Spin and interaction effects on charge distribution and currents in one-dimensional conductors and rings within the Hartree-Fock approximation

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Using the self–consistent Hartree-Fock approximation for electrons with spin at zero temperature, we study the effect of the electronic interactions on the charge distribution in a one-dimensional continuous ring containing a single δ scatterer. We reestablish that the interaction suppresses the decay of the Friedel oscillations. Based on this result, we show that in an infinite one dimensional conductor containing a weak scatterer, the current is totally suppressed because of a gap opened at the Fermi energy. In a canonical ensemble of continuous rings containing many scatterers, the interactions enhance the average and the typical persistent current.

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The effects of electronic interactions on characteristic properties, such as charge fluctuations, persistent currents (PC's) and the conductance of electronic systems are very rich and interesting. [1] They strongly depend on the strength and range of the interactions, [2,3,4] on the dimensionality of the system, and on whether the space is discrete or continuous. [5,6] Approximate calculations, like Hartree-Fock, introduce a great deal of simplifications, but at the same time many effects may be washed out. However, approximate calculations may be used to shed more light on specific problems, while keeping in mind their limitations. In this work we consider e-e interactions within the self-consistent Hartree-Fock approximation (SCHFA) for electrons with spin at zero temperature. For simplicity we assume an equal number of electrons of opposite spin states.

Our aim is to study numerically the interaction effects on the charge distribution and the currents in continuous one-dimensional (1D) isolated rings and open conductors containing a single δ scatterer, [4,7,8,9,10] as well as on the PC's in rings containing many scatterers. [11,12] Even within the Hartree-Fock approximation we recover the bosonization [4] and the density-matrix renormalization-group result: [10] We show that for a single scatterer in a ring the repulsive electronic interaction suppresses the decay of the charge oscillations. Based on this we show, as a central result, that for an open conductor with a weak scatterer the electronic conduction at the Fermi energy vanishes because of Bragg reflection coexisting with a gap at the Fermi energy. The zero conduction of the interacting system was obtained in Refs. [7,8,9] by exact and by renormalization group calculations. Within the first iteration of the SCHFA, it was shown [8,9] that an attempt to explain this result by a scattering perturbation series is inadequate because of logarithmic divergences of the transmission amplitude at the Fermi energy in all orders of the series.

Although the dissipative conductance of the infinite conductor is suppressed by the interactions, the PC in a ring is not. This is because the conductance depends on the properties of the levels close to the Fermi energy but the PC is a thermodynamic property that depends on the response of all occupied levels. [11] Moreover, we show that once many scatterers are considered, the interactions not only do not suppress the PC, but even enhance it. We write the HF equation for electrons in a ring of radius R with angular coordinate θ and energy units $\hbar^2/m_eR^2 = 1$ (we drop the background term) as

$$-\left[\frac{1}{2}\frac{\partial^2}{\partial\theta^2} + V_{\rm dis}(\theta) + \frac{R}{r_0}\int_0^{2\pi}\frac{\sum_{l'=1}^{Ne}|\psi_{l'}(\theta')|^2}{\sqrt{(\theta-\theta')^2+\epsilon^2}}d\theta'\right]\psi_l(\theta)$$
$$-\delta_{s_{l'},s_l}\frac{R}{r_0}\int_0^{2\pi}\frac{\sum_{l'=1}^{Ne}\Psi^*_{l'}(\theta')\Psi_{l'}(\theta)}{\sqrt{(\theta-\theta')^2+\epsilon^2}}\psi_l(\theta')d\theta' = E\psi_l(\theta)\,. \quad (1)$$

