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PERSISTENT CURRENT OSCILLATIONS IN ELECTRON-HOLE QUANTUM DOTS

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A system of Kohn-Sham equations was solved self-consistently for the two-dimensional, spatially separated electrons and holes. A series of magic numbers were found for the total angular momentum of the electrons and holes in a strong magnetic field. The change of the angular momentum of the charge carriers was shown to lead to oscillations of the persistent current.

Keywords: electron-hole quantum dots, the Kohn-Sham equations, persistent current.

1. Introduction

In recent years, quantum effects in mesoscopic and nanoscale structures have been actively studied. The superconducting transition temperature is well documented to have an oscillatory form in thin superconducting rings with a period equal to half of the magnetic flux quantum $\Phi_0 = h/e$. The situation is much more complicated in quantum rings due to electron-electron interactions. Little-Parks oscillations and oscillations of the persistent current in semiconductor quantum rings are associated with the change of the energy in a magnetic field. Particularly, in two-dimensional systems with axial symmetry, both effects are explained by changes in the angular momentum of the electrons in quantum rings and order parameter in superconducting rings. The oscillations of the persistent current in semiconductor quantum rings have been studied actively both theoretically [1] and experimentally [2]. Systems with two-dimensional electron-hole (EH) complexes have been studied to a lesser degree.

2. Theoretical model

In the present paper the total energy of spatially separated EH quantum dots was calculated with a finite number N electron-hole pairs in a transverse magnetic field B. Density functional theory was used to calculate the total energy of the EH system. The total energy is written for a two-component system (electrons and holes) as

$$E_t[n_e, n_h] = T_e[n_e] + T_h[n_h] + E_c[n_e, n_h] + E_{xc}[n_e, n_h], \quad (1)$$

where T_e, T_h — the kinetic energy of the carriers, E_c – electrostatic energy, E_{xc} — exchange-correlation energy, n_e and n_h — the density of electrons and holes.

It should be noted that for a small number of particles it is necessary to exclude their self-interaction in the expression (1). Exclusion of particles self-interaction leads to good agreement with the exact results for quantum dots with a small number of electrons [3].

We obtain Kohn-Sham equations for electrons and holes by varying the expression (1) according to the densities n_e and n_h:

$$\left[-\frac{\mu}{m_e}\frac{1}{r_e}\frac{\partial}{\partial r_e}\left(r_e\frac{\partial}{\partial r_e}\right)+\frac{\mu}{m_e}\frac{k_e^2}{r_e^2}+\frac{\mu}{m_e}\frac{k_e}{L^2}+\frac{\mu}{m_e}\frac{r_e^2}{4L^4}+V_{eff,e}(r_e)\right]\psi_{e,k_e}(r_e)=E_{e,k_e}\psi_{e,k_e}(r_e), \tag{2}$$

$$\left[-\frac{\mu}{m_h}\frac{1}{r_h}\frac{\partial}{\partial r_h}\left(r_h\frac{\partial}{\partial r_h}\right)+\frac{\mu}{m_h}\frac{k_h^2}{r_h^2}+\frac{\mu}{m_h}\frac{k_h}{L^2}+\frac{\mu}{m_h}\frac{r_h^2}{4L^4}+V_{eff,h}(r_h)\right]\psi_{h,k_h}(r_e)=E_{h,k_h}\psi_{h,k_h}(r_h), \tag{3}$$

