LETTER TO THE EDITOR

A Hartree–Fock study of charge redistribution in a two-dimensional mesoscopic structure

A Kambili[1], H Fehrmann[2], C J Lambert[2] and J H Jefferson[3]

[1] Department of Physics, University of Bath, Claverton Down, Bath BA2 7AY, UK
[2] School of Physics and Chemistry, Lancaster University, Lancaster LA1 4YB, UK
[3] Defence Evaluation and Research Agency, St Andrews Road, Malvern, Worcs WR14 3PS, UK

E-mail: pysak@bath.ac.uk (A Kambili)

Abstract
In this letter, we investigate the ground state of two-dimensional disordered cylinders which contain spinless, interacting electrons using the Hartree–Fock approximation. Calculations of the deviation of the polarization from uniformity reveal a tendency of the charge to rearrange towards the ends of the system. The presence of disorder results in fluctuations of the deviation around its mean value, which are more pronounced when the disorder strength is of the order of the interaction between the electrons.

The existence of persistent currents in normal mesoscopic rings threaded by a magnetic flux [1] has stimulated a great deal of experimental and theoretical work [2–13]. More recently, there have been studies of the ground state of one-dimensional rings containing spinless fermions [14–16] which take into account both electron–electron interactions and disorder. Strongly disordered rings with short-range interactions and a half-filled band exhibit a reorganization of the charge in the ground state. The charge density changes from an inhomogeneous configuration due to the presence of the strong disorder to a periodic array of charges as a result of the interactions.

In the present letter, we study the ground state of two-dimensional cylinders which contain spinless, interacting electrons via Coulomb interactions, by solving self-consistently the Hartree–Fock equation. The validity of the method has already been established [17] by studying the ground state of one-dimensional disordered rings and finding good agreement with the exact calculations [16]. Our aim is to examine reorganization of the charge in the ground state and, in particular, the manner in which charge tends to polarize towards the ends of the cylinder, thereby producing spontaneous dipole or quadrupole moments.

The system under investigation is a two-dimensional cylinder, formed by a tight-binding lattice with M sites in the longitudinal direction (x) and L sites in the transverse direction (y). We take periodic boundary conditions along the longitudinal direction and free boundary

conditions along the transverse direction. The cylinder contains N spinless electrons described by the Hamiltonian

$$H = \sum_{l=1}^{LM} \varepsilon_l \hat{c}_l^\dagger \hat{c}_l + \sum_{l,k=1}^{LM} V_{lk} \hat{c}_l^\dagger \hat{c}_k + \frac{1}{2} \sum_{l,k=1}^{LM} U_{lk} \hat{c}_l^\dagger \hat{c}_l \hat{c}_k^\dagger \hat{c}_k \tag{1}$$

where each site l has coordinates $l = (x, y)$. The operators $\hat{c}_l^\dagger$, $\hat{c}_l$ create and destroy a particle at site l, respectively. V_{lk} is the element for hopping between different sites. In the following, we will restrict ourselves just to nearest-neighbour hopping elements of strength $V_{lk} = -V$. ε_l is the on-site energy which is equal to $\varepsilon_l = 4V + r_l$, where r_l are random numbers uniformly distributed over the range $[-W/2, +W/2]$. W is the strength of the disorder, and in the clean case $W = 0$. U_{lk} is the interaction between the particles, which has been taken to be long range:

$$U_{lk} = \frac{U}{|r_1 - r_2|} \tag{2}$$

where r_n is the position of the nth particle. The Hartree–Fock equation which corresponds to the Hamiltonian (1) is of the form

$$\varepsilon_l \Psi^n(l) - V \sum_{l'=\text{n.n. of } l} \Psi^n(l') + \sum_{m=1}^{N} \sum_{k=1}^{LM} |\Psi^m(k)|^2 U_{lk} \Psi^n(l) - \sum_{m=1}^{N} \sum_{k=1}^{LM} \Psi^{*m}(k) \Psi^m(l) U_{lk} \Psi^n(k)$$

$$= E_n \Psi^n(l) \tag{3}$$

where $\Psi^n(l)$ is the amplitude of the nth single-particle wavefunction on site l and E_n is the corresponding single-particle energy. The third and fourth terms are the direct and exchange potentials, respectively.