The twisted boundary condition $\psi(\theta+2\pi) = \psi(\theta)\exp(i2\pi\phi/\phi_0)$ accounts for a flux ϕ threading the ring. $\phi_0 \equiv hc/e$ is the flux quantum. $V_{\rm dis}(\theta)$ is the disorder potential which may include a single or many scatterers. The first (second) integral term is the Hartree (Fock) term. The electronic wave functions $\Psi_l(\theta) \equiv \psi_l(\theta)\exp(-i\theta\phi/\phi_0)$ in the Fock term are 2π periodic for any value of flux. l enumerates the energy levels together with the spin state s_l. N_e is the total number of electrons in the ring. The cutoff ϵ^2 allows (as in quasi 1D) using the 3D Coulomb law [5] and makes the integrations finite. The square of the distance between the particles is defined [13] by $(\theta-\theta')^2 \equiv \min[|\theta-\theta'|^2, (2\pi-|\theta-\theta'|)^2]$. In Eq. (1), $r_0 \equiv \varepsilon\hbar^2/m_ee^2$ denotes the Bohr radius with dielectric constant ε (to be distinguished from the cutoff ϵ). We define the coefficient $g \equiv R/r_0$ to be the interaction strength. $g \sim 1$ corresponds to semiconductors.

[14] Because the sum $\sum_{l'=1}^{Ne} \Psi^*_{l'}(\theta')\Psi_{l'}(\theta)$ represents almost a closure relation we replace, as discussed in Refs. [14] and [15], the integrodifferential equation (Eq. (1)) by an ordinary Schrödinger equation that we solve *self–consistently*:

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial\theta^2} + V_{\rm dis}(\theta) + gV_{\rm eff}(\theta)\right]\psi_l(\theta) = E\psi_l(\theta). \qquad (2)$$

Here $V_{\rm eff}(\theta)$ is given by

$$\int_0^{2\pi} \frac{\sum_{l'=1}^{Ne}|\psi_{l'}(\theta')|^2 - \delta_{s_{l'},s_l}{\rm Re}\{\Psi^*_{l'}(\theta')\Psi_{l'}(\theta)\}}{\sqrt{(\theta-\theta')^2+\epsilon^2}}d\theta'$$

where Re stands for real part. The spin degree of freedom is very important. For spinless electrons the interaction effect is weak because the Fock and Hartree terms tend to cancel each other due to opposite signs and similar absolute values. Taking into account the spin degree of freedom, the Hartree term is twice as large as the exchange term. Then the former dominates $V_{\rm eff}$ and enhances screening; therefore we expect the interaction effects to be stronger for electrons with spin. This explains the importance of considering spin [16] in order to understand disordered interacting systems.

We begin by studying the interaction effect on the charge oscillations in a ring with a single scatterer,

$$V_{\rm dis}(\theta) = \lambda\delta(\theta). \qquad (3)$$

For a strong scatterer, $\lambda \geq E_f$ (E_f is the Fermi energy), the interaction effect on the decay of the charge oscillations is weak and may even be neglected because the scatterer is dominating. For a weak scatterer, $\lambda << E_f$, at the level of the SCHFA we recover the numerical result of Ref. [10] based on the density-matrix renormalization group: With increasing repulsive interaction g the decay of the Friedel oscillations is suppressed (indicating also the reliability of our SCHFA). Figure 1 depicts the decay rate for the strongest interaction for which the SCHFA still converges. As Fig. 2 shows, the effective potential tends to be periodic with half a Fermi wavelength periodicity. Both (direct and exchange) terms tend to have this periodicity which is independent of the interaction strength. This behavior holds for a larger number of electrons on a ring for a given constant charge density.

The above results may be used to study the effect on the charge oscillations and on the conduction in the case of a single weak scatterer $\hat\lambda\delta(x)$ embedded in an *infinite* 1D conductor (x is the spatial coordinate).

For noninteracting electrons the orthogonal wave functions, with a given spin state, are [8,9]

$$\phi_k^{(1)}(x) = \begin{cases} e^{ikx} + r(k,\lambda)e^{-ikx}, & x<0 \\ t(k,\lambda)e^{ikx}, & x>0, \end{cases} \qquad (4)$$

$$\phi_k^{(2)}(x) = \begin{cases} t'(k,\lambda)e^{-ikx}, & x<0 \\ e^{-ikx} + r'(k,\lambda)e^{ikx}, & x>0, \end{cases} \qquad (5)$$