where k_e (k_h) — the angular momentum of the electron (hole), m_e (m_h) — mass of the electron (hole), L — magnetic length,
$\mu = m_e m_h/(m_e+m_h)$, $V_{eff,e}(r) = -V_h(r,d)+V_e(r,0)-V_{e,k_e}(r,0)+V_{xc,e}(r)$,
$V_{eff,h}(r) = -V_e(r,d)+V_h(r,0)-V_{h,k_h}(r,0)+V_{xc,h}(r)$, $V_e(r,d) = 2\int\frac{n_e(r')dr'}{\sqrt{|r-r'|^2+d^2}}$,
$V_{e,k_e}(r,d) = 2\int\frac{\psi_{e,k_e}^2(r')dr'}{\sqrt{|r-r'|^2+d^2}}$, $V_h(r,d) = 2\int\frac{n_h(r')dr'}{\sqrt{|r-r'|^2+d^2}}$, $V_{h,k_h}(r,d) = 2\int\frac{\psi_{h,k_h}^2(r')dr'}{\sqrt{|r-r'|^2+d^2}}$,
$n_{e,k_e}(r)=\psi_{e,k_e}^2(r)$, $n_e(r)=\sum_{k_e} n_{e,k_e}(r)$, $n_{h,k_h}(r)=\psi_{h,k_h}^2(r)$, $n_h(r)=\sum_{k_h} n_{h,k_h}(r)$,
d — the distance between the electron and hole quantum dots.

Here and below the exciton system units were used: the energy was measured in units of $Ry_{ex}=e^2/2\varepsilon a_{ex}$, and the length in units $a_{ex}=\varepsilon\hbar^2/\mu e^2$.

The electrons and holes were assumed to be spin-polarized. Electron-hole correlations may be neglected for spatially separated quantum dots, then

$$E_{xc}=\int\varepsilon_{x,e}(n_e)n_e(r)dr-\sum_{k_e}\int\varepsilon_{x,e}(n_{e,k_e})n_{e,k_e}dr+$$
$$\int\varepsilon_{x,h}(n_h)n_h(r)dr-\sum_{k_h}\int\varepsilon_{x,h}(n_{h,k_h})n_{h,k_h}dr,$$

where $\varepsilon_{x,e}=\alpha n_e$, $\varepsilon_{x,h}=\alpha n_h$, $\alpha=\pi\sqrt{2\pi}L$

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

$$I_e=-\frac{\mu}{m_e}\sum_{k_e}\int\frac{2k_e}{r}\psi_{e,k_e}^2(r)dr+\frac{\mu}{m_e}\frac{N}{2\pi L^2},$$

$$I_h=\frac{\mu}{m_h}\sum_{k_h}\int\frac{2k_h}{r}\psi_{h,k_e}^2(r)dr-\frac{\mu}{m_h}\frac{N}{2\pi L^2}$$

3. Numerical results

Kohn-Sham equations were solved numerically for different values of the magnetic field and the distance between the quantum dots. The calculations were performed for different sets of k_e and k_h and the minimum energy was achieved in a compact configuration of particles (neighboring states are populated). This result is shown in Fig. 1 for $N=3$ and $m_e=m_h=0,077m_0$ (m_0 is the free electron mass). The total energy has a minimum when the total angular momentum of the holes is $K_h=3$ (k_h=0,1,2), $K_h=6$ ($k_h=1,2,3$) and $K_h=9$ ($k_h=2,3,4$), i.e. period of magic number is 3. When we increased N (up to ten EH pairs), the period of magic numbers for the total angular momentum of the electrons and holes was equal to N as well. The results presented in Fig. 1 correspond to the magnetic field value, near which occurs transition from one configuration of particles to another. This transition is important to study persistent current oscillations and the fractional quantum Hall effect. At the value of magnetic field $= 3,2$ T, a total energy minimum was achieved for $K_e = 3$ and $K_h = 3$. When the magnetic field was increased, the ground state became the one with $K_e = 6$ and $K_h = 6$.

Changing the angular momentum of the electrons and holes resulted in a jump in the persistent current. Fig. 2 shows the dependence of persistent current of electrons and holes on the magnetic field. The persistent current had an oscillatory form with almost linear segments. Different segments corresponded to different values of K_e and K_h which increased as the magnetic field increased. The first segment in Fig. 2 corresponded to the values of $K_e = K_h = 6$, and for the subsequent segments values K_e and K_h, were equal to 9, 12, 15 and 18. The oscillation period decreased slightly as the magnetic field increased. The amplitude of the oscillations decreased because with largeK_e and K_h the diamagnetic current compensated for the paramagnetic one.

