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Persistent currents in 1D rings and the metal–insulator transition under strong long-range Coulomb repulsion

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Abstract. A perturbative approach for large (in comparison with electron overlap and on-site disorder) long-range Coulomb interaction is developed for a 1D ring model. The explicit expression for low-lying energy levels has been obtained. It is shown that in the case of strong repulsive long-range interaction persistent current does not depend exclusively on the filling factor $\nu = p/q$ but is extremely sensitive to its denominator q. It also depends on the common factor M of electrons and sites number. In the absence of a common factor ($M = 1$) there exists only one quasiparticle that experiences no strong Coulomb interaction, thus moving freely with bare electron overlap, which provides an unexpectedly large persistent current. For the case of an arbitrary M and a large enough q a system of M weakly interacting quasiparticles has been introduced, which undergoes a metal–insulator transition at unusually small overlap even for a filling factor close to one half. Suppression of the persistent current by disorder is taken into account. Comparison of analytically obtained expressions with the results of numerical calculations shows a reasonable agreement.

Recent measurements of the persistent current of small mesoscopic rings have aroused much interest in this field [1–3]. Due to discrepancies between the prediction of a single-electron theory for the persistent current of a disordered ring [15–19] and the values measured in experiment [1, 2], many theoretical studies regarding the influence of electron–electron (e–e) interactions on the persistent current of rings threaded by a magnetic flux were initiated [4–14]. The main goal was to check whether e–e interactions could increase the average persistent current of a disordered system.

In [11] it was shown that for a 1D half-filled single-band spinless lattice model e–e interactions do not lead to a dramatic increase of the persistent current above its non-interacting value. The result was also checked for an arbitrary filled ring [14], and, based on variational methods and numerical studies, it has been shown that for any amount of disorder the current must decrease. An interesting behaviour was observed for an ordered ring, where for certain filling factors in the limit of large interactions the current approaches zero, while for other fillng factors, termed the 'frustrated' cases, the current approaches a small but finite value. Hence, for these models e–e interactions cannot explain the high values of current observed in experiment. The reason for the absence of any dramatic increase in the average current is that for interactions strong enough to counter the influence of disorder the electrons are already in a pinned Wigner crystal, for which the current is suppressed.

In this paper we shall approach the arbitrary filled ring model using a perturbative method. We shall show that for an ordered ring the magnitude of persistent current depends

strongly on the common factor M but not on the filling factor $\nu = p/q$. In the case of $M = 1$ there exists a quasiparticle that exhibits no Coulomb interactions and carries large persistent current. If $M \neq 1$ and q is large enough a system of weakly interacting quasiparticles can be introduced, which undergoes the metal–insulator transition at unusually small overlap even for filling factor close to one half. For the case of an on-site disorder we shall obtain an explicit expression for the persistent current, which, compared with the results of numerical calculations, will demonstrate a reasonable fit.

Let us consider a 1D ring with $N = Mq$ sites threaded by magnetic flux ϕ and containing $N_e = Mp$ electrons. The Coulomb e–e interaction is assumed to be strong in the sense that the overlap t is much smaller than the change in Coulomb energy, denoted by V, under the displacement of one electron by one lattice spacing.

To develop the perturbative approach in the small parameter $t/V \ll 1$ we shall use a zeroth-order approximation the well known Hubbard solution of the unperturbed ($t = 0$) problem [20]. In [20] Hubbard proposed a rigorous procedure to construct the ground-state (GS) configuration for a system consisting of particles interacting with each other by a long-range potential, which is assumed to be repulsive and convex. For a given filling factor ν, defined as the ratio of the number of particles N_e to the number of sites N, the Hamiltonian

$$\mathcal{H}_{\text{Coul}} = \sum_{ij} V_{ij} n_i n_j \tag{1}$$

(where V_{ij} is the interelectron interaction energy and n_i are the electron occupation number operators), determines uniquely the arrangement of particles minimizing the interaction energy. This arrangement represents a 1D classical Wigner lattice, which is the configuration of the GS of Hamiltonian (1). To build up this configuration one has to expand filling factor ν into a continued fraction

