

# FRIEDEL OSCILLATIONS IN A ONE-DIMENSIONAL NON-INTERACTING ELECTRON GAS IN THE PRESENCE OF TWO IMPURITIES

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**ABSTRACT.** Using the linear response theory, we analyze Friedel oscillations in a one-dimensional non-interacting electron gas in the presence of two impurities with different potential strengths. The impurities potentials are modeled using Dirac delta function, as well as Lorentzian and Gaussian distribution functions. Our findings show that the density oscillations are strongly sensitive to both the distance between the impurities and their respective potential strengths.

**Keywords:** *One-dimensional electron gas, one impurity, two impurities, Friedel oscillations*

## INTRODUCTION

Friedel oscillations describe the oscillatory behavior of electron density around impurities in a material, arising from the quantum character of electrons and their interactions with the crystal lattice [1,2]. The electron density exhibits periodic oscillations as a function of distance from the impurity, with the wavelength depending on the Fermi wavevector. The amplitude of the oscillations decreases with increasing distance from the impurity, and temperature can reduce the amplitude of the oscillations. The specific form of the oscillations is affected by the shape and the curvature of the Fermi surface. Impurities in the crystal scatter electrons leading to

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perturbations of the electron density. The scattered electrons interfere giving rise to a standing wave pattern. Due to the Pauli exclusion principle, scattered electrons avoid regions where there are already other electrons, leading to formation of density oscillations. The distance dependence of charge oscillations is influenced by the dimensionality of the system. These oscillations can affect the electrical conductivity of materials, particularly in low dimensional systems, with graphene a special case [3]. The problem of Friedel oscillations in one-dimensional non-interacting electron gas in the presence of a single impurity was analyzed by Giuliani et al. [4], and later further extended to two impurities and a chain of dense impurities [5-7]. The Friedel oscillations have been theoretically studied in two- and three-dimensional electron Fermi liquids [8]. Additionally, Friedel oscillations in a nanowire symmetrically connected to two macroscopic electrodes with different chemical potentials have been investigated using the nonequilibrium Keldysh Green functions formalism [9]. The problem of Friedel oscillations in superconductors was also discussed within the framework of Bogoliubov-de Gennes theory [10]. More recently, Friedel oscillations in the presence of a non-Hermitian, imaginary impurity, have been studied using non-Hermitian linear response theory [11]. These theoretical results can be connected to experimental measurements, such as nuclear magnetic resonance [12], Mössbauer spectroscopy [13], scanning tunneling microscopy [14], and X-ray diffraction [15].

In this paper we analyze Friedel oscillations in a one-dimensional non-interacting electron gas, induced by two large impurities, modeled using Lorentzian and Gaussian distribution functions. The impurities have different potential strengths. The main goal of the present work is to study the effect of asymmetry in potential strengths on the Friedel oscillations. Additionally, we compare the numerically obtained results for the two models with the exact analytical results derived when the impurities are described by Dirac delta potentials.

## MODEL

The two impurities are first modeled with a Dirac delta function [4,5,7] of different potential strengths ( $C_1$  and  $C_2$ ):

$$V_{ext}^D(x) = C_1 \delta(x) + C_2 \delta(x - a), \quad (1)$$

where  $x$  and  $a$  represent the distance from the perturbing impurity and the distance between impurities, respectively. We approximate the Dirac delta potential  $V_{ext}^D(x)$  with a Lorentzian distribution function

$$V_{ext}^L(x) = \frac{C_1}{\pi} \frac{\varepsilon}{x^2 + \varepsilon^2} + \frac{C_2}{\pi} \frac{\varepsilon}{(x-a)^2 + \varepsilon^2}, \quad (2)$$

for small values of  $\varepsilon$  ( $\varepsilon \rightarrow 0^+$ ), and a Gaussian distribution function

$$V_{ext}^G(x) = \frac{C_1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} + \frac{C_2}{\sigma\sqrt{2\pi}} e^{-\frac{(x-a)^2}{2\sigma^2}}, \quad (3)$$

when  $\sigma \rightarrow 0^+$ , respectively.