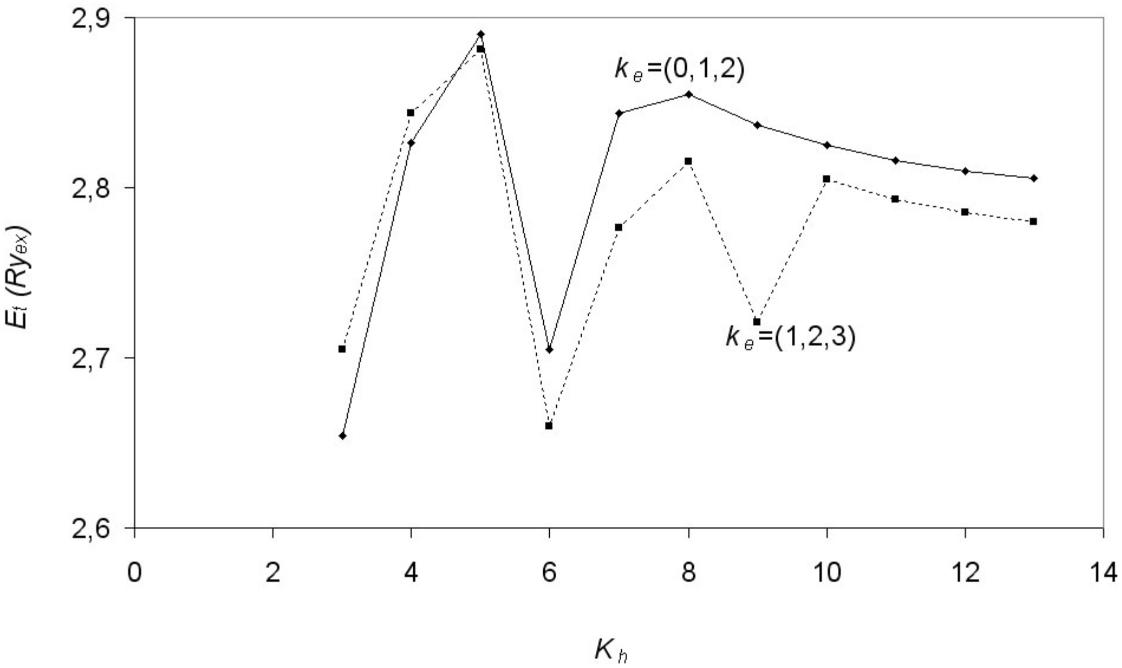

Fig. 1. The total energy versus the total angular momentum of the holes ($N = 3,\ d = 2,\ B = 3,2$ T, $m_e = m_h = 0,077m_0$). The points are connected by lines for illustrative purposes

Fig. 3 shows the phase diagram for the transition from a state with $K_e = K_h = 3$ into the state with $K_e = K_h = 6$. The transition to a new state for small d was possible only in very strong magnetic fields, and this value of the magnetic field increased along with the mass of the hole. When the mass of the holes was doubled, a transition to a new state occurred also with $K_e = K_h$, so the persistent current oscillation period of the electrons and holes were equal (Fig. 4). It should be noted that the oscillation's amplitude of the persistent current was smaller for holes than for electrons, and the oscillation period became longer than in case of $m_e = m_h$.

4. Conclusion

Thus, the system of Kohn-Sham equations were solved numerically for two-dimensional electrons and holes in a strong magnetic field. The total energy of the electron-hole

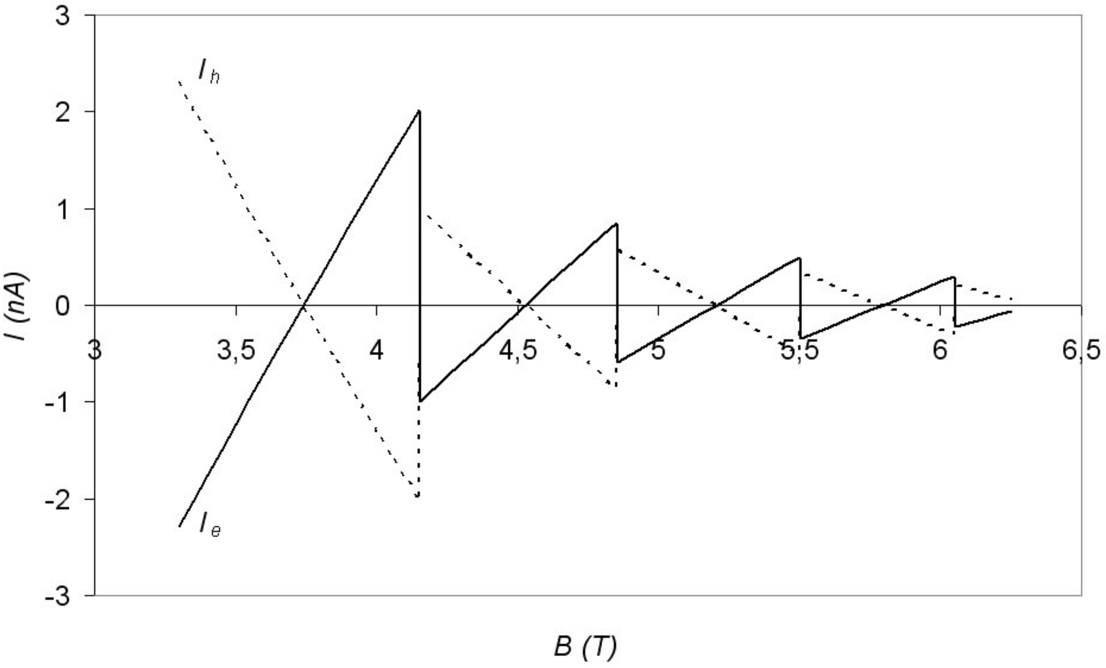

Fig. 2. The persistent current versus the magnetic field ($N = 3$, $d = 2$, $m_e = m_h = 0,077m_0$)

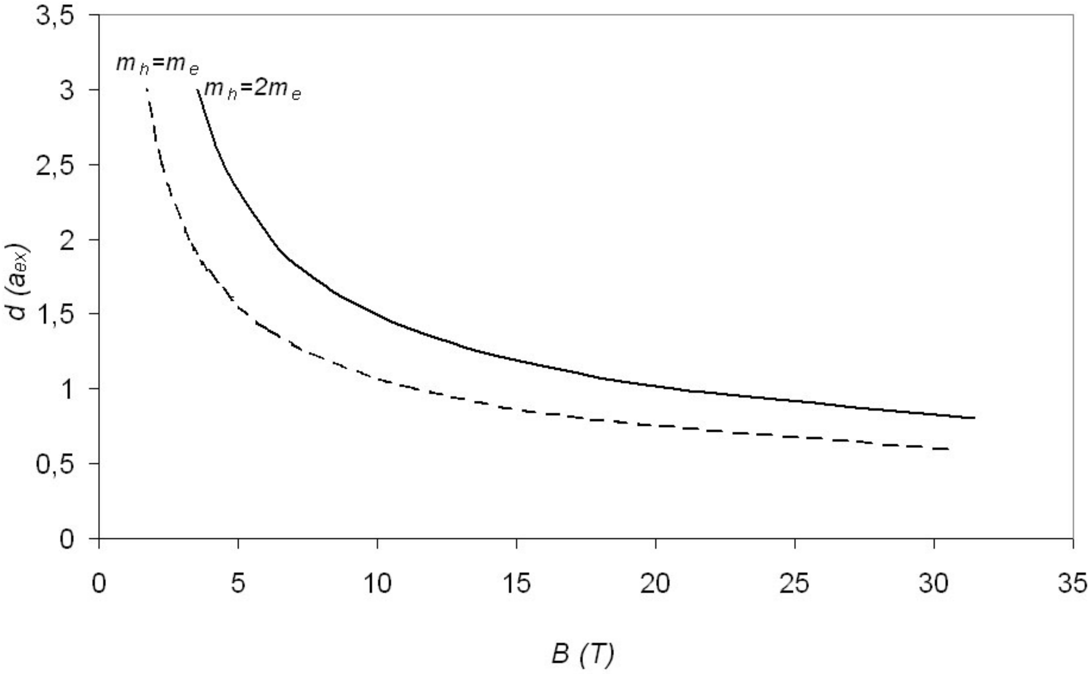

Fig. 3. The phase diagram of transition from state $k_e = (0, 1, 2)$ and $k_h = (0, 1, 2)$ to state $k_e = (1, 2, 3)$ and $k_h = (1, 2, 3)$ (N=3, $m_e = 0,077m_0$)

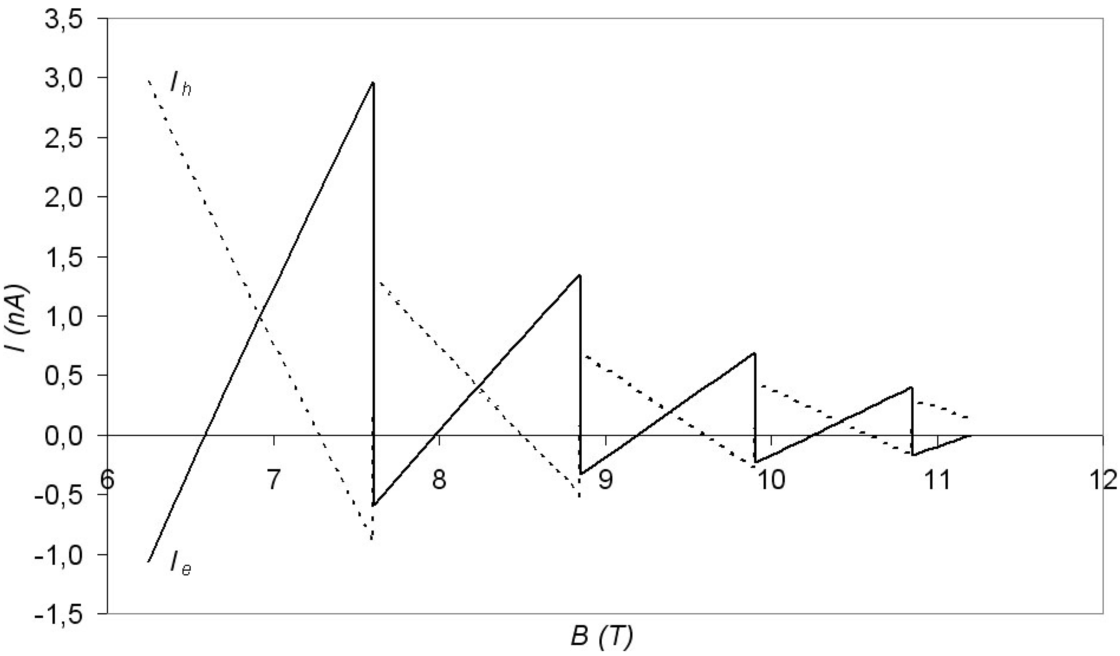

Fig. 4. The persistent current versus the magnetic field ($N = 3$, $d = 2$, $m_h = 2m_e$, $m_e = 0,077m_0$)

system was calculated and a series of magic numbers were found for the total angular momentum of the electrons and holes. Changes in the total angular moment of electrons and holes were shown to lead to oscillations in the persistent current of electrons and holes.

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