$$\nu = 1/\{n + \alpha/[n_1 + \alpha_1/(n_2 + \cdots + \alpha_{m-1}/n_m)]\} \tag{2}$$

where all n_i are positive integers and $\alpha_i = \pm 1$ are chosen to provide the modulus of the remainders at any step to be less than one half. The configuration corresponding to the value $\nu = p/q$ (p, q are integers with no common factor) is periodic with a period q and has p electrons in each period. Configurations are described by a sequence of the distances between the nearest particles. In the GS configuration distances take two values only: n and $n + \alpha$. We follow Hubbard by denoting the configuration of i particles spaced by a distances X as $[X]^i$ and define the sequences $\{X_j\}$ and $\{Y_j\}$ by

$$X_{i+1} = [X_i]^{n_i - 1} Y_i \qquad X_1 = n \qquad Y_{i+1} = [X_i]^{n_i + \alpha_i - 1} Y_i \qquad Y_1 = n + \alpha \tag{3}$$

then the required arrangement for the filling factor (2) in each period is given by X_m.

Built up in this way the GS configuration enables us to develop the perturbative approach for a small overlap t in order to obtain a persistent current. We will further treat the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + T \qquad \mathcal{H}_0 = \sum_{ij} V_{ij} n_i n_j + \sum_i \varepsilon_i n_i \qquad T = -t e^{i\theta} \sum_i c_{i+1}^+ c_i + \text{HC} \tag{4}$$

where $c_i (c_i^+)$ are the annihilation (creation) operators, $n_i = c_i^+ c_i$ is the particle number operator, $\theta = 2\pi\phi/N\phi_0$ allows for magnetic flux ϕ threading a ring of N sites and $\phi_0 = hc/e$ is the flux quantum.

As follows from Hubbard's algorithm the GS configuration for filling factor $v = p/q$ is q-fold degenerate.

To construct a perturbation approach in a case of GS degeneracy we need to introduce the operator $\mathbf{P}$, which projects onto the subspace of the GS eigenfunctions of $\mathcal{H}_0$ and an operator $\mathbf{Q} = 1 - \mathbf{P}$, which projects onto the orthogonal subspace. Then dividing an arbitrary wavefunction Ψ into two parts belonging to the different subspaces $\Psi = \mathbf{P}\Psi + \mathbf{Q}\Psi$ and projecting the Schrödinger equation $\mathcal{H}\Psi = E\Psi$ onto these two subspaces

$$\mathbf{P}\mathcal{H}\mathbf{P} \cdot \mathbf{P}\Psi + \mathbf{P}\mathcal{H}\mathbf{Q} \cdot \mathbf{Q}\Psi = E \cdot \mathbf{P}\Psi \qquad \mathbf{Q}\mathcal{H}\mathbf{Q} \cdot \mathbf{Q}\Psi + \mathbf{Q}\mathcal{H}\mathbf{P} \cdot \mathbf{P}\Psi = E \cdot \mathbf{Q}\Psi \qquad (5)$$

one can eliminate the part of the wavefunction lying outside the GS subspace

$$\mathbf{Q}\Psi = [1/(E - \mathbf{Q}\mathcal{H}\mathbf{Q})]\mathbf{Q}\mathcal{H}\mathbf{P} \cdot \mathbf{P}\Psi \qquad (6)$$

in order to obtain an effective Hamiltonian in the GS subspace

$$\mathcal{H}_{\text{eff}}\mathbf{P}\Psi = E \cdot \mathbf{P}\Psi \qquad \mathcal{H}_{\text{eff}} = \mathbf{P}\mathcal{H}\mathbf{P} + \mathbf{P}\mathcal{H}\mathbf{Q} \cdot [1/(E - \mathbf{Q}\mathcal{H}\mathbf{Q})] \cdot \mathbf{Q}\mathcal{H}\mathbf{P}. \qquad (7)$$

