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PERSISTENT CURRENTS IN TWISTED TORI MADE OF CHIRAL NANOTUBES*

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Mesoscopic metal rings can carry persistent currents driven by a constant magnetic field. The geometrical structure of a toroidal carbon nanotube can be characterized by four independent parameters. We derive the formula for persistent currents driven by a constant Bohm–Aharonov type of field perpendicular to the plane of the torus. The dependencies of the currents on the chirality, twist and circumference of the torus are discussed.

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1. Persistent currents in a metal ring

The existence of persistent currents is one of the most beautiful proofs that there are plenty interesting phenomena in the physics of mesoscopic systems, which are impossible in macroscopic solid state physics. In a small (of an order of a few μm) metal ring, threaded by a constant magnetic flux (like in Bohm–Aharonov effect) currents appear, with no varying magnetic fields or any electric potential. The idea that such currents might exist comes from Büttiker *et al.* [1], and was further explored by Gefen *et al.* in [2].

Since we are dealing with a closed system, the very first step is to define the boundary conditions. For the wave function of an electron on a ring of circumference L, the most comfortable way of defining them is to consider the system as one-dimensional and periodic with period L:

$$\psi(L) = \exp\left(i2\pi\frac{\phi}{\phi_0}\right)\psi(0), \tag{1}$$

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where ϕ is the magnetic flux through the ring and ϕ_0 is the flux unit, $\phi_0 = hc/e$. The system is one-dimensional, with the Bohm–Aharonov effect duly taken into account. Our job is to investigate the possible currents in the ring. As the system is finite, the momentum is quantized. The n-th momentum state carries the current:

$$I_n = -\frac{ev_n}{L} = -\frac{e}{L}\frac{1}{\hbar}\frac{\partial E_n}{\partial k_n} = -\frac{e}{\hbar L}\frac{\partial E_n}{\partial \phi}\frac{\partial \phi}{\partial k_n} = -c\frac{\partial E_n}{\partial \phi}. \tag{2}$$

The formula above is valid for any closed system, provided that the boundary conditions are of the form (1). The simplest Hamiltonian is sufficient to understand the nature of persistent currents, so we will work in the free electron approximation, and in a gauge in which the vector potential does not enter directly in the Hamiltonian. If our ring is free from impurities and there is no external potential $V(x)$, the energy and the current of the n-th state are

$$E_n = \frac{\hbar^2}{2m}\left[\frac{2\pi}{L}\left(n + \frac{\phi}{\phi_0}\right)\right]^2, \tag{3}$$

$$I_n = -\frac{2\pi e\hbar}{mL^2}\left(n + \frac{\phi}{\phi_0}\right). \tag{4}$$

The result above is not surprising, an electron with a nonzero momentum always carries a current, but usually the currents carried by all the electrons in the system cancel out, so there is no macroscopic current. Here they do not cancel out, and this is easier to understand when we look at the Fig. 1.

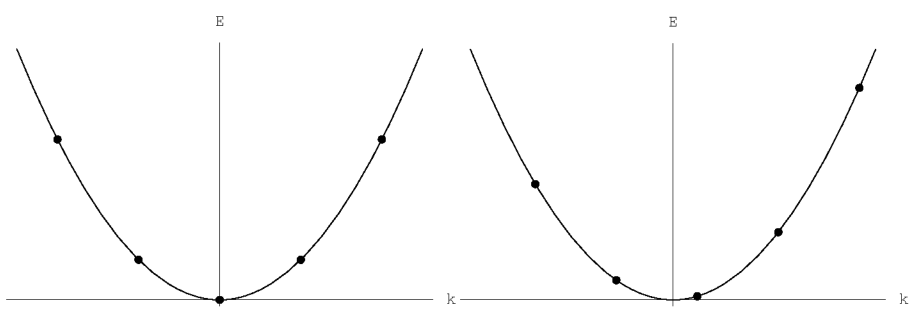

Fig. 1. The left figure is the plot of general energy *versus* momentum relation in a ring with no magnetic flux inside — note that the states are arranged in perfect symmetry on both sides of the E axis. The second figure shows the general shape of the dispersion relation in the system with the magnetic flux switched on and equal $\phi = 0.3\phi_0$.

