Oscillatory persistent currents in quantum rings

Alexander A. Vasilchenko*
National Research Tomsk State University, 634050 Tomsk, Russia

Abstract. The density functional theory is used to study persistent currents in two-dimensional quantum rings containing several electrons. We find a series of magic numbers for the total angular momentum of electrons in the strong magnetic field and show that changes in the angular momentum of electrons lead to persistent current oscillations. We suggest an empirical expression for the period of persistent current in quantum rings and examine the effect of Coulomb interaction on the properties of persistent currents.

1 Introduction

It is well known that persistent current can exist in mesoscopic metallic rings placed into the magnetic field [1-12]. Over the past decades, researchers have succeeded in experimentally observing the persistent current oscillations in metallic rings. Let us note that there have been many studies on a similar effect in superconducting rings (Little-Parks effect [13]). The Little-Parks oscillations and persistent current oscillations in quantum rings are associated with the change in energy of the system in the magnetic field. In two-dimensional systems with axial symmetry, both effects are explained by the change in the angular momentum of electrons in quantum rings and in the order parameter in superconducting rings.

A theoretical paper [1] has stimulated the study of persistent currents in mesoscopic metallic rings. Over the recent years, many theoretical [2-8] and experimental [9-12] works have focused on this matter. It is believed that in metallic rings one can disregard the interaction of electrons when calculating the persistent current [5, 9]. Experimental results confirm this assumption [9].

Properties of persistent currents in semiconductor structures have been studied less extensively. Theoretical [14-26] and experimental [27-29] works examine the properties of persistent currents in semiconductor quantum rings. The authors of [29] measured the persistent current in InAs/GaAs quantum rings with one electron. They determined the persistent current via the magnetic moment of electrons in the assembly of quantum rings. In order to interpret this result, they solved the Schrödinger equation numerically for different types of confinement potentials. The calculation results are in good agreement with experimental results [29].

Electron-electron interaction plays an important role in such phenomena as the fractional quantum Hall effect, metal-dielectric transition [30], conductivity quantization [31], Wigner crystallization [32], and spontaneous spin polarization in quantum wires [33]. The purpose of this paper is to report on the effect of electron-electron interaction on the persistent current in a quantum ring. We use the density functional theory to study persistent currents in two-dimensional quantum rings containing several electrons.

* e-mail: a_vas2002@mail.ru
2 Theoretical model

Hereinafter, the atomic system of units is used, where energy is expressed in units of \( \text{Ry} = \frac{e^2}{2\epsilon a_B} \), and length in units of \( a_B = \frac{\varepsilon \hbar^2}{m_e e^2} \), where \( m_e \) is the effective electron mass, \( \varepsilon \) is the dielectric constant. All calculations are performed for the two-dimensional GaAs quantum rings, for which \( \varepsilon = 12.4 \) and \( m_e = 0.067 m_0 \) (\( m_0 \) is the free electron mass). For GaAs we get \( a_B = 9.8 \text{ nm}, \text{Ry} = 5.9 \text{ meV} \).

According to the density functional theory, the total energy of the many-electron system in the external potential \( V_{\text{ext}}(r) \) is the functional of electron density \( n(r) \):

\[
E[n] = T[n] + E_H[n] + E_{\text{xc}}[n] + \int V_{\text{ext}}(r)n(r)dr,
\]

where \( T[n] \) is the kinetic energy of non-interacting electrons in the perpendicular magnetic field \( B \), \( E_{\text{xc}}[n] \) is the exchange-correlation energy.