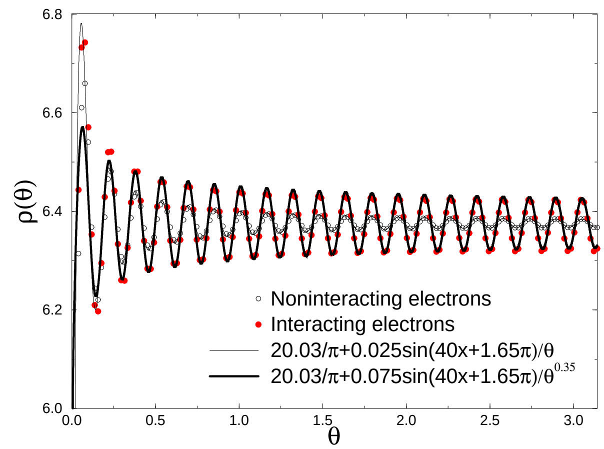

FIG. 1. Charge oscillations per spin, along half circumference of a 1D continuous ring, induced by a *weak* single scatterer $\lambda\delta(\theta)$ ($\lambda = 3.8$). Thin (bold) symbols stand for noninteracting (interacting) electrons. The interactions, at self-consistency of the Hartree-Fock calculations, tend to make $\rho(\theta)$ periodic and to minimize $\rho(0)$ further. The interaction strength is $g = 3$, and the flux threading the ring is $\phi/\phi_0 = 0.05$ (see text). The total number of electrons per spin is 40. The curves are the estimations by the indicated formulas.

with $k > 0$ and $\lambda \equiv \hat\lambda/(\hbar^2/m_e)$ having units of inverse length. $r(k,\lambda) = -i\lambda/(k+i\lambda)$ and $t(k,\lambda) = k/(k+i\lambda)$. Because of time-reversal symmetry and the symmetry of the potential under coordinate inversion, $t' = t$ and $r' \equiv -(r/t)^*t = r$. The fluctuating density per spin is

$$\Delta\rho(x) = 2\int_0^{K_f} \frac{-\lambda^2\cos 2kx + \lambda k\ \sin 2k|x|}{k^2+\lambda^2}dk$$
$$= -2\lambda e^{2\lambda|x|}{\rm Im}\{E_1(-iz)\}. \qquad (6)$$

Im takes the imaginary part of the exponential integral E_1, $z \equiv 2|x|(K_f + i\lambda)$, and K_f is the Fermi wave vector. $\Delta\rho(0) = -2\lambda\tan^{-1}(K_f/\lambda)$ is a minimum. For $K_f x > 1$, the asymptotic expansion of E_1 implies

$$\Delta\rho(x) = -\frac{\lambda(K_f\cos 2K_f x + \lambda\sin 2K_f|x|)}{|x|(\lambda^2+K_f^2)}. \qquad (7)$$

Using $r \equiv |r|e^{i\eta}$ and $|r_f| = |\lambda|/\sqrt{K_f^2+\lambda^2}$, $\sin\eta_f = -k/\sqrt{K_f^2+\lambda^2}$, one finds [8,9]

$$\Delta\rho(x) = \frac{|r_f|\sin(2K_f|x| + \eta_f)}{|x|}. \qquad (8)$$

For the SCHFA the initial $V_{\rm eff}$ is calculated using the wave functions of noninteracting electrons. The charge fluctuations define the Hartree potential

$$V_H(x) = g_s\int_0^\infty \left[\frac{1}{|x+x'|} + \frac{1}{|x-x'|}\right]\Delta\rho(x')dx', \qquad (9)$$

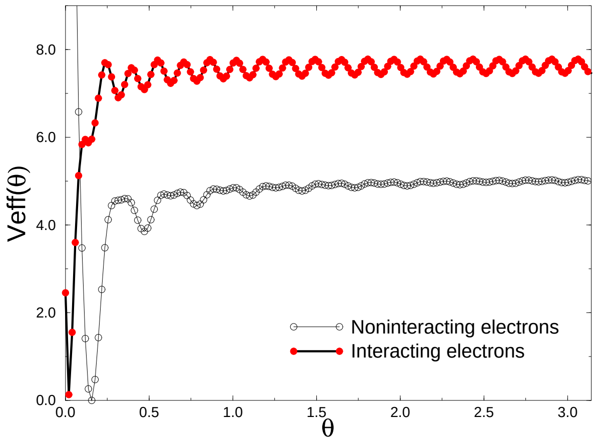

FIG. 2. The effective potential along the half circumference of the ring of Fig. 1. The thin (bold) symbol is the noninteracting (interacting) result. Note the clear tendency of $V_{\rm eff}(\theta)$ at self-consistency to become periodic, and to screen the scattering potential $\lambda\delta(\theta)$ (not shown).