When the magnetic flux is present in the system, the states on the positive momentum side go up, the states on the negative side slide down, and the currents (proportional to the slope of E_n at the k_n point) on both sides do not cancel out any more. When $T = 0$, all occupied states have the same weight, and the total current in the system is a function periodic in ϕ/ϕ_0, with period 1, given by the formula (*cf.* [3]):

$$I(\phi) = -\frac{2\pi e\hbar N}{mL^2}\begin{cases} \frac{\phi}{\phi_0}, & \text{for } N \text{ odd and } -\frac{1}{2} \leq \frac{\phi}{\phi_0} < \frac{1}{2} \\ \frac{\phi}{\phi_0} - \frac{1}{2}, & \text{for } N \text{ even and } 0 \leq \frac{\phi}{\phi_0} < 1 \end{cases} .$$

The plots of the current for N odd and N even are presented in the Fig. 2.

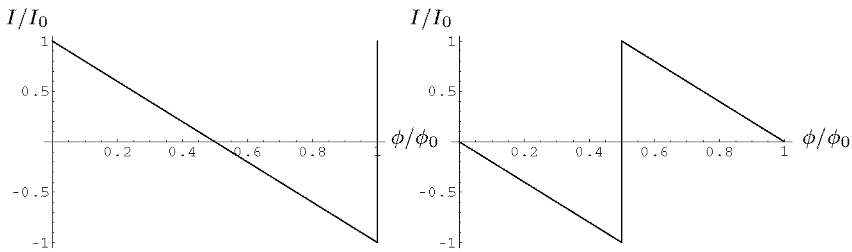

Fig. 2. The left plot corresponds to a system with N even, the right one to N odd, where $I_0 = \frac{\pi e\hbar N}{mL^2}$. The sudden leaps in the current are due to some states being shifted above the Fermi level, thus becoming unavailable, while their negative counterparts are lowered into the spectrum of available states at exactly the same flux.

2. The structure of a nanotube

A nanotube basically is just a strip of graphene sheet, rolled up, with opposite edges glued. (We see already that a boundary condition will be necessary.) When we want to close it into a torus, we bend it and glue the opposite edges once again. (Another boundary condition appears.)

We work here in the basis and approximation used by González *et al.* in the Ref. [4]. $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$ are vectors generating the honeycomb lattice, given in our basis by $\boldsymbol{T}_1 = \sqrt{3}e_x$ and $\boldsymbol{T}_2 = \frac{\sqrt{3}}{2}e_x + \frac{3}{2}e_y$. Both the circumference of the nanotube $\boldsymbol{L}_n$ and the circumference of the torus $\boldsymbol{L}_t$ can be expressed as linear combinations of these two vectors, with parameters m_1, m_2, p_1 and p_2:

$$\boldsymbol{L}_n = m_1\boldsymbol{T}_1 + m_2\boldsymbol{T}_2, \quad \boldsymbol{L}_t = p_1\boldsymbol{T}_1 + p_2\boldsymbol{T}_2. \tag{5}$$

We cannot roll this strip in any arbitrary way, but only so that the "gluing" edges correspond exactly. The nanotorus is thus uniquely defined by four parameters: m_1, m_2 corresponding to the gluing of a nanotube, and p_1, p_2 defining the gluing of the nanotube to make a torus. We shall refer to it as the $(m_1, m_2) \times (p_1, p_2)$ torus. The meaning of these parameters is illustrated by the Fig. 3.

