \le 1$ [5,6]. In that case, Eq. (8) becomes simply

$$F_n^{(\mu)}(x) = \frac{\pi g_\mu}{|\omega_n|} \exp\left[-\frac{|g_\mu \omega_n x|}{v_F} \right].$$

Finally, the quantity $\mathcal{B}$ in Eq. (6) is an average in q space; all dependency on impurity properties is contained in this factor. With Matsubara components $q_{\mu,n}$, we find

$$\mathcal{B}(x, \lambda_\mu, V) = \left\langle \prod_\mu \exp\left[\frac{i\lambda_\mu}{\beta} \sum_{n=-\infty}^{\infty} q_{\mu,n} \frac{F_n^{(\mu)}(x)}{F_n^{(\mu)}(0)} \right] \right\rangle_q .$$

The q bracket stands for an average taking the action

$$S[q_\mu] = \frac{1}{\beta} \sum_\mu \sum_{n=1}^{\infty} \frac{|q_{\mu,n}|^2}{F_n^{(\mu)}(0)} + V \int_0^\beta d\tau \cos[q_\sigma(\tau)] \cos[q_\rho(\tau)].$$

The first term is the standard influence functional [6]. From these equations (or generalizations with additional θ fields at some other position x'), one may obtain all desired information about density profiles and correlations in the presence of an arbitrarily high barrier. The results of Refs. [5,8] for the clean system ($V = 0$) are easily recovered. Similar expressions incorporating the ϕ fields reproduce the results of Refs. [6,9].

Let us now consider the expectation value $\langle \hat\rho(x) \rangle$. From Eq. (6), one finds $\langle \theta_\mu(x) \rangle = 0$. The long-wavelength part in $\hat\rho$ [first term in Eq. (2)] does not feel the impurity since H_{imp} does not contain forward scattering terms. However, Friedel oscillations follow for the $2k_F$ and (in the spin-$\frac{1}{2}$ case) for the $4k_F$ component in Eq. (2).

For a spinless Luttinger liquid, we obtain the Friedel oscillation

$$\langle \hat\rho(x) \rangle / \rho_0 = -P(|x|, g, V)\, W(|x|, g) \cos(2k_F x), \quad (9)$$

where $\rho_0 = k_F/\pi$. Evaluation of $\mathcal{B}$ gives the *pinning function*

$$P(x, g, V) = -\left\langle \cos\left[\frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-gx|\omega_n|/v_F} q_n \right] \right\rangle_q . \quad (10)$$

This function determines the amplitude of the Friedel oscillation and hence the ability of the scatterer to pin charge density waves.

In the following, we discuss the ground-state properties of the Friedel oscillation (9) in some detail. From Eq. (7), we find

$$W(x, g) = (1 + x/\alpha)^{-g}, \quad (11)$$

where $\alpha = v_F/2g\omega_c$ is a microscopic length scale, say, a lattice spacing. The properties of the pinning function P can be studied using either numerically exact quantum Monte Carlo (QMC) simulations or simple approximations. For transmittance one ($V = 0$), the "charge" q is free and $P = 0$. For zero transmittance ($V \to \infty$), the potential $V \cos q$ locks q at odd multiples of π, and P takes its maximal value, $P = 1$, for all x.

To estimate P for arbitrary V/ω_c, we first discuss a simple variational procedure based on a quadratic trial Hamiltonian [self-consistent harmonic approximation (SCHA)] [19,20]. Replacing the cosine term by a Gaussian with frequency Ω, Feynman's variational principle leads to the self-consistency equation

$$\Omega = V\left(1 + \frac{\omega_c}{2\pi g\Omega}\right)^{-g}. \quad (12)$$

Within the SCHA, Eq. (10) is a Gaussian average, and one finds

$$P(x,g,V) = \exp[-g\, e^{(x+\alpha)/x_0} E_1((x + \alpha)/x_0)] \quad (13)$$

with the exponential integral $E_1(y)$ [21] and the crossover scale

$$x_0 = \frac{\alpha}{2\pi g}\frac{\omega_c}{\Omega}. \quad (14)$$

In the strong-scattering limit, $\pi V/\omega_c \gg 1$, Eq. (12) yields $\Omega = V$. In this limit, only small fluctuations around the minima of the cosine potential are possible, with interwell tunneling being forbidden by an exponentially small WKB factor. Since x_0 is even smaller than α, see Eq. (14), the term "crossover" is not meaningful in this limit. Using asymptotic properties of $E_1(y)$, Eq. (13) becomes for $x \gg \alpha$

$$P = e^{-gx_0/x} \simeq 1, \quad (15)$$

in accordance with our QMC results and a recent study of Friedel oscillations by open boundary bosonization [22].