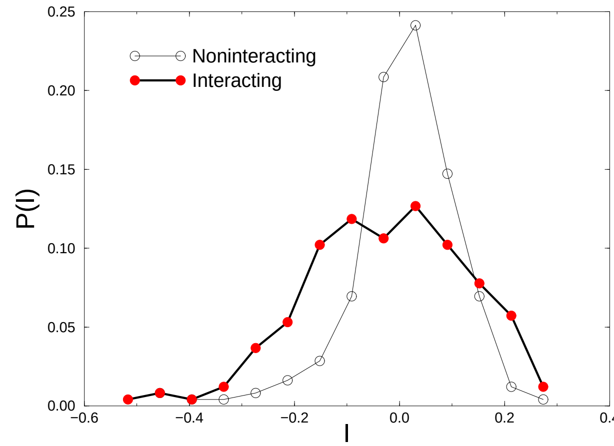

FIG. 3. The interaction effect on the statistics of the sample persistent current (in units of the PC of the clean ring of noninteracting electrons). Thin (bold) symbols stand for noninteracting (interacting) electrons for the same canonical ensemble of 201 realizations. The interaction ($g=1,\ \phi/\phi_0=0.325$) enhances the persistent current.

where $g_s = 1$ (2) for electrons without (with) spin. Our approximated Fock potential is

$$V_{\scriptscriptstyle F}(x) = -\int_{-\infty}^{+\infty} \frac{\int_0^{K_f}\sum_{i=1}^{2}{\rm Re}\{\phi_k^{(i)*}(x')\phi_k^{(i)}(x)\}dk}{|x-x'|}dx'$$
$$= -\int_0^{\infty}\left[\frac{1}{|x+x'|}+\frac{1}{|x-x'|}\right]\Delta\rho(x+x')dx'. \quad (10)$$

Clearly, $V_{\rm eff} = V_{\scriptscriptstyle H} + V_{\scriptscriptstyle F}$ is a function of $|x|$, and will change during the iterations until self-consistency is reached. $V_{\rm eff}$ is small due to a weak coupling constant ($g \sim 1$). At this point we invoke an approximate self-consistency by adopting a suppression [4,10] of the decay of the Friedel oscillations, as was demonstrated above to be valid in the SCHFA. We substitute by hand the limit [4] $\delta = 0$ in

$$\Delta\rho(x) = \frac{|r_f|\sin(2K_f|x|+\eta_f)}{|x|^{\delta}} \quad (11)$$

for Eqs. (9) and (10), assuming that this yields a $V_{\rm eff}$ close to that from the SCHFA. To carry out the integration [in Eqs. (9) and (10)], we use a *cutoff* that allows contributions only from $|x-x'| \ge \epsilon$. This cutoff is equivalent to that used in Eq. (1). For $K_f x \gg 1$, we then obtain, up to an additive constant,

$$V_{eff}(x) = U[g_s\sin(2K_f x+\eta_f) - \sin(4K_f x+\eta_f)], \quad (12)$$

where $U \equiv -2|r_f|\mathbf{c}_i(2K_f\epsilon)$, and $\mathbf{c}_i$ is the cosine integral. Equation (12) shows that $V_{\rm eff}$ has two periodicities: $\lambda_f/2$ from the direct potential ($\lambda_f \equiv 2\pi/K_f$), and $\lambda_f/4$ from the exchange potential. The overall periodicity is given by the larger period. The electrons at the Fermi energy exactly obey the Bragg condition [17] for total reflection, i.e.,

$$2\frac{\lambda_f}{2}\sin\frac{\pi}{2} = n\lambda_f\,. \quad (13)$$

All the states with $|k| < K_f$ remain practically unaffected by the weak and periodic $V_{\rm eff}$. Note that consistently with Eq. (13) there is a gap [17] of order U at the Fermi energy. Thus the current vanishes at the Fermi energy.