Bearing in mind that such an approach can be useful only for the case when the Coulomb interaction is the largest energy in the problem, it is convenient to expand the effective Hamiltonian (7) in the kinetic energy operator T

$$\mathcal{H}_{\text{eff}} = \mathbf{P}\mathcal{H}_0\mathbf{P} + \mathbf{P}T \cdot \sum_{s=0}^{\infty} \left(\frac{1}{E - \mathcal{H}_0} \cdot \mathbf{Q}T\mathbf{Q} \right)^s \cdot \mathbf{P}. \qquad (8)$$

If we express the projecting operator $\mathbf{P}$ through the set $\{|\alpha\rangle\}_{\alpha=1}^{q}$ of the GS eigenfunction $\mathcal{H}_0|\alpha\rangle = E_\alpha|\alpha\rangle$ as follows:

$$\mathbf{P} = \sum_{\alpha=1}^{q} |\alpha\rangle \langle\alpha|$$

the effective Hamiltonian takes the form

$$\mathcal{H}_{\text{eff}} = \sum_{\alpha} |\alpha\rangle E_\alpha \langle\alpha| + \sum_{\alpha\beta} |\alpha\rangle \tilde{T}_{\alpha\beta} \langle\beta| \qquad (9)$$

where

$$\tilde{T}_{\alpha\beta} = \langle\alpha|T \sum_{s=0}^{\infty} \left(\frac{1}{E - \mathcal{H}_0} \mathbf{Q}T\mathbf{Q} \right)^s |\beta\rangle \qquad (10)$$

and

$$E_\alpha = \sum_{ij \in \alpha} V_{ij} + \sum_{i \in \alpha} \varepsilon_i. \qquad (11)$$

Here the electron positions i and j belong to one of the GS configurations α. The first term in (11) is the unperturbed GS energy, which does not depend on α and will be taken as zero.

Herefoth we assume that the gap between the GS energy and the first excited level in the absence of the overlap element (equal to the smallest loss in the Coulomb energy under one spacing shift of any electron from its GS position) is much larger than the GS level split

due to disorder and overlap t. This lets us restrict ourselves by the first non-zeroth term in $\tilde{T}_{\alpha\beta}$ (10) and take E as equal to the unperturbed GS energy there.

As apparently follows from (10) the leading term in overlap is diagonal and equal to

$$\tilde{T}_{\alpha\alpha} = t^2 \sum_{\substack{i\in\alpha \\ \sigma=\pm}} \left(\frac{1}{V_{i\sigma}} \right) \tag{12}$$

where $V_{i\sigma}$ denotes the extra Coulomb energy under a shift of the ith particle to the left ($\sigma = -$) or right ($\sigma = +$) by one spacing. It is important to note that this term is ϕ independent because in the lowest approximation (12) it describes the displacement and then the return of each electron to the same site and therefore the phase factors θ cancel out. It may seem that the flux-dependent contribution will appear in the N_eth order correction to the GS energy only, which corresponds to the rotation of the electron system as a whole by a lattice constant, but what actually happens is that we need to shift only M electrons to transfer one unperturbed vacuum state $|\alpha\rangle$ to some other vacuum state $|\beta\rangle$. To prove our statement we will point to the quickest way of such a transformation which, in accordance with (10), gives us the leading ϕ-dependent term of $\tilde{T}_{\alpha\beta}$. With this aim we should treat in detail the unperturbed GS configuration.

The position of the ith electron in the GS configuration described by the Hubbard algorithm can be expressed in the analytical form

$$x_i = [i/\nu - \xi] \tag{13}$$

where square brackets denote an integer part, the particle coordinates are measured in lattice units and ξ is an arbitrary parameter corresponding to the different choices of origin. The proof of the equivalence between GS configurations constructed following the Hubbard algorithm and (13) lies in the fact that the GS energy E_{GS} calculated with the use of (13) has the form

$$\frac{E_{GS}}{N_e} = \sum_{n=1}^{N_e-1} \left(1 - \left\{ \frac{n}{\nu} \right\} \right) V_{[i/\nu]} + \left\{ \frac{n}{\nu} \right\} V_{[i/\nu]+1} \tag{14}$$