The probability of finding an electron on site (l) is

$$\nu_{x,y} = \sum_{n=1}^{N} |\Psi^n(x, y)|^2$$

and hence the mean number of electrons per unit length in the transverse direction is

$$\rho(y) = \sum_{x=1}^{M} \nu_{x,y} \tag{4}$$

We then define

$$p(y) = \frac{\rho(y)}{N} \tag{5}$$

where $p(y)\,\Delta y$ is the probability of finding an electron in the interval $[y, y + \Delta y]$. A measure of the deviation of the charge from uniformity is the standard deviation of $p(y)$:

$$\sigma^2 = \langle y^2 \rangle - \langle y \rangle^2 \tag{6}$$

where

$$\langle y^n \rangle = \sum y^n p(y)\,\Delta y.$$

In the case of a clean system ($W = 0$) the electron density for a uniform distribution must be $\rho(y) = N/L$, where L is the system size in the transverse direction (number of chains). This gives $\sigma^2/L^2 = 1/12$. On the other hand, for the extreme case in which half the charge is at $L/2$ and the other half at $-L/2$,

$$\rho(y) = \frac{N}{2} \delta\left(y + \frac{L}{2}\right) + \frac{N}{2} \delta\left(y - \frac{L}{2}\right)$$

which gives $\sigma^2/L^2 = 1/4$. Thus, the length-normalized deviation of $p(y)$ can take values in the interval $[1/12, 1/4]$, the minimum and the maximum values corresponding to a uniform distribution and a maximally 'polarized' one, respectively.

In figure 1 we present the normalized deviation with respect to the number of particles N, for different values of U, and $V = 1$. The system has no disorder and its size is $L = M = 10$. As we increase the interactions between the particles, for small N, σ^2/L^2 approaches its maximum value, which indicates total 'polarization'. This is the expected result since we are approaching the electrostatic limit. When the system contains more electrons there is still an increase in σ^2/L^2 as U increases, but not all electrons move towards the ends of the cylinder. We have confirmed that this again approaches the expected minimum-electrostatic-energy configuration.
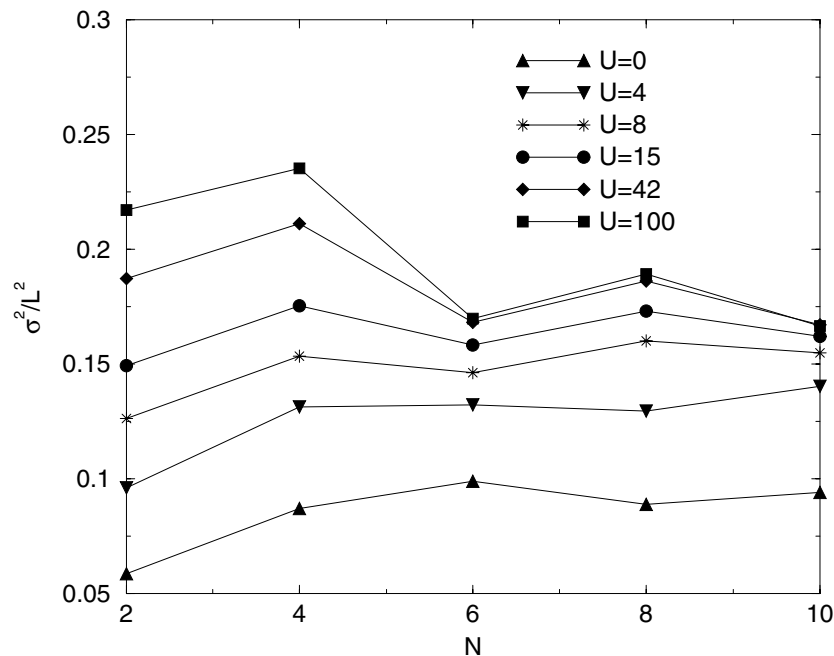

Figure 1. The length-normalized deviation of $p(y)$ with respect to the number of particles N for a clean cylinder of size $L = M = 10$, for different values of the interaction strength U.

In figures 2 and 3 we show σ^2 for a system with non-zero disorder. In figure 2 we plot the ensemble average of σ^2 versus U, for disorder strength $W = 2$ and $N = 10$ along with σ^2 for three individual samples. Individual samples show small fluctuations around the mean value of σ^2 indicating that the charge tends to separate. Increasing the disorder, as in figure 3 where $W = 4$, one can see that the fluctuations increase with disorder, even though the average (dots) remains practically unaffected by it. However, the behaviour of the first moment $\langle y \rangle$ for individual samples is more pronounced than that for σ^2. In figures 4 and 5 we have plotted $\langle y \rangle$ for two different strengths of disorder, $W = 2$ and $W = 4$, respectively. In the insets of figures 4 and 5, the ensemble average of the absolute value of the first moment is shown.