For a ring with a weak scatterer the interaction will not destroy the PC even if the current at the Fermi energy (assuming a large ring) is totally suppressed by the periodic effective potential. This follows from the fact that all occupied levels contribute to the PC, except at E_f, where Eq. (13) is assumed to be relevant.

In the following we will consider the general case of a large number of scatterers in a ring. Figure 2 already shows the importance of screening for a single scatterer. This indicates that screening is of particular relevance for the case of many random scatterers:

$$V_{\rm dis}(\theta) = \sum_{j=1}^{N_s}\lambda_j\delta(\theta-\theta_j). \quad (14)$$

Here the location and strength of the jth scatterer are uniformly distributed in $(0,2\pi)$ and $(-\Lambda,\Lambda)$, respectively. N_s is the total number of scatterers in a ring. For the numerics we use $\Lambda = 14$ (in scaled units).

The characteristic features of disordered noninteracting samples were, e.g., discussed by Imry and Shiren. [18] For noninteracting electrons, the localization length [14] at $E_f = 200$ is $\xi \sim \pi/2$. This should reduce the average current in open conductors by a factor $\sim 1/50$. The average sample PC of noninteracting electrons was reduced by factor $\sim 1/40$ which is slightly greater than predicted

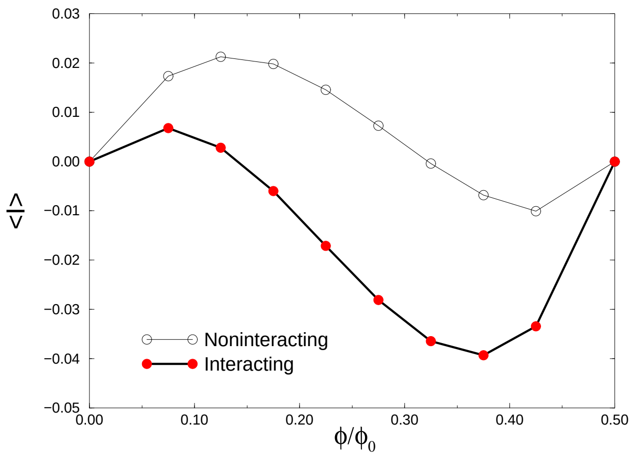

FIG. 4. The interaction ($g = 1.75$) enhances the average sample persistent current (in units of the PC of the clean ring) and introduces a preffered diamagnetic current direction. Thin (bold) symbols represent noninteracting (interacting) electrons for the same 150 realizations.

for open conductors. The typical sample PC, $\sqrt{\langle I^2\rangle}$, was reduced by factor $\sim 1/10$ which indicates the importance of a statistical study. The fixed total number of electrons in a ring was 32 ± 4.

Figure 3 shows the interaction effect on the sample PC statistics for an interaction coupling constant $g = 1$. The interaction reduces the peak, centered at zero, while broadening the distribution. Furthermore, the distribution gains more weight at negative values of the PC, which indicates a diamagnetic tendency. We found that the interaction enhances the typical PC (by factor $\sim$2); the average PC is neither enhanced nor suppressed. Figure 4 shows that for increasing interaction, $g = 1.75$, the average PC is also enhanced by factor $\sim$2. Figures 3 and 4 both show a clear tendency of the interaction to enhance the PC for electrons with spin. For spinless electrons the PC was found [14] to be rather unaffected by interaction. This shows an essential difference between models of electrons with or without spin. In addition, a clear difference between tight-binding models and continuous models [19] becomes apparent: In the former it was concluded, [20] using exact diagonalization and the SCHFA, that switching on the *e*-*e* interaction in the regime of moderate disorder further suppresses the PC because of the Mott transition. [21] In continuous models this transition appears to be irrelevant, since the continuous models correspond to tight-binding models at very low fillings. [16,7]

In conclusion, using the SCHFA in one-dimension, we showed the tendency of the electronic interaction to build up nondecaying charge oscillations in a ring containing a single weak scatterer. Adopting this result for an infinite conductor implies a periodic effective potential. The electronic conduction was shown to vanish, because of Bragg reflection that coexists with a gap at the Fermi energy. This shows that, even in the HF limit the influence of the interactions on the Friedel oscillations and on conduction in one-dimension, calculated by exact and renormalization methods, may be reproduced. In rings the PC is not suppressed by the interaction. It is even enhanced in the case of many moderate scatterers due to screening. To demonstrate these effects, we considered the spin degree of freedom and used continuous conductors and rings.