The Coulomb energy has the form

\[
E_H[n] = \frac{1}{2} \int V_H(r)n(r)dr,
\]

where

\[
V_H(r) = 2\int \frac{n(r')}{|r-r'|}dr'.
\]

The challenge of the functional density theory is that the type of exchange-correlation energy \( E_{\text{xc}}[n] \) is unknown in the general case. In practice, different approximations are used for the exchange-correlation energy. Hereinafter, we take into account only the exchange energy and use the local density approximation for it:

\[
E_x[n] = \int \varepsilon_x(n)n(r)dr - \sum_m \left( \varepsilon_x(n_m) + \frac{1}{2} V_{H,m}(n) n_m(r)dr \right),
\]

where \( V_{H,m}(r) = 2\int \frac{n_m(r')}{|r-r'|}dr' \), \( n_m(r) \) is the density of electron with angular momentum \( m \), \( \varepsilon_x(n) \) is the exchange energy per electron for uniform electron gas that looks as follows for the lower spin Landau level:

\[
\varepsilon_x(n) = -\sqrt{2\pi} \alpha L n(r),
\]

where \( L \) is the magnetic length.

Let us consider equation (4) in greater detail. In local density approximation, the compensation of electron self-action in the exchange and Coulomb energy turns out to be incomplete. When the number of electrons is finite and small, one needs to exclude the self-action of electrons, which is what is done in expression (4). The use of equation (4) in the Kohn-Sham equations results in good agreement with the exact diagonalization results [34, 35]. The difference between the energy calculated using the Kohn-Sham equations and the exact results was less than 5
percent for quantum dots with a number of electrons \( N = 3 \) [34] and around 13 percent for \( N = 7 \) [35]. Most importantly, the same sets and periods of magic numbers were obtained for the total angular momentum of electrons, as in exact calculations [34, 35].

We perform the calculations for the magnetic fields, at which all two-dimensional electrons are spin-polarized. Varying the energy (1) and taking into account the circular symmetry, we obtain the Kohn-Sham equations for spin-polarized electrons

\[
\left\{-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{1}{r} \frac{\partial}{\partial r} + \frac{m^2}{r^2} + V_{\text{eff}}(r)\right\}\phi_n(r) = E_n\phi_n(r),
\]

with the effective single-particle potential

\[
V_{\text{eff}}(r) = V_H(r) - V_{H,m}(r) + 2\alpha(n(r) - n_m(r)) + V_{\text{ext}}(r),
\]

where \( m \) is the angular momentum of an electron, \( n_m(r) = \left| \phi_m(r) \right|^2 \), \( n(r) = \sum_{\text{occ } m} n_m(r) \), \( \alpha = -\sqrt{2}\pi \alpha_N \).

Let us take the parabolic confinement potential with frequency \( \omega_0 \) and ring radius \( r_0 \):

\[
V_{\text{ext}}(r) = \frac{\omega_0^2}{4}(r - r_0)^2.
\]

The persistent current is the sum of the paramagnetic and the diamagnetic currents:

\[
I = -\sum_m \frac{2m}{r} \phi_m^2(r) dr + \frac{N}{2\pi d^2},
\]

where \( N \) is the number of electrons in a quantum ring.

### 3 Numerical results and discussion

The Kohn-Sham equations (6) – (7) with external potential (8) are solved numerically. Calculations are performed for different sets of \( m \) values, and the state with minimal energy is taken as the ground state for the given value of the total angular momentum of electrons \( M \). Figure 1 presents the results of electron energy calculations depending on the total angular momentum of electrons. One can see that magic numbers have a period \( \Delta M = N \), and the ground and the metastable states are only possible when

\[
M_p = M_0 + pN,
\]

where \( M_0 = N(N-1)/2 \), \( p = 0, 1, 2 \ldots \).

These magic numbers were also found in quantum dots [34]. The presence of magic numbers with a period \( \Delta M = N \) is explained by the compact configuration of electrons in the angular momentum space. Let us note that with the increase in the
ring radius, the ground state shifts towards larger $M$. This is because the electrons are localized near $r_0$ in the ground state.

The presence of magic numbers leads to quantization of the total angular momentum of electrons (Fig. 2), while the dependence $M(B)$ is a series of angular momentum plateaus separated by the height $N$. The midpoints of all plateaus $B_p$ are close to the direct proportion to the total angular momentum (see Fig. 2):

$$B_p = c M_p,$$  \(11\)

where $c$ is the constant.