and coincides with that obtained in [22] from the Hubbard algorithm for finite-range interaction if one replaces the interaction range with the ring circumference (curly brackets in (14) denote the fractional part). Since the GS energy does not include the parameter ξ, all configurations related to its different values are GS ones. As is obvious from (13) the changing of ξ by unity corresponds to the rotation of all electrons as a whole by one lattice spacing and after changing ξ by q the configuration will coincide with itself. This means that the 'evolution' of ξ transfers between different vacuums of Hamiltonian (1). To trace how this transfer occurs let us follow what happens with particles $i = 0, 1, \ldots, p-1$ (one period) on increasing ξ from zero to unity (rotation of the whole electron system by one lattice spacing). To do this it is convenient to rewrite (13) in the form

$$x_i = [[i/\nu] + \{i/\nu\} - \xi]. \tag{15}$$

In our case (filling factor $\nu = p/q$, p and q have no common factor) the following property exists:

$$\{s/\nu\} = \{s'/\nu\} \qquad \text{only for } s = s' \qquad \text{if } s, s' = 0, 1, \ldots, p-1. \tag{16}$$

Statement (16) is true because otherwise $(s - s')/\nu$ would be proportional to an integer, which contradicts the fact that p and q do not have a common factor. Property (16) means that we can order fractional parts appearing in (15):

$$\{i_0/\nu\} < \{i_1/\nu\} < \ldots < \{i_{p-2}/\nu\} < \{i_{p-1}/\nu\}.$$

When $\xi = 0$ the initial configuration is given by $x_i = [i/\nu]$. Within the interval $0 < \xi < \{i_1/\nu\}$ we obtain one new configuration defined by

$$x_i = [i/\nu] \qquad \text{for } i \neq i_0, x_{i_0} = -1.$$

This configuration differs from the initial one just by shifting the i_0th electron by one spacing to the left. In the interval $\{i_1/\nu\} < \xi < \{i_2/\nu\}$ we find two electrons shifted by one spacing to the left

$$x_i = [i/\nu] \qquad \text{for } i \neq i_0, i_1 \qquad x_{i_0} = -1, \ x_{i_1} = [i_1/\nu] - 1.$$

Proceeding with the evolution we will transfer different vacuums from one to another and within p steps rotate the whole electron system on one lattice spacing. At each step we should move only one electron in the period. Therefore we have finished the proof of our statement mentioned above: with no overlap, the GS configuration of $N_e = Mp$ electrons on a ring with $N = Mq$ sites is such that it is enough to shift only M electrons to transfer one vacuum state (the GS configuration) to another.

Returning to the calculation of the parameter $\tilde{T}_{\alpha\beta}$ in Hamiltonian (9), for the leading order in the overlap t we may retain only transitions between $|\alpha\rangle$ states corresponding to the largest hopping term (which corresponds to the shift of M special electrons, described above). If we label the nearest (in the sense of transferring probability, i.e. magnitude of matrix elements (10)) states as $|\alpha\rangle$ and $|\alpha \pm 1\rangle$, we obtain a tight-binding Hamiltonian with nearest-neighbour hopping

$$\mathcal{H}_{\text{eff}} = \sum_\alpha |\alpha\rangle E_\alpha \langle\alpha| - \tilde{t}e^{iM\theta}|\alpha + 1\rangle\langle\alpha| - \tilde{t}e^{-iM\theta}|\alpha\rangle\langle\alpha + 1| \qquad (17)$$

where

$$\tilde{t} = \left| \langle \alpha \pm 1|T(-(1/\mathcal{H}_0)\mathbf{Q}T\mathbf{Q})^{M-1}|\alpha\rangle \right| \simeq t(2t/V)^{M-1}. \qquad (18)$$

Here V is the characteristic Coulomb excitation energy, which is of the order of the energy of the first excited level and related to the discreteness of lattice. Therefore, the problem is reduced to the problem of one 'particle' moving with a renormalized hopping term

$$\tilde{t} = t(2t/V)^{M-1} \qquad (19)$$

through a ring with q sites. According to our previous consideration the q low-lying energy levels appearing due to the GS degeneracy removal are given by

$$E_n(\varphi) = -2t(2t/V)^{M-1}\cos(2\pi/q)(n + \varphi) \qquad n = 0, 1, \ldots, q - 1 \qquad (20)$$

where $\varphi = \phi/\phi_0$ is the dimensionless flux.

(20) shows that the φ-dependent energy shift (and therefore the persistent current) depends not on the filling factor $\nu = p/q$ as might be expected, but on its denominator q only. It also depends on the common factor M and not on the number of electrons.

What is most surprising is the fact that in a case where no common factor exists ($N_e = p, N = q, M = 1$) there are only two special electrons whose displacements lead to the transform of a vacuum state $|\alpha\rangle$ into another one distinguishing only by the position of the defect Y_{m-1}. This defect can be regarded as a freely moving quasiparticle with the bare electron overlap t and feeling no Coulomb interactions at all. In the situation when the numbers of sites and electrons have no common factor the GS energy does not depend on N_e:

$$E_n(\varphi) = -2t \cos(2\pi/q)(n + \varphi). \tag{21}$$

The persistent current can be easily calculated using the well known relation

$$I(\varphi) = -(e/h)\partial E_{GS}(\varphi)/\partial\varphi$$

where $E_{GS}(\varphi) = \min(E_n(\varphi))$ is the GS energy, which is periodic in φ with unit period:

$$I(\varphi) = -(e/h)t(4\pi/q)\sin(2\pi/q)\varphi \qquad -\tfrac{1}{2} \leqslant \varphi \leqslant \tfrac{1}{2}. \tag{22}$$

In the case of $M \neq 1$ the persistent current can be obtained in the same way:

$$I(\varphi) = -(e/h)t(2t/V)^{M-1}(4\pi/q)\sin(2\pi/q)\varphi \qquad -\tfrac{1}{2} \leqslant \varphi \leqslant \tfrac{1}{2}. \tag{23}$$

In the case of small flux ($2\pi\phi/q \ll 1$) (22) and (23) coincide with the result obtained in [14] by the variational method. Expression (23) explicitly demonstrates insensitivity to the number p of electrons per elementary cell of the Wigner crystal. This insensitivity can be easily understood in the terms of M quasiparticles described above. The weakness of their interaction stems from the fact that the change in Coulomb energy under the displacement of one special electron is governed by interactions between these special electrons only (the Coulomb energy of the interaction of the special electron with the rest of them is not changed under this displacement). In other words, the energy U_{ij} of their interaction is equal to the Coulomb energy of a one-spacing shift for particles separated by a distance $|i - j|q$, i.e. $U_{|i-j|} = V_{|i-j|q}$.

The fact that in the leading order we can introduce M weakly coupled 'particles', insensitive to the rest of the electrons composing the Wigner lattice, leads to an unexpected behaviour of the coherence length in the insulating regime as a function of filling factor and, accordingly, to a drastical change of metal–insulator transition criteria even in the case when the filling factor is of the order of unity. To obtain these features it is sufficient to note that expression (20) contains a factor exponential in the electron number, which implies a metal–insulator transition (in the thermodynamical limit $M \to \infty$) when the characteristic Coulomb energy becomes equal to the electron overlap, but as has been mentioned above, the typical energy in the denominator of (20) is that $V(q)$ of a defect pair creation in the electron lattice gas with filling factor $1/q$ (a defect providing the smallest increase of the Coulomb energy corresponds to the structure ... $[q][q]$ ... $[q + 1][q][q]$ ... $[q][q - 1][q][q]$ ...; $V(q)$ is the extra Coulomb energy when pair $[q + 1]$ and $[q - 1]$ are infinitely moved apart). This means that even for filling factor close to unity the metal–insulator transition occurs at small enough overlap if q is large enough. One can easily check that stiffness coefficient