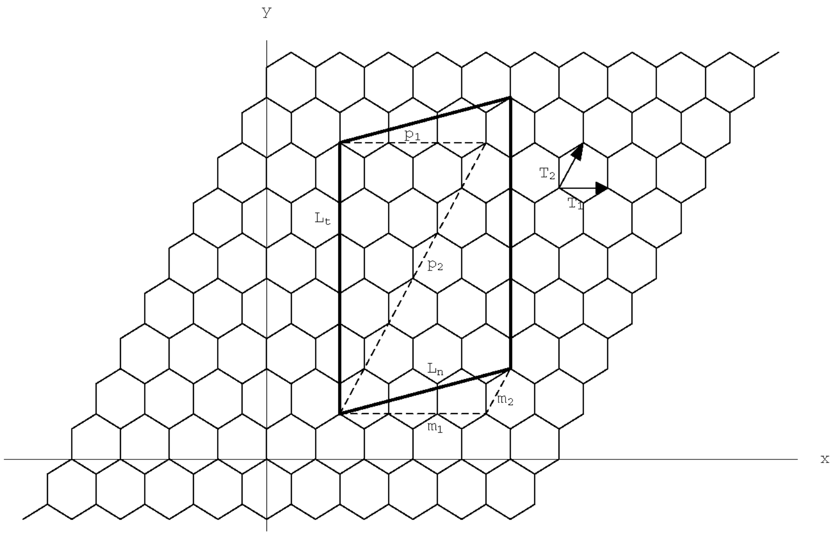

Fig. 3. The structure of a graphene sheet and the patch of the $(3,1) \times (-3,6)$ torus ($m_1 = 3$, $m_2 = 1$, $p_1 = -3$, $p_2 = 6$).

Note that $\boldsymbol{L}_n$ and $\boldsymbol{L}_t$ do not have to be perpendicular — the torus is then twisted, but this is allowed. In fact, most of the experimentally obtained tori are twisted, as we gather from the paper by Ceulemans *et al.* (Ref. [5]).

Upon trying out different ways of rolling a nanotube, we meet with a few cases so special that they got given names. The first is the one when $m_2 = 0$, thereby producing a "zigzag" structure along the circumference of the tube. The second is $m_1 = m_2$, which has a characteristic "armchair" structure along the circumference.

It turns out that every armchair nanotube and the zigzag tubes with m_1 divisible by 3 are metallic. This is due to a specific property of the energy spectrum of the graphene sheet, which in the tight-binding approximation is given by the formula:

$$E(\boldsymbol{k}) = \pm\sqrt{1 + 4\cos^2\left(\frac{\sqrt{3}}{2}k_x\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_x\right)\cos\left(\frac{3}{2}k_y\right)} \qquad (6)$$

and, when plotted, looks like a double crown, of which we only show the lower part, corresponding to the '$-$' sign in the equation (6). The existence

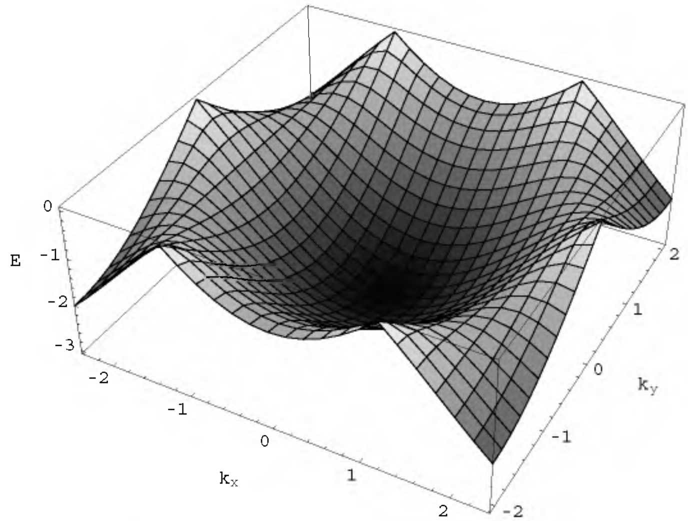

Fig. 4. This is the negative part of the honeycomb lattice dispersion relation, plotted against k_x and k_y. A very interesting feature of this spectrum is that it does not have Fermi surface — or rather, the Fermi surface is limited to six points at the peaks of the crown. Also, only two of these points are independent. This will turn out to be very important when we will calculate the conducting properties of the nanotubes.

of Fermi *points* only, instead of a whole Fermi surface, is the very feature responsible for different conducting properties of differently folded nanotubes. As can be seen after performing some careful calculations, only the tubes which satisfy the relation $(m_1 - m_2)|_{\mathrm{mod}3} = 0$ have Fermi points among their allowed momentum states (*cf.* Ref. [6]). The armchair ($m_1 = m_2$) and "triple zigzag" ($m_1 = 3k, m_2 = 0$) tubes are just special cases of this general rule.