Figures 2, 3, 4 and 5 illustrate behaviour which we expect to be typical of small systems with free-end boundary conditions in at least one direction—namely that with increasing U the dipole moment $\langle y \rangle$ induced by random potential fluctuations (i.e. $W \neq 0$) tends to zero, and the charge distribution becomes sharply peaked at the ends of the samples. A key feature revealed
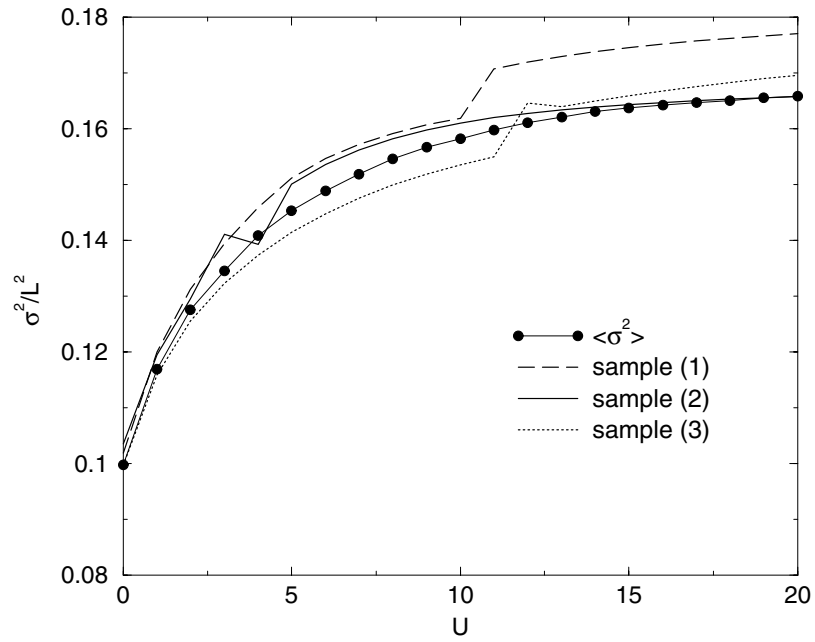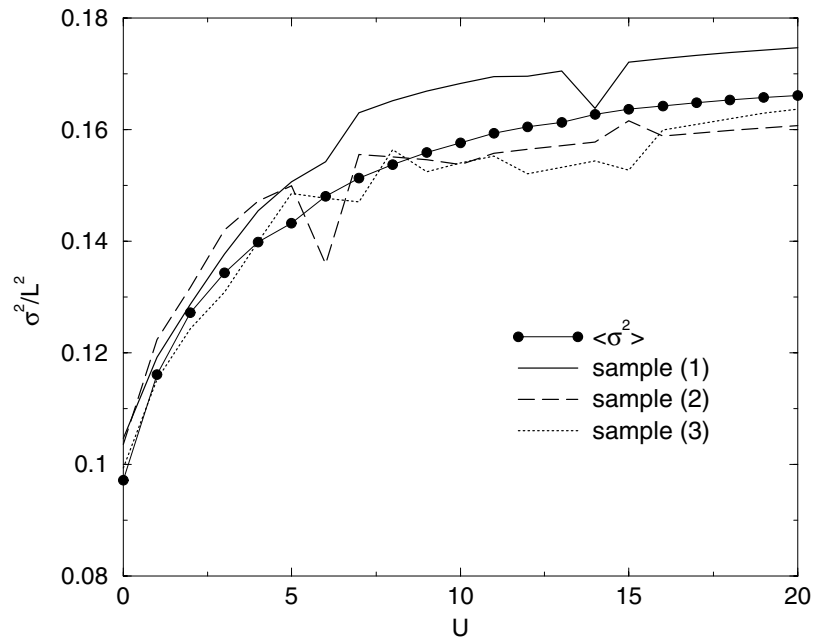
Figure 2. The length-normalized deviation of $p(y)$ with respect to the interaction for disordered cylinders of size $L = M = 10$ and $N = 10$ electrons, with $W = 2$. The dots represent the ensemble average of σ^2 obtained from 200 samples. The different lines represent individual disorder realizations.