$D (D = (N/\varphi^2)\partial^2 E/\partial\varphi^2)$ calculated with the use of (20) is proportional to the small exponent under the thermodynamic limit $(M \to \infty)$

$$D = Nt(2\pi/q)^2 e^{-N/\xi} \tag{24}$$

as it should be in the insulating regime, but the coherence length ξ

$$\xi = q \ln^{-1}(V(q)/2t) \tag{25}$$

tends to infinity when q increases. A metal–insulator transition $(\xi = \infty)$ occurs at overlap $t = V(q)/2$ which is essentially less than that of the half-filled case. It is important to note that this conclusion is valid as long as $q \gg 1$ even if $\nu = p/q$ is close to one half.
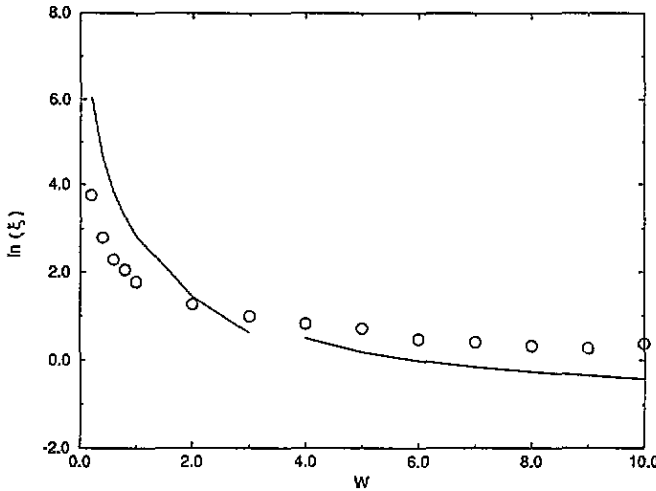
Figure 1. The localization length as a function of disorder. The line represents (28) (with $\tilde{W} = 2.5$) while the symbols correspond to the localization length extracted from the numerical data according to (26). The ensemble average is performed over 500 realizations of disorder.

Some predictions concerning the disorder effect can be made due to the reduction of the initial many-body problem to a rather simple Hamiltonian (17), where E_α are 'disorder' energies of different vacuums (the second term in (11)). Since the effective Hamiltonian (17) describes a tight-binding model with disorder (and no longer contains Coulomb interactions explicitly) we can use the well known results for the persistent current of a non-interacting system [16], replacing the number of sites with q and the overlap with the renormalized one $\tilde{t}$ (18):

$$I = I_0 \exp(-q/\zeta) \tag{26}$$

where I_0 is the amplitude of the persistent current of one particle on an ordered ring with q sites and overlap $\tilde{t}$:

$$I(\varphi) = -(e/h)\tilde{t}4\pi/q \qquad -\tfrac{1}{2} \leqslant \varphi \leqslant \tfrac{1}{2} \tag{27}$$

and ζ is an effective localization length

$$\zeta = \begin{cases} 105(\tilde{t}/\tilde{W})^2 & \tilde{W} \ll \tilde{t} \\ \ln^{-1}(\tilde{W}/2e\tilde{t}) & \tilde{W} \gg \tilde{t} \end{cases} \tag{28}$$

where $\tilde{W}$ is the effective width of distribution of the on-site energy E_α for a particular GS $|\alpha\rangle$. One should note that since the random part depends on the summation of the relevant on-site energies ε_i of the original Hamiltonian ($E_\alpha = \sum_{i \in \alpha} \varepsilon_i$) it is no longer uniformly distributed between $-W/2$ and $W/2$ as for ε_i. Nevertheless, as a zero approximation the effective width of distribution may be estimated as $\tilde{W} \sim \sqrt{N_e} W$. In order to verify this assumption we have performed an exact diagonalization numerical calculation of the persistent current following a method presented in [11] and [14] for a system of four electrons and 11 sites. Using (26), ζ is extracted from the numerical current and compared with the non-interacting results of (28) (figure 1). For $\tilde{W} = 2.5$ a reasonable fit is obtained between the theory and the numerical results.

In conclusion, a perturbative calculation for the persistent current of a strongly interacting 1D ring has been presented. The system in the limit of small overlap can be represented by M weakly interacting quasi-particles. The current is proportional to $(t/V)^{M-1}$. For the disordered case the current decreases proportionally to an effective non-interacting localization length.

Acknowledgments

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