In the weak-scattering limit, $\pi V/\omega_c \ll 1$, the pinning function exhibits more structure. From Eq. (12) one has

$$\Omega = V\,(2\pi gV/\omega_c)^{g/(1-g)},$$

which together with Eq. (14) implies that the crossover scale goes to infinity as $V \to 0$, namely, $x_0 \sim V^{-1/(1-g)}$. For $x \gg x_0$, SCHA always gives $P \simeq 1$ according to Eq. (15). This failure is due to the complete neglect of interwell tunneling in the SCHA, as can be seen by considering the $x \to \infty$ value of the pinning function (10), $P_\infty = -\langle \cos\bar{q}\rangle_q$, where $\bar{q}$ is the time average value of the imaginary-time path $q(\tau)$. Without tunneling transitions $\bar{q}$ is an odd multiple of π and one finds $P_\infty = 1$ as predicted by SCHA. However, taking into account excursions to neighboring wells, it is readily seen that in general $P_\infty < 1$. Despite these shortcomings, the effective Gaussian treatment indicates that for weak scatterers there is a crossover, with a slower decay of the Friedel oscillation at intermediate distances than the asymptotic x^{-g} decay. In fact, Eq. (13) predicts $P \sim x^g$ for $x \ll x_0$.

To investigate the weak-scattering limit further, we have evaluated Eq. (10) in powers of V giving to lowest order

$$P(x,g,V) = \gamma_g \frac{\pi V}{\omega_c}\left(\frac{x}{\alpha}\right)^{1-g} + \mathcal{O}(V^3), \quad (16)$$

with $\gamma_g = (4^{g-1}/\pi)B(1/2, g - 1/2)$, where $B(x,y)$ is the Beta function [21]. This perturbative result is only valid for $g > 1/2$ (otherwise γ_g diverges). Furthermore, since higher orders of the perturbation series grow faster $\sim x^{n(1-g)}$ with $n = 3, 5, \ldots$, the lowest-order result (16) is only valid for $x \ll x_0$, where x_0 is found to be given by the SCHA crossover scale (14). Hence, for intermediate distance from the barrier, the Friedel oscillation decays *slower* than x^{-g}, namely, like x^{1-2g}. As a consequence, there is a nontrivial limit for the pinning function as $x \to \infty$ and $V \to 0$.

The behavior of the pinning function for arbitrary V/ω_c and g can be computed by means of QMC simulations. In Fig. 1, we show results for $g = 2/3$ and two (relatively small) barrier heights V. For small-to-intermediate x, our data display a power law $P \sim x^{\delta_g}$ with $\delta_{2/3} = 0.24 \pm 0.03$. This is in crude accordance with the perturbational result $\delta_g = 1 - g$ valid for weak interactions. On the other hand, for $x \gg x_0$, the pinning function P is essentially constant, and the asymptotic decay of the Friedel oscillation is therefore $\sim x^{-g}$. A similar behavior is found at $g = 1/3$, where direct perturbation theory is inapplicable. Figure 2 shows QMC results for the pinning function. The small-to-intermediate x behavior is again a power

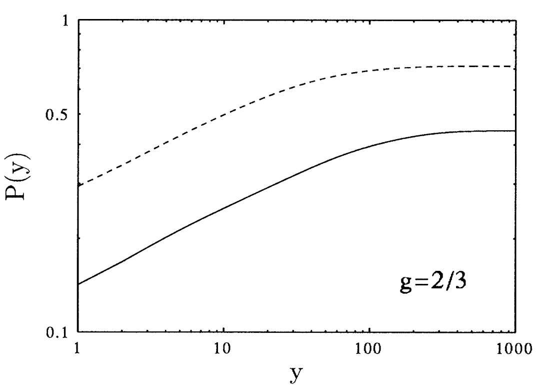

FIG. 1. QMC results for the pinning function $P(y)$ at $g = 2/3$ and two barrier heights: $V/\omega_c = 0.05$ (solid curve) and 0.1 (dashed curve). The dimensionless space variable is $y = \omega_c x/v_F$. Note the logarithmic scales.

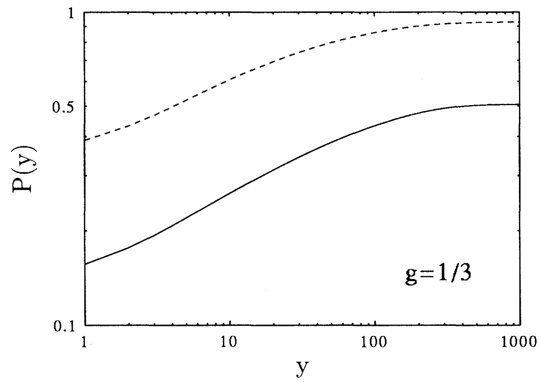

FIG. 2. QMC results for the pinning function $P(y)$ at $g = 1/3$ and two barrier heights: $V/\omega_c = 0.01$ (solid curve) and 0.05 (dashed curve).

law, now with exponent $\delta_{1/3} = 0.22 \pm 0.03$. This is in crude accordance with the SCHA prediction $\delta_g = g$, which holds for very strong interactions. Based on our numerical data, the exponents δ_g are independent of the barrier height, while the region where the intermediate decay is seen shrinks rapidly as V grows.