Figure 3. The length-normalized deviation of $p(y)$ with respect to the interaction for disordered cylinders of size $L = M = 10$ and $N = 10$ electrons, with $W = 4$. The dots represent the ensemble average of σ^2 obtained from 200 samples. The different lines represent individual disorder realizations.
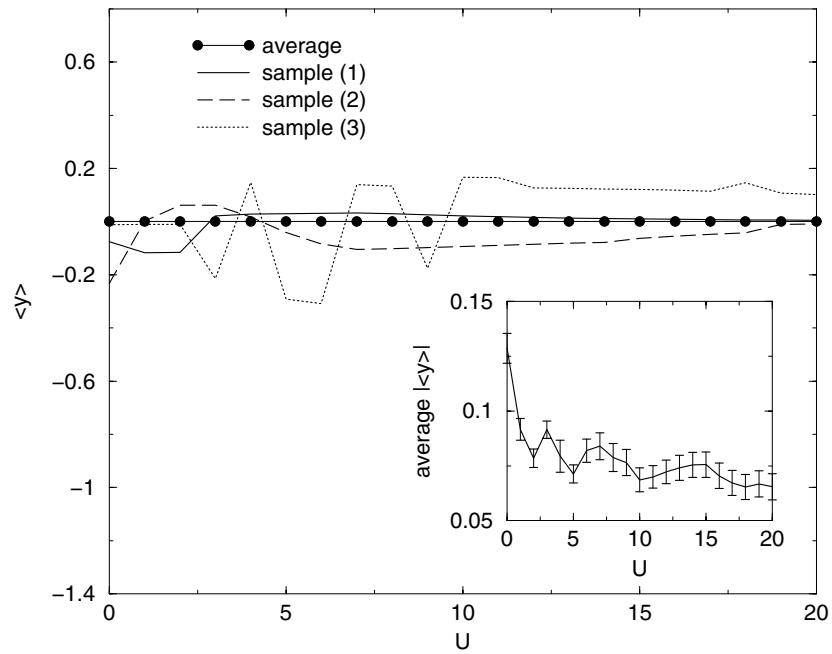
Figure 4. The first moment of $p(y)$ versus U for disordered cylinders of size $L = M = 10$ and $N = 10$ electrons, with $W = 2$. The dots represent the ensemble average. The different lines represent individual disorder realizations. The inset shows the average of $|\langle y \rangle|$ versus U.
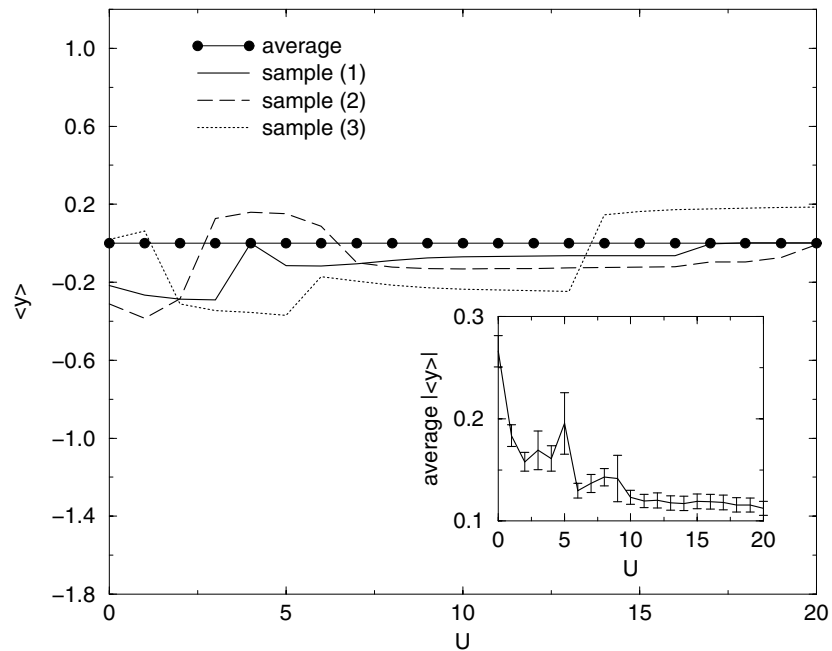

Figure 5. The first moment of $p(y)$ versus U for disordered cylinders of size $L = M = 10$ and $N = 10$ electrons, with $W = 4$. The dots represent the ensemble average. The different lines represent individual disorder realizations. The inset shows the average of $|\langle y \rangle|$ versus U.

by these figures is that at intermediate values of U (of order W), both σ^2 and $\langle y \rangle$ exhibit large sample-to-sample fluctuations about their means and large fluctuations with increasing U, associated with charge redistribution of the ground state.