By imposing the nanotube boundary condition on our graphene sheet we reduced the momenta spectrum to a set of lines (which may or may not cross the Fermi points). When we glue it into a torus, we impose the second boundary condition, and the set of allowed momentum states becomes just a set of points. Here again, we can make our torus either in such a way that Fermi points belong to the spectrum, or in such that they do not. It turns out that when both $(m_1 - m_2)|_{\mathrm{mod}3} = 0$ and $(p_1 - p_2)|_{\mathrm{mod}3} = 0$, the tori are metallic. When the m's fulfill this condition but the p's do not, the torus is a narrow-gap semiconductor. Why? Because the tori which are stable (and without topological defects, which would spoil our Hamiltonian) are much longer than they are wide. Therefore the momentum states are more narrowly spaced along the momentum lines corresponding to the $\boldsymbol{L}_t$

direction, than the $\boldsymbol{L}_n$ direction. So, once they are on a momentum line which passes through a Fermi point, they can miss it only by very little. When the nanotube is not metallic, we have wide-gap semiconductors, which are beyond the scope of our paper.

3. Persistent currents in toroidal nanotubes

We take now our torus and thread it with a line of magnetic flux. What current will the Bohm–Aharonov effect produce? Finding an answer to this question can proceed along similar lines as before, in the case of one-dimensional metallic ring — with a few important differences:

- the energy is given by a different formula;
- the system is 2-dimensional, therefore there are two boundary conditions to be taken into account;
- the number of electrons is always even and, more precisely, equal $2(m_1p_2 - p_1m_2)$.

Let us deal with these points in the proper order. The formula for energy is the same as in case of the flat graphene sheet and was given in the previous section. The boundary conditions for $\boldsymbol{k}$ are

$$\begin{aligned} \boldsymbol{k}\cdot\boldsymbol{L}_n = 2\pi l_n \;&\Rightarrow\; \frac{\sqrt{3}}{2}(2m_1+m_2)k_x + \frac{3}{2}m_2k_y = 2\pi l_n, \\ \boldsymbol{k}\cdot\boldsymbol{L}_t = 2\pi(l_t + \frac{\phi}{\phi_0}) \;&\Rightarrow\; \frac{\sqrt{3}}{2}(2p_1+p_2)k_x + \frac{3}{2}p_2k_y = 2\pi(l_t + \frac{\phi}{\phi_0}). \end{aligned} \tag{7}$$

Since the flux influences only the motion along the torus, it enters into the second condition, but not the first one. From these equations we can calculate currents associated with every state. The resulting formula has the following, rather complicated shape:

$$\begin{aligned} I_n = &\frac{2\pi}{m_1p_2 - m_2p_1}\{2m_2\cos\alpha(\phi)\sin\alpha(\phi) + m_2\cos\beta(\phi)\sin\alpha(\phi) \\ &-(2m_1+m_2)\cos\alpha(\phi)\sin\beta(\phi)\}\left(1 + 4\cos^2\alpha(\phi) + 4\cos\alpha(\phi)\cos\beta(\phi)\right)^{-1/2}, \end{aligned} \tag{8}$$

where

$$\begin{aligned} \alpha(\phi) &= \frac{\pi(p_2l_n - m_2(l_t+\phi))}{m_1p_2 - p_1m_2}, \\ \beta(\phi) &= \frac{\pi(-(2p_1+p_2)l_n + (2m_1+m_2)(l_t+\phi)}{m_1p_2 - p_1m_2}. \end{aligned}$$