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[1] For reviews see: *Mesoscopic Phenomena in Solids*, edited by B. L. Altshuler, P. A. Lee, and R. A. Webb (North-Holland, Amsterdam, 1990); *Exactly Solvable Models of Strongly Correlated Electrons*, edited by V. A. Korepin and F. H. L. Eßler (World Scientific, Amsterdam, 1994); K. Richter, D. Ullmo, and R. A. Jalabert, Phys. Rep. **276**, 1 (1996).

[2] W. Apel and T. M. Rice, Phys. Rev. B **26**, 7063 (1982).

[3] M. Fabrizio, A. O. Gogolin and S. Scheidl, Phys. Rev. Lett. **72**, 2235 (1994); Y. Oreg and A. M. Finkelstein, *ibid.* **76**, 4230 (1997).

[4] R. Egger and H. Grabert, Phys. Rev. Lett. **75**, 3505 (1995).

[5] H. Schulz, Phys. Rev. Lett. **71**, 1864 (1993).

[6] E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).

[7] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. **68**, 1220 (1992); Phys. Rev. B **46**, 15233 (1992).

[8] K. A. Matveev, D. Yue, and L. I. Glazman, Phys. Rev. Lett. **71**, 3351 (1993); D. Yue, L. I. Glazman, and K. A. Matveev, Phys. Rev. B **49**, 1966 (1994).

[9] M. P. A. Fisher and L. I. Glazman, cond-mat/9610037 (unpublished).

[10] P. Schmitteckert and U. Eckern, Phys. Rev. B **53**, 15397 (1996).

[11] R. Berkovits and Y. Avishai, Phys. Rev. Lett. **76**, 291 (1996).

[12] N. Byers and C. N. Yang, Phys. Rev. Lett. **7**, 46 (1961); L. P. Levy, G. Dolan, J. Dunsmuir, and H. Bouchiat, *ibid.* **64**, 2074 (1990); V. Chandrasekhar. R. A. Webb, M. J. Brady, M. B. Ketchen, W. J. Gallagher, and A. Kleinsasser, *ibid.* **67**, 3578 (1991); D. Mailly, C. Chapelier, and A. Benoit, *ibid.* **70**, 2020 (1993).

[13] This definition of the distance is close to $2\ \sin(|\theta - \theta'|/2)$ and does not introduce any qualitative changes. Also, the small cutoff has a negligible influence on the numerical results.

[14] A. Cohen, R. Berkovits, and A. Heinrich, Int. J. Mod. Phys. B. **11**, 1845 (1997).

[15] *Quantum mechanics II*, by Rubin H. Landau (Wiley, New York, 1990), p.194.

[16] T. Giamarchi and B. S. Shastry, Phys. Rev. B. **51**, 10915 (1995); M. Kamal, Z. H. Musslimani, and A. Auerbach, J. Phys. France I **5**, 1487 (1995).

[17] *Introduction to Solid State Physics* by C. Kittel (Wiley, New York, 1996).

[18] Y. Imry and N. S. Shiren, Phys. Rev. B **33**, 7992 (1986).

[19] A. Müller-Groeling, H. A. Weidenmüller, and C. H. Lewnkopf, Europhys. Lett. **22**, 193 (1993); A. Müller-Groeling and H. A. Weidenmüller, Phys. Rev. B **49**, 4752 (1994).

[20] M. Abraham and R. Berkovits, Phys. Rev. Lett. **70**, 1509 (1993); G. Bouzerar, D. Poilblanc, and G. Montambaux, Phys. Rev. B **49**, 8258 (1994); H. Kato and D. Yoshioka, *ibid.* **50**, 4943 (1994).

[21] N. Mott, Proc. R. Soc. London, Ser. A **382**, 1 (1982).