Finally, in figures 6, 7 and 8 we present σ^2, $\langle y \rangle$ and the current I, respectively, as functions of the phase $\phi = 2\pi \Phi / \Phi_0$, where Φ is the magnetic flux threading the cylinder and Φ_0 is the flux quantum. The current is equal to

$$I = -\frac{\delta E_g}{\delta \phi} \tag{7}$$

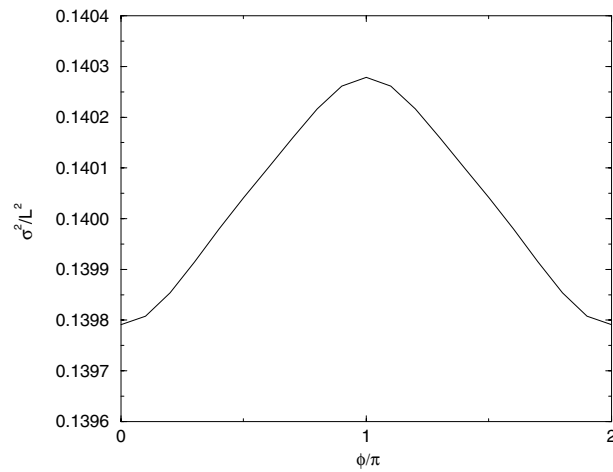where E_g is the Hartree–Fock ground-state energy.

Figure 6. The length-normalized deviation of $p(y)$ for an individual disorder realization, as a function of the magnetic field. The cylinder is of size $L = M = 10$ and contains $N = 10$ electrons, with $W = 2$. The results have been obtained for $U = 4$.

Figure 7. The first moment of $p(y)$ for an individual disorder realization, with respect the magnetic field. The cylinder is of size $L = M = 10$ and contains $N = 10$ electrons, with $W = 2$. The results have been obtained for $U = 4$.
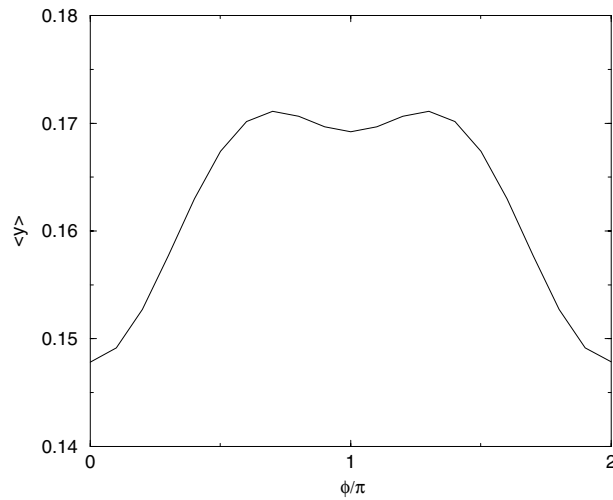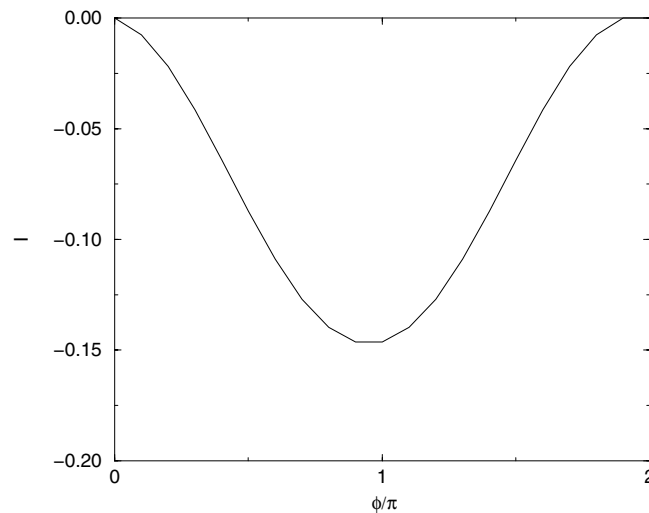
Figure 8. Current versus magnetic field for an individual disorder realization. The cylinder is of size $L = M = 10$ and contains $N = 10$ electrons, with $W = 2$. The results have been obtained for $U = 4$.

The results show the behaviour of one disordered cylinder, for the case of $W = 2$ and for one value of the interaction strength ($U = 4$) such that it is of the order of the disorder strength. A common feature of these three figures is that all quantities are symmetrical around the value of the phase ϕ which corresponds to a magnetic field of half a flux quantum. Such charge fluctuations could possibly be detected experimentally by placing a SET in the vicinity of a sample, which couples to the electric field generated by such a non-uniform charge distribution.

In this letter, we have made a Hartree–Fock study of the ground state of two-dimensional cylinders which contain spinless, interacting electrons. We found that the charge in the ground state shows a separation towards the ends of the cylinder, which is reflected in the polarization of the system. The polarization shows fluctuations around its mean value in the presence of disorder. These fluctuations are stronger in the first moment of the charge distribution when the disorder, bandwidth and interaction between the electrons are of the same order, reflecting the competition between Mott and Anderson localization [18].

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