This formula for the persistent current, in the special cases of the zigzag and armchair nanotubes, has been found by Lin and Chuu in the Ref. [7]. In our system we have one unbound (or π-) electron per lattice site, therefore the Fermi level lies at $E = 0$. The summation over all states in the first Brillouin zone gives the total current in the torus at zero temperature. This current depends on four parameters — two of them define the nanotube and the remaining two define the torus. We want to check the currents' dependencies on:

- the chirality of the nanotube (m_1/m_2);
- the twist with which we glue together the edges of the tube in order to obtain the torus (the angle between L_n and L_t), proportional to $\frac{m_1(2p_1+p_2)+m_2(p_1+2p_2)}{\sqrt{(m_1^2+m_1m_2+m_2^2)(p_1^2+p_1p_2+p_2^2)}}$;
- the circumference of the torus, $\sqrt{3(p_1^2+p_1p_2+p_2^2)}$.

Fig. 5 illustrates the dependence of the current on the chirality of the original nanotube. One should understand, though, that a nanotube is not a continuous object and it is impossible to keep fixed its length and chirality, while changing only the twist. So, when we say "we compare the nanotubes of the same length and chirality and varying twist", it must be understood that the length will also vary — albeit very slightly. Out of the three main features of the torus, the most important turns out to be the chirality of the nanotube which made it. Once we fix $m_1 - m_2 = 3k$, the current is relatively big and has the characteristic "sawtooth" shape, always crossing the ϕ/ϕ_0 axis at integer and half-integer values of ϕ/ϕ_0 (see Fig. 5 (b), (e)).

The current depends on the explicit difference $(p_1 - p_2)|_{\mathrm{mod}3}$. If $p_1 - p_2$ is not divisible by 3, it is a zigzag crossing the ϕ/ϕ_0 axis also at $1/3$ and $2/3$, if it is divisible by 3 it has no additional zero points. (See Fig. 6.)

While we keep $(p_1 - p_2)|_{\mathrm{mod}3}$ constant, we can still play with p_1 and p_2 separately, varying the circumference and twist of the torus. The current is then inversely proportional to the circumference of the torus (see Fig. 7) and it has no essential dependence on the twist. When the tube itself is not metallic, the current is sinusoidal and definitely smaller (as can be seen on the Fig. 5(a), (c) and (d)), for any value of $p_1 - p_2$. It does not depend much on the $p_1 - p_2$, but it decreases strongly with increasing circumference of the torus.

These effects can be understood by analysing the structure of the Brillouin zone. There are two main factors influencing the amplitude of the current. First, the number of states shifted through the edge of the Brillouin zone with increasing magnetic flux: if many states are shifted at once out of the Brillouin zone while their counterparts appear on the opposite side