![Fig. 1. Total electron energy as a function of the total angular momentum of electrons. $N = 7$, $B = 6.5$ T, $\omega_0 = 0.67$. The points mark the lowest energy for each value of the total angular momentum. The lines connect the points for visual clarity.](image1)

From expressions (10) and (11), we get the following expression for the plateau widths:

$$\Delta B = \frac{2B_1}{N + 1},$$  \(12\)

where $B_1$ corresponds to the midpoint of the first plateau with $M = N(N-1)/2 + N$.

![Fig. 2. Total angular momentum of electrons as a function of magnetic field. $N = 7$, $\omega_0 = 0.67$, $r_0 = 1$. The straight line corresponds to expression (11).](image2)

With a change in the angular momentum of electrons, one ought to expect a change in the persistent current in a quantum ring. Figure 3 presents the calculation
results. The first linear segments on the curves in Fig. 3 correspond to value $M = 28$. Further on, with the increase in the magnetic field, the value of total angular momentum increases with a period $N = 7$. The period of persistent current oscillations is well described by expression (12) and increases with the increase in the ring radius. One can see that the oscillation amplitude weakly depends on the ring radius.

Calculations performed for different values of $N$ and $\omega_0$ ($N < 14$, values of $\omega_0$ are taken as 0.67, 1.0 and 2.0) also show that the period of persistent current oscillations is well described by expression (12). In these calculations, it is assumed that the electrons have a compact configuration.

![Graph of persistent current versus magnetic field](image.png)

**Fig. 3.** Persistent current in a quantum ring as a function of magnetic field. $N = 7$, $\omega_0 = 0.67$.

It is of great interest to study the impact of electron-electron interaction on the properties of persistent current in quantum rings. For this, we perform the calculations without taking into account the electron interaction. In this case, in the Kohn-Sham equations the effective potential equals the external potential: $V_{\text{eff}}(r) = V_{\text{ext}}(r)$. Figure 4 presents the calculation results. Comparison of results presented in Fig. 3 and 4 shows the strong effect of the electron-electron interaction on the persistent current characteristics depending on the magnetic field. Without taking into account the electron-electron interaction, there is an approximately twofold decrease in the persistent current amplitude, but the most crucial difference is associated with the increase in the oscillation period and the shifting of the ground state with the given $M$ towards larger magnetic fields. For instance, at $r_0 = 3$, value $B_1$ in Fig. 4 is 1.7 times larger than in Fig. 3. An even bigger difference in the values of $B_1$ and oscillation periods is observed when $r_0$ goes down. For instance, for radii $r_0 = 2$ and $r_0 = 1$, values of $B_1$ are $B_1 = 5.1$ T and $B_1 = 7.1$ T, respectively (Fig. 3), while in the absence of interaction $B_1 = 13.7$ T (Fig. 4) and $B_1 = 56$ T (not shown in Fig. 4). For non-interacting electrons, persistent current oscillations are close to Aharonov-Bohm oscillations with a period $\Phi_0 = h/e$, whereas for interacting electrons the period is much smaller than $\Phi_0$. The period $\Phi_0$ corresponds to $\Delta B = 13.7/r_0^2$ in the atomic system of units.

Let us estimate value $B_1$ for the non-interacting electrons. In the magnetic field, the wave function of an electron with angular momentum $m$ has a maximum at $r_m = (2m)^{1/2}L$. In order to achieve the energy minimum, the electrons ought to be
localized near \( r_0 \), and all electrons ought to have a compact configuration. For the state with \( M = M_0 + N \), the electrons have configuration \((1, 2, \ldots, N)\) and the energy of electrons will have a minimum at \((N+1)^{1/2}L \approx r_0\). From the latter expression, we get:

\[
B_1 \approx \frac{6.9(N + 1)}{r_0^2}.
\]  

(13)

Fig. 4. Persistent current in a quantum ring as a function of magnetic field without taking into account the electron-electron interaction. \( N = 7, \omega_0 = 0.67 \).