In the linear response theory, the dependence of the electron density deviation on the distance is expressed as follows [4-8]:

$$n(x) = \int_0^\infty \frac{dq}{\pi} \chi_0(q) V_{ext}(q) \cos(qx), \quad (4)$$

where  $\chi_0(q)$  is the static Lindhard response function for one-dimensional non-interacting electron gas ( $\hbar = 1$ ):

$$\chi_0(q) = \frac{2m}{\pi q} \ln \left| \frac{2k_F + q}{2k_F - q} \right|, \quad (5)$$

where  $m$  is the electron mass, and  $k_F$  stands for the Fermi wave number. The Fourier transform of the perturbing impurities potential  $V_{ext}(q)$  is

$$V_{ext}^D(q) = C_1 + C_2 \cos(qa), \quad (6)$$

for the Dirac delta function. In the case of the Lorentzian and Gaussian distribution function based models, the Fourier transforms of the potentials are expressed as

$$V_{ext}^L(q) = [C_1 + C_2 \cos(qa)] e^{-\varepsilon|q|}, \quad (7)$$

and

$$V_{ext}^G(q) = [C_1 + C_2 \cos(qa)] e^{-\frac{\sigma^2 q^2}{2}}, \quad (8)$$

respectively. Using Eqs. (4)-(6) and applying the method outlined in Refs. [5-7], the electron density deviation can be analytically calculated as

$$n(x) = -\frac{2m}{\pi} \left\{ C_1 si(2k_F x) + \frac{C_2}{2} [si[2k_F(x+a)] + si[2k_F(x-a)]] \right\}, \quad (9)$$

where  $si(x)$  is the shifted sine-integral function, with  $x > a$ . In the case where  $C_1 = C_2$ , the expression for  $n(x)$  from Eq. (9) reduces to that found in Ref. [5]. The distance dependence of the electron density within the Lorentzian distribution function model is expressed as

$$n(x) = \frac{2m}{\pi} \left[ \frac{C_1}{\pi} \int_0^\infty \frac{dy}{y} \ln \left| \frac{1+y}{1-y} \right| \cos(2k_F x y) e^{-2\varepsilon k_F y} + \frac{C_2}{\pi} \int_0^\infty \frac{dy}{y} \ln \left| \frac{1+y}{1-y} \right| \cos(2k_F x y) \cos(2k_F a y) e^{-2\varepsilon k_F y} \right], \quad (10)$$

while for the Gaussian distribution function model, it reads

$$n(x) = \frac{2m}{\pi} \left[ \frac{C_1}{\pi} \int_0^\infty \frac{dy}{y} \ln \left| \frac{1+y}{1-y} \right| \cos(2k_F x y) e^{-2\sigma^2 k_F^2 y^2} + \frac{C_2}{\pi} \int_0^\infty \frac{dy}{y} \ln \left| \frac{1+y}{1-y} \right| \cos(2k_F x y) \cos(2k_F a y) e^{-2\sigma^2 k_F^2 y^2} \right], \quad (11)$$

with a new variable  $y = q/2k_F$ . Eqs. (10) and (11) are numerically evaluated.

## RESULTS AND DISCUSSION

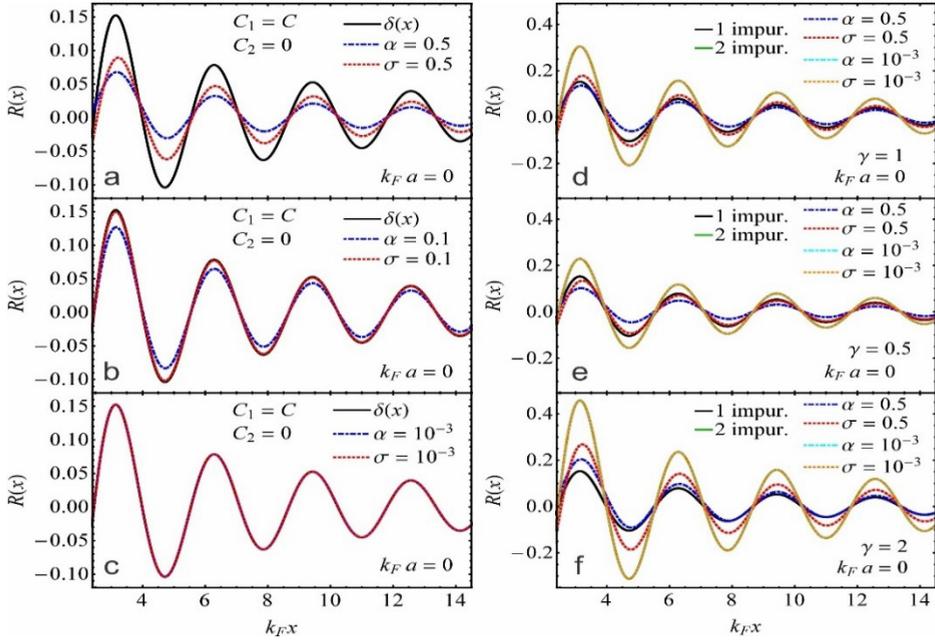
In this section, we present our results for one-dimensional non-interacting electron gas in the presence of two impurities, modeled by Dirac delta potentials, as well as Lorentzian and Gaussian distribution functions. The Fermi wave number is used as the energy unit, i.e.,  $k_F = 1$ .

We first model the asymmetry in potential strengths as  $\gamma = C_2/C_1$  with potential strength of the impurity located at  $x = 0$  fixed, i.e.,  $C_1 = C$ . For simplicity, we introduce a normalized electron density  $R(x) = n(x)/(2mC/\pi)$ .

In Figures 1(a)-(c), we plot  $R(x)$  as a function of the distance  $k_F x$  for a single impurity within the three models discussed above, for different values of the scale parameters  $\varepsilon$  and  $\sigma$ , respectively. We observe that the analytical results obtained for the Dirac delta potential can be well approximated using either a Lorentzian or Gaussian distribution function when their scale parameters,  $\varepsilon$  and  $\sigma$ , are small. Additionally, it can be seen that when we use a Gaussian distribution function to approximate the impurity potential, our results will converge faster to the analytical result obtained for Dirac delta potential, as the half-width at half-maximum approaches zero. At the same time, the approximation of the impurity potential using a Lorentzian distribution function converges more slowly to the analytical result as the half-width at half-maximum decreases. This tendency can be clearly seen from the Fourier transforms of the potentials, given by Eqs. (6)-(8), respectively.

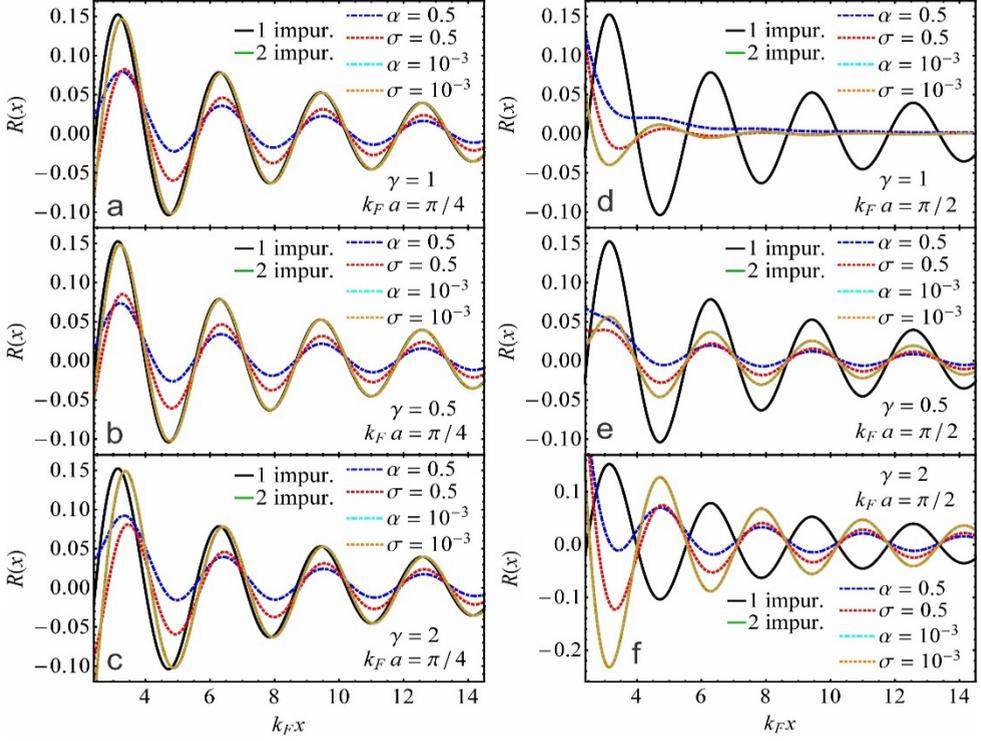
In Figures 1(d)-(f), the normalized density  $R(x)$  is plotted as a function of the distance  $k_F x$  for both one impurity and two impurities with different values of the potential strength parameter  $\gamma = C_2/C_1$  (where  $C_1 = C$ ) when the distance between impurities is  $k_F a = 0$ . We observe that the magnitude of the oscillations increases with the addition of a second impurity, while their phase remains unchanged at  $k_F a = 0$ , consistent with the findings in Ref. [5]. In addition, we find that the amplitude of the oscillations decreases or increases as the potential strength of the second impurity decreases or increases, respectively [see Figures 1(d)-(f)].

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**Fig. 1(a)-(c):**  $R(x) = n(x)/(2mC/\pi)$  as a function of  $k_F x$  for a single impurity ( $\gamma = 0$ ) at  $k_F a = 0$  within different models. The black solid line corresponds to the analytical result obtained using the Dirac delta potential. The parameter values are indicated in the figures. **(d)-(f):**  $R(x)$  as a function of  $k_F x$  for one impurity (black solid line) and two impurities (green solid line), calculated analytically for  $k_F a = 0$  with  $k_F = 1$ . The dotted lines represent the results based on the Lorentzian and Gaussian distribution function models, with different values of the scale parameters  $k_F \varepsilon$  and  $k_F \sigma$ . The asymmetry in potential strengths is indicated in the figures.

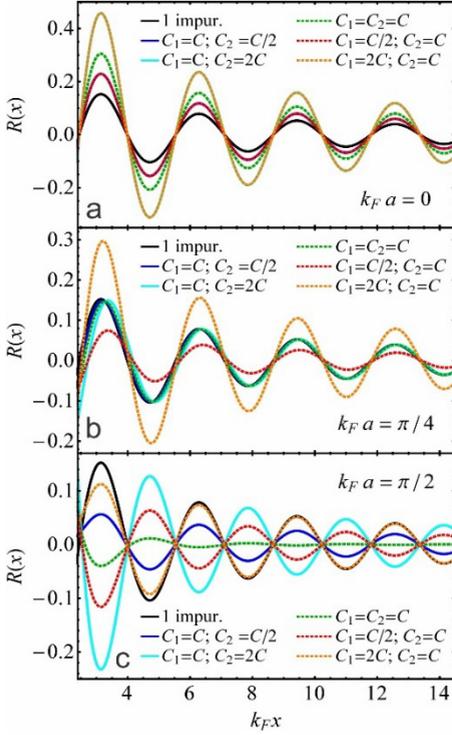
Figures 2(a)-(f) show the results for  $R(x)$  as a function of the distance  $k_F x$  for one impurity and two impurities, when varying potential strength parameter  $\gamma = C_2/C_1$  (where  $C_1 = C$ ) with finite values of the distance between impurities,  $k_F a \neq 0$ . By changing the distance between the impurities and the potential asymmetry  $\gamma$ , a phase shift in the oscillations can be observed for smaller values of  $k_F x$  [see Figures 2(a)-(c) for  $k_F a = \pi/4$ ], due to the interference effects, as noted in Ref. [5]. A possible asymmetry in potential strengths has less impact on the magnitude of the oscillations at  $k_F a = \pi/4$ , in contrast to the  $k_F a = 0$  case. A further increase in the distance  $k_F a$  can lead to the formation of an antiphase between the oscillations caused by the two perturbing impurities and those caused by a single impurity [see Figures 2(d) and (f) for  $k_F a = \pi/2$ ]. Note that the magnitude of the oscillations is significantly reduced in the presence of a second impurity with  $\gamma = 1$  and  $k_F a = \pi/2$ . A deviation in potential strengths ( $\gamma \neq 1$ ) can strongly influence the amplitude of the oscillations at  $k_F a = \pi/2$ .



**Fig. 2:** The normalized density  $R(x) = n(x)/(2mC/\pi)$  as a function of distance  $k_F x$  for one impurity (black solid line,  $\gamma = 0$ ) and two impurities (green solid line), calculated analytically. The dotted lines represent the results based on the Lorentzian and Gaussian distribution function models, with different values of the scale parameters  $k_F \varepsilon$  and  $k_F \sigma$ . The distance between impurities  $k_F a$  is: (a)-(c)  $k_F a = \pi/4$  and (d)-(f)  $k_F a = \pi/2$ . The asymmetry in potential strengths  $\gamma$  is indicated in the figure.

Figures 3(a)-(c) present the results for  $R(x)$  as a function of the distance  $k_F x$  for one impurity and two impurities for different values of the distance between impurities  $k_F a$  when the potential strengths ( $C_1$  and  $C_2$ ) are differently varied. We note that in the presence of two impurities, when the distance between them is  $k_F a = 0$ , Eq. (9) for the density variation  $n(x)$  reduces to  $n(x) = -(2m/\pi)(C_1 + C_2) \text{si}(2k_F x)$ . Thus, this system with two impurities can be viewed as a single impurity located at  $a = 0$ , with a potential amplitude of  $C_1 + C_2$ . This can be seen by changing the values of  $C_1$  while keeping  $C_2$  fixed, or varying  $C_2$  while keeping  $C_1$  fixed in a similar manner, the oscillations show equal deviations from the results corresponding to the symmetrical  $C_1 = C_2$  case [see Figure 3(a)]. Note that the large-distance ( $x \gg a$ ) behavior of the electron density deviation  $n(x)$  [4-7] is obtained as  $n(x) \sim [m(C_1 + C_2)/\pi k_F] \cos(2k_F x)/x$ .

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**Fig. 3:** The normalized density  $R(x) = n(x)/(2mC/\pi)$  as a function of  $k_F x$  for one impurity (black solid line,  $C_1 = C$  and  $C_2 = 0$ ) and two impurities, calculated analytically. The distance between the impurities is: (a)  $k_F a = 0$ , (b)  $k_F a = \pi/4$  and (c)  $k_F a = \pi/2$ , with  $k_F = 1$ . The asymmetry in potential strengths is indicated in the figure.