For spin-$\frac{1}{2}$ electrons, we find asymptotically a slightly faster decay $\sim x^{-(1+g)/2}$ at zero temperature. This can be rationalized by noticing that the additional spin channel has $g_\sigma = 1$ and the exponent $-g$ in Eq. (9) has to be replaced by $-(g_\sigma + g_\rho)/2$. Remarkably, for spin-$\frac{1}{2}$ electrons, there is also a $4k_F$ Friedel oscillation component

$$\langle \hat{\rho}(x) \rangle \sim \cos(4k_F x)\, x^{-2g},$$

which dominates over the $2k_F$ contribution for strong enough correlations, $g < 1/3$. Since $4k_F$ corresponds to the interparticle spacing, this suggests that for $g < 1/3$ signatures of Wigner crystal behavior are induced by the impurity.

Wigner crystal behavior has also been found by Schulz [8] for the clean system with long-ranged $1/r$ correlations. For $1/r$ interactions, the $4k_F$ Friedel oscillation decay is extremely slow. While the spin degrees of freedom involve again the $x^{-1/2}$ factor suppressing the $2k_F$ component, the $4k_F$ Friedel oscillations decay like $\exp(-c\sqrt{\ln x})$, i.e., slower than any power law. Effectively, one will then only observe the $4k_F$ component. In the spinless case, the same quasi-long-ranged behavior appears for the $2k_F$ component already because the spin channel is absent now.

Apparently, Friedel oscillations are always present in 1D for arbitrary electron-electron interaction. Moreover, due to reduced screening in low dimensions, their decay is always slower than the Fermi liquid $1/x$ prediction. We wish to stress that inclusion of backscattering is not expected to alter these findings substantially. In the spinless case, backscattering is treated as an exchange event of forward scattering and can be absorbed by a redefinition of g. The asymptotic decay of the Friedel oscillation is then always x^{-g}. In the spin-$\frac{1}{2}$ case, based on the renormalization group analysis [2], there are at most weak logarithmic corrections.

To conclude, we have computed the Friedel oscillations in an interacting 1D electron liquid. These results should show up in NMR experiments or as strong quasi Bragg peaks in x-ray scattering. They are also of relevance for studies of quasi-one-dimensional conductors at low doping concentrations, or the case of a magnetic impurity.

We wish to thank P. Riseborough, M. Sassetti, and U. Weiss for useful discussions.

[1] J. M. Luttinger, J. Math. Phys. **4**, 1154 (1963).
[2] J. Solyom, Adv. Phys. **28**, 201 (1979).
[3] A. Luther and I. Peschel, Phys. Rev. B **9**, 2911 (1975).
[4] V. J. Emery, in *Highly Conducting One-Dimensional Solids,* edited by J. T. Devreese *et al.* (Plenum, New York, 1979).
[5] F. D. M. Haldane, J. Phys. C **14**, 2585 (1981); Phys. Rev. Lett. **47**, 1840 (1981).
[6] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992); Phys. Rev. B **46**, 15 233 (1992).
[7] K. A. Matveev, D. Yue, and L. I. Glazman, Phys. Rev. Lett. **71**, 3351 (1993).
[8] H. J. Schulz, Phys. Rev. Lett. **71**, 1864 (1993).
[9] M. Fabrizio, A. O. Gogolin, and S. Scheidl, Phys. Rev. Lett. **72**, 2235 (1994).
[10] L. I. Glazman, I. M. Ruzin, and B. I. Shklovskii, Phys. Rev. B **45**, 8454 (1992).
[11] G. Grüner, *Density Waves in Solids* (Addison-Wesley, Reading, 1994).
[12] *Single Charge Tunneling,* edited by H. Grabert and M. H. Devoret, NATO ASI Ser. B, Vol. 294 (Plenum, New York, 1992).
[13] *Mesoscopic Phenomena in Solids,* edited by B. L. Al'tshuler *et al.* (North-Holland, Amsterdam, 1991).
[14] J. Friedel, Nuovo Cimento Suppl. **7**, 287 (1958).
[15] I. Tüttö and A. Zawadowski, Phys. Rev. B **32**, 2449 (1985).
[16] It is crucial to view ω_c as a physically meaningful bandwidth parameter instead of a regulator which has to be sent to infinity at any prize.
[17] R. Egger and H. Grabert (unpublished).
[18] We note that the $n = 0$ infrared divergence of Eq. (8) cancels in Eq. (7).
[19] Y. Saito, Z. Phys. B **32**, 75 (1978); M. P. A. Fisher and W. Zwerger, Phys. Rev. B **32**, 6190 (1985).
[20] A. O. Gogolin, Phys. Rev. Lett. **71**, 2995 (1993); N. V. Prokof'ev, Phys. Rev. B **49**, 2243 (1994).
[21] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1971).
[22] M. Fabrizio and A. O. Gogolin, Phys. Rev. B **51**, 17 827 (1995).