Let us note that values \( B_1 \) calculated based on expressions (13) agree rather well with the numerical results presented in Fig. 4. The electron-electron interaction leads to the shift of the electron density profile in relation to the confinement potential minimum.

One should expect that with the increase in electron density, the Coulomb interaction would play a smaller role. To study this phenomenon, we perform the calculations with different confinement potential strengths. Figures 5 and 6 present the results of these calculations. Without taking electron-electron interaction into account (Fig. 6), the oscillation period practically does not depend on \( \omega_0 \), and the frequency of confinement potential affects only the persistent current amplitude. Taking electron-electron interaction into account, one observes a change in the persistent current period and amplitude depending on the confinement potential frequency. The persistent current amplitude increases with the increase in frequency (Fig. 5). Such a dependence was obtained for mesoscopic rings in [22, 24]. At sufficiently high values of \( \omega_0 \), the curves of dependence \( I(B) \) in both cases are close to one another (curves with \( \omega_0 = 4 \) in Fig. 5 and 6). The calculation results show that at \( \omega_0 > 4 \), the amplitude and the oscillation period practically do not depend on the confinement potential frequency, both when the electron-electron interaction is present and when it is absent. Therefore, at high \( \omega_0 \) (high electron densities) the effect of Coulomb interaction on the persistent current characteristics goes down. The persistent current period depending on magnetic flux is close to \( \Phi_0 \) both for non-interacting electrons (Fig. 6) and for interacting electrons for high \( \omega_0 \) (curves with \( \omega_0 = 4 \) in Fig. 5). A similar result was obtained in [20] for magnetization in quantum rings. For high \( \omega_0 \), electron-electron
interaction does not affect the magnetic moment (associated with persistent current) of electrons in quantum rings. With the decrease in $\omega_0$, there emerges a slight phase shift between the results for interacting and non-interacting electrons.

Fig. 5. Persistent current in a quantum ring as a function of magnetic field. $N = 7$, $r_0 = 3$.

Fig. 6. Persistent current in a quantum ring as a function of magnetic field without electron-electron interaction. $N = 7$, $r_0 = 3$.

4 Conclusions

The system of Kohn-Sham equations is solved numerically for two-dimensional electrons in the strong magnetic field. We calculate the total energy of electrons and find a series of magic numbers for the total angular momentum of electrons. We calculate the value of persistent current in two-dimensional quantum rings depending on the magnetic field and suggest an empirical expression for the period of persistent current oscillations. We also show that the effect of electron-electron interaction on the persistent current characteristics decreases with the increase in electron density.

Acknowledgements

This work was supported by the State Assignment of the Ministry of Science and Higher Education of the Russian Federation (project No. 0721-2020-0048).
References

1. M. Buttiker, Y. Imry, R. Landauer, S. Pinhas, Phys. Rev. B 31, 6207 (1985).
2. M. Buttiker, Y. Imry, R. Landauer, Phys. Lett. A 96, 365 (1983).
3. B. Reulet, H. Bouchiat, Phys. Rev. B 50, 2259 (1994).
4. F. Marchesoni, J. of Stat. Phys. 70, 247 (1993).
5. E.K. Riedel, F. von Oppen, Phys. Rev. B 47, 15449 (1993).
6. E.M.Q. Jariwala, P. Mohanty, M.B. Ketchen, R.A. Webb, Phys. Rev. Lett. 86, 1594 (2001).
7. H. Bary-Soroker, O. Entin-Wohlman, Y. Imry, Phys. Rev. B 82, 144202 (2010).
8. H. Bluhm, N.C. Koshnick, J.A. Bert, M.E. Huber, K.A. Moler, Phys. Rev. Lett. 102, 136802 (2009).
9. A.C. Bleszynski-Jayich, W.E. Shanks, B. Peaudecerf, E. Ginossar, F. von Oppen, J.G.E. Harris, Science 326, 272 (2009).
10. V. Chandrasekhar, R.A. Webb, M.J. Brady, M.B. Ketchen, W.J. Gallagher, A. Kleinsasser, Phys. Rev. Lett. 67, 3578 (1991).
11. E.M.Q. Jariwala, P. Mohanty, M.B. Ketchen, R.A. Webb, Phys. Rev. Lett. 86, 1594 (2001).
12. H. Bluhm, N.C. Koshnick, J.A. Bert, M.E. Huber, K.A. Moler, Phys. Rev. Lett. 102, 136802 (2009).
13. W.A. Little, R.D. Parks, Phys. Rev. Lett. 9, 9 (1962).
14. V.M. Fomin, V.N. Gladilin, S.N. Klimin, J.T. Devreese, N.A.J.M. Kleemans, P.M. Koenraad, Phys. Rev. B 76, 235320 (2007).
15. V.M. Fomin, V.N. Gladilin, J.T. Devreese, N.A.J.M. Kleemans, P.M. Koenraad, Phys. Rev. B 77, 205326 (2008).
16. L.K. Castelano, G.Q. Hai, B. Partoens, F.M. Peeters, Phys Rev. B 78, 195315 (2008).
17. L.L. Li, D. Moldovan, P. Vasilopoulos, F.M. Peeters, Phys. Rev. B 95, 205426 (2017).
18. S. Viefers, P. Singha Deo, S.M. Reimann, M. Manninen, M. Koskinen, Phys. Rev. B 62, 10668 (2000).
19. J.C. Lin, G.Y. Guo, Phys. Rev. B 65, 035304 (2001).
20. T. Chakraborty, P. Pietilainen, Phys. Rev. B 50, 8460 (1994).
21. W-C. Tan, J.C. Inkso, Phys. Rev. B 60, 5626 (1999).
22. L. Wendler, V.M. Fomin, Phys. Stat. Sol. (b) 191, 409 (1995).
23. L. Wendler, V.M. Fomin, Phys. Rev. B 51, 17814 (1995).
24. L. Wendler, V.M. Fomin, A.V. Chaplik, Solid State Commun. 96, 809 (1995).
25. L. Wendler, V.M. Fomin, A.V. Chaplik, A.O. Govorov, Phys. Rev. B 54, 4794 (1996).
26. D. Bejan, C. Stan, Eur. Phys. J. Plus 134, 127 (2019).
27. R. Debloock, R. Bel, B. Reulet, H. Bouchiat, D. Mailly, Phys. Rev. Lett. 89, 206803 (2002).
28. D. Mailly, C. Chapelier, A. Benoit, Phys. Rev. Lett. 70, 2020 (1993).
29. N.A.J.M. Kleemans, I.M.A. Bominaar-Silkens, V.M. Fomin, V.N. Gladilin, D. Granados, A.G. Taboada, J.M. Garcia, P. Offermans, U. Zeitler, P.C.M. Christianen, J.C. Maan, J.T. Devreese, P.M. Koenraad, Phys. Rev. Lett. 99, 146808 (2007).
30. S.V. Kravchenko, M.P. Sarachik, Rep. Prog. Phys. 67, 1 (2004).
31. R. Crook, J. Prance, K.J. Thomas, S.J. Chorley, I. Farrer, D.A. Ritchie, M. Pepper, C.G. Smith, Science 312, 1359 (2006).
32. J.S. Meyer, K.A. Matveev, J. Phys.: Condens. Matter 21, 023203 (2009).
33. A.A. Vasilchenko, Phys. Lett. A 379, 3013 (2015).
34. P.A. Maksym, Physica B 184, 385 (1993).
35. C. Yannouleas, U. Landman, Phys. Rev. B 70, 235319 (2004).