In the case of  $k_F a \neq 0$ , the density oscillations become highly sensitive to any asymmetry appearing in potential strengths. Depending on the values of  $k_F a$ , the magnitude of the oscillations can be amplified by varying the potential strengths. In addition, for  $k_F a \neq 0$ , the large-distance behavior of the electron density deviation  $n(x)$  is expressed as

$$n(x) \sim \frac{m}{\pi k_F} \left\{ C_1 \frac{\cos(2k_F x)}{x} + C_2 \left[ \cos(2k_F a) \frac{\cos(2k_F x)}{x} + a \sin(2k_F a) \frac{\sin(2k_F x)}{x^2} \right] \right\}, \quad (12)$$

which reduces to the results in Ref. [5] when  $C_1 = C_2$ . Note that, in the symmetrical case ( $C_1 = C_2$ ), at large distances and for values of  $2k_F a = (2n + 1)\pi$  (where  $n$  is a positive integer), the density oscillations vanish [5]. In the case of asymmetrical potential strengths, for  $2k_F a = (2n + 1)\pi$ , the large-distance behavior of the density  $n(x)$ , as given by Eq. (12), reduces to the form  $n(x) \sim [m(C_1 - C_2)/\pi k_F] \cos(2k_F x)/x$ , which remains finite as long as  $C_1 \neq C_2$ .

## CONCLUSIONS

In this work, we have investigated Friedel oscillations in a one-dimensional non-interacting electron gas induced by a single impurity and by two impurities with different potential strengths. The impurities have been modeled using a Dirac delta potential, as well as Lorentzian and Gaussian distribution functions. We have shown that the analytical results obtained with the Dirac delta potential can be well approximated using either a Lorentzian or Gaussian distribution function model. We have found that by further adding an impurity to a single-impurity system, the magnitude of the density oscillations can be significantly increased by appropriately adjusting the value of the distance between impurities. We have established that any asymmetry in the potential strengths of the impurities can strongly influence both the magnitude and phase of oscillations, depending on the values of the distance between the impurities.

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## REFERENCES

- [1] J. Friedel, *Lond. Edinburgh Dublin Philos. Mag. J. Sci.* **43** (1952) 153
- [2] J. Villain, M. Lavagna, P. Bruno, *C. R. Physique* **17** (2016) 276–290
- [3] C. Bena, *C. R. Physique* **17** (2016) 302–321
- [4] G. F. Giuliani, G. Vignale, T. Datta, *Phys. Rev. B* **72** (2005) 033411
- [5] I. Grosu, L. Tugulan, *J. Supercond. Nov. Magn.* **21** (2008) 65–68
- [6] I. Grosu, L. Tugulan, *Stud. Univ. Babeş-Bolyai, Physica*, **LII**, **2** (2007) 79–84
- [7] L. Tugulan, *Stud. Univ. Babeş-Bolyai, Physica*, **LIII**, **1** (2008) 33–41
- [8] G. E. Simion, G. F. Giuliani, *Phys. Rev. B* **72** (2005) 045127
- [9] A. Gorczyca, M. M. Maška, M. Mierzejewski, *Phys. Rev. B* **76** (2007) 165419
- [10] M. Stosiek, C. Baretzky, T. Balashov, F. Evers, W. Wulfhchel, *Phys. Rev. B* **105** (2022) L140504
- [11] B. Dóra, D. Sticlet, C. P. Moca, *Phys. Rev. B* **104** (2021) 125113
- [12] C. Berthier, *J. Phys. C: Solid State Phys.* **11** (1978) 797–814
- [13] T. Mitsui, S. Sakai, S. Li, T. Ueno, T. Watanuki, Y. Kobayashi, R. Masuda, M. Seto, H. Akai, *Phys. Rev. Lett.* **125** (2020) 236806
- [14] P. Hofmann, B. G. Briner, M. Doering, H.-P. Rust, E. W. Plummer, A. M. Bradshaw, *Phys. Rev. Lett.* **79** (1997) 265–268
- [15] S. Rouzière, S. Ravy, J.-P. Pouget, S. Brazovskii, *Phys. Rev. B* **62** (2000) R16231(R)