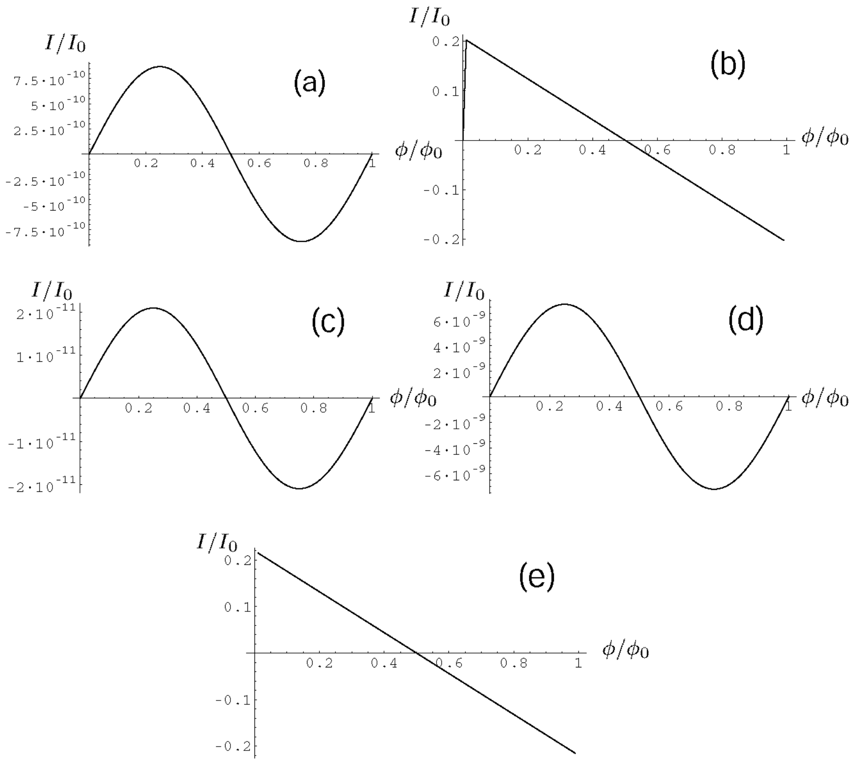

Fig. 5. The examples of normalised persistent currents $\frac{I}{I_0}$ *versus* $\frac{\phi}{\phi_0}$ in tori made with nanotubes of different chiralities, with approximately the same length and twist. The tori whose currents are presented here are (a) $(4,0)\times(-30,60)$, (b) $(4,1)\times(-39,60)$, (c) $(4,2)\times(-44,55)$, (d) $(4,3)\times(-51,55)$ and (e) $(4,4)\times(-50,49)$. Also, we keep fixed $(p_1-p_2)|_{\mathrm{mod}3}=0$.

of the hexagon, the current is strong. Second, the distance of the shifted states from the Fermi points. The states close to the "Fermi peaks" carry the greatest currents, so if they are present, the overall current is significantly greater than when we shift even many states, but far from the peaks.

The case of the metallic tube $((m_1-m_2)|_{\mathrm{mod}3}=0)$, when $(p_1-p_2)|_{\mathrm{mod}3}=0$ as well, is the one where the conditions are most favourable for the persistent currents. The Fermi points belong to the momentum spectrum at $\phi=0$, and when we switch on the flux, many states at once cross the edge of the first Brillouin zone.

When the tube is metallic, but $p_1-p_2\neq 3k$, there are many states but they lie only close to the Fermi points: at $1/3$ or $2/3$ from them, hence the specific zigzag shape of $I(\phi)$. Both cases are illustrated on the Fig. 6. When

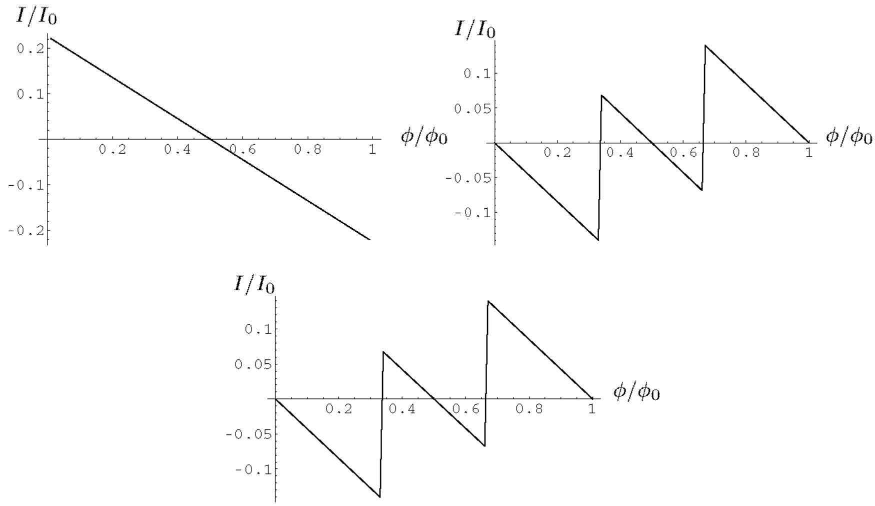

Fig. 6. Current *versus* flux of the tori $(4,1) \times (-30,60)$, $(4,1) \times (-31,60)$, and $(4,1) \times (-32,60)$. They all have the same nanotube chirality and similar circumference and twist, