Oscillations of the energy, magnetic moment, and current with a period equal to the normal or superconducting flux quantum in cyclic systems

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Oscillations with a period equal to the normal or superconducting flux quantum occur in the current density and the orbital parts of the energy and the magnetic moment in cyclic systems. Transitions between these regimes can be induced by changing the number of electrons or by switching between states with different energies.

Oscillations of the resistance with a period equal to the normal flux quantum $\Phi_0 = \text{cosh}/e$ or the superconducting flux quantum $\Phi_S = \text{cosh}/2e$ occur[1] in the region of hopping conductivity. In the present letter we show that oscillations of the current and the orbital parts of the energy and the magnetic moment with a period equal to the normal or superconducting flux quantum can occur in cyclic systems. Certain properties may oscillate with a period which is a multiple of the normal flux quantum; this effect corresponds to a replacement of the electron charge e by a fractional value of this charge in the expression for Φ_0.

We consider a system of one electron and three lattice sites at the vertices of an equilateral triangle. A three-site system of this sort arises, for example, in the triphenylcyclopropanyl molecule. The Hamiltonian is

$$\mathcal{H} = -|L| \sum_{g=1}^{3} (e^{-i\varphi_g} a_{g\sigma}^+ a_{g+1,\sigma} + e^{i\varphi_g} a_{g+1,\sigma}^+ a_{g\sigma}) - \mu_B H \sum_{g=1}^{3} (n_{g\uparrow} - n_{g\downarrow}), \qquad a_{4\sigma} = a_{1\sigma}, \tag{1}$$

where L is the transport integral, the operators $a_{g\sigma}^+$ ($a_{g\sigma}$) create (annihilate) an electron with a spin projection σ at site g ($g = 1,2,3$); $n_{g\sigma} = a_{g\sigma}^+ a_{g\sigma}$; φ_1, φ_2, φ_3 are the phase shifts which result from the orbital effect of the magnetic field; H is the magnetic field; and μ_B is the Bohr magneton. Solving the Schrödinger equation with Hamiltonian (1), we find the energies

$$E_n = -2|L|\cos\frac{2\pi}{3}\left[\frac{\Phi}{\Phi_0} + 2(n-1)\right] \pm \mu_B H, \quad n = 1, 2, 3, \tag{2}$$

where $\Phi = \oint_S H_n \, dS$ is the magnetic flux through the equilateral triangle, and S is the area of this triangle. The orbital parts of the energies in (2) are oscillatory functions of the magnetic flux, with a period of $3\Phi_0$. This period is found from the expression $\Phi_0 = \text{cosh}/e$ for the normal flux quantum by replacing the charge e by the fractional charge $e/3$. The magnetic moment M is given by the expression $M = -\partial E/\partial H$ [see, for example, (1.22) in Ref. 2]. We thus find from (2)

$$M_n = M_0 \sin\left\{\frac{2\pi}{3}\left[\frac{\Phi}{\Phi_0} + 2(n-1)\right]\right\} \pm \mu_B , \quad n = 1, 2, 3 . \tag{3}$$

Analogously, for the current density we find

$$j_n = j_0 \sin\left\{\frac{2\pi}{3}\left[\frac{\Phi}{\Phi_0} + 2(n-1)\right]\right\} + \mu_B , \quad n = 1, 2, 3 . \tag{4}$$

It follows from (3) and (4) that the orbital parts of the magnetic moments M_1, M_2, and M_3 and of the current densities j_1, j_2, and j_3 also oscillate with a period of $3\Phi_0$. The energy ($E_{\rm I}$) of the ground level and those ($E_{\rm II}$ and $E_{\rm III}$) of the first and second excited levels can be represented by the series

$$\begin{aligned} E_{\rm I} &= -\frac{6\sqrt{3}}{\pi}|L|\left[\frac{1}{2} + \sum_{n=1}^{\infty}\frac{(-1)^n}{1-9n^2}\cos\left(\frac{2\pi n\Phi}{\Phi_0}\right)\right] + \mu_B H \\ E_{\rm II} &= -\frac{6\sqrt{3}}{\pi}|L|\left[\sum_{n=1}^{\infty}\frac{1-(-1)^n}{1-9n^2}\cos\left(\frac{2\pi n\Phi}{\Phi_0}\right)\right] \pm \mu_B H \\ E_{\rm III} &= \frac{6\sqrt{3}}{\pi}|L|\left[\frac{1}{2} + \sum_{n=1}^{\infty}\frac{1}{1-9n^2}\cos\left(\frac{2\pi n\Phi}{\Phi_0}\right)\right] \pm \mu_B H . \end{aligned} \tag{5}$$

According to (5), the orbital parts of $E_{\rm I}$, $E_{\rm II}$, and $E_{\rm III}$ oscillate with a period of Φ_0. The orbital parts of the magnetic moments $M_{\rm I}$, $M_{\rm II}$, and $M_{\rm III}$ and of the current densities $j_{\rm I}$, $j_{\rm II}$, and $j_{\rm III}$ oscillate with the same period.

The one-electron states of this system can be filled by a number (N_e) of electrons 0, 1, 2, 3, 4, 5, or 6. When the two possible spin projections are taken into account, we find that there are six orbitals. Consequently, for a given value of N_e there are $Z(N_e) = 6!/[N_e!(6-N_e)!]$ states. There are a total of $2^6 = 64$ states (since each of the six orbitals may be vacant or occupied by one electron). In the case of a two-electron system (e.g., the triphenylcyclopropanyl cation), a stable structure corresponds to the case with two electrons with opposite spin projections in the level $E_{\rm I}$. According to (5), in this case the energy of the ground state, the magnetic moment, and the current density oscillate with the normal period Φ_0. In the case of a neutral three-electron system (we are assuming that the ion at each of the three sites has a charge $|e|$), the third electron must be placed in a higher level. If two electrons with opposite spin projections are placed in level $E_{\rm I}$, and a third is placed in $E_{\rm II}$, the energy of this system is, according to (5),

$$2E_{\rm I} + E_{\rm II} = -\frac{6\sqrt{3}}{\pi}|L|\left[1 + 2\sum_{n=1}^{\infty}\frac{1}{1-36n^2}\cos\left(\frac{4\pi n\Phi}{\Phi_0}\right)\right] \pm \mu_B H . \tag{6}$$

It follows from (6) that in this case the oscillation period of the orbital part of the energy is equal to the superconducting flux quantum $\Phi_S = (1/2)\Phi_0$. In this case the orbital part of the magnetic moment and the current density oscillate with the same period. Analogously, when there is one electron in level E_{II}, and there are two electrons with opposite spin projections in level E_{III}, the energy of the system is, according to (5),

$$E_{II} + 2E_{III} = \frac{6\sqrt{3}}{\pi}|L|\left[1 + 2\sum_{n=1}^{\infty}\frac{1}{1-36n^2}\cos\left(\frac{4\pi n\Phi}{\Phi_0}\right)\right] \pm \mu_B H. \quad (7)$$

In this case the orbital part of the energy, the orbital part of the magnetic moment, and the current density also oscillate with period Φ_S. If there are two electrons, with opposite spin projections, in level E_I, while there is a third electron in level E_{III}, the energy of the system is

$$2E_I + E_{III} = \frac{6\sqrt{3}}{\pi}|L|\left[-\frac{1}{2} + \sum_{n=1}^{\infty}\frac{1-2(-1)^n}{1-9n^2}\cos\frac{2\pi n\Phi}{\Phi_0}\right] \pm \mu_B H. \quad (8)$$

In this case the current density and the orbital parts of the energy and the magnetic moment oscillate with a period Φ_0.

Let us consider the case of a circle of radius r_0, which is the limiting case of a polygon as the number of vertices increases without bound. In this case the energy levels are $E_m = (e^2r_0^2/8m_ec^2)H^2 + (\hbar^2/2m_er_0^2)m^2 + m\mu_BH$, where $m = 0, \pm 1, \pm 2...$. In this case the ground-state energy E_g periodically undergoes a change in its H dependence. At $\Phi < \Phi_S$, E_g is equal to E_0, and M decreases with increasing H, from 0 to $-(1/2)\mu_B$. At $\Phi_S < \Phi < \Phi_S + \Phi_0$, E_g is equal to E_{-1}, and M decreases with increasing H, from $(1/2)\mu_B$ to $-(1/2)\mu_B$. At $\Phi_S + \Phi_0 < \Phi < \Phi_S + 2\Phi_0$, E_g is equal to E_{-2}, and M decreases with increasing H, from $(1/2)\mu_B$ to $-(1/2)\mu_B$; etc. These oscillations are analogous to the change in the sign of the magnetic moment in the model of a two-dimensional gas of free electrons which has been used to explain the de Haas-van Alphen effect (Refs. 3 and 4, for example). In this case, however, the oscillations are not related to the displacement of some of the electrons from one level to another, above the Landau level. The oscillations also occur in excited states. For example, the energy of the first excited state undergoes a change in H dependence with a period Φ_S. With $\Delta\Phi \sim hc/e$ and $S \sim 1$ mm^2 we find $\Delta H \sim 10^{-5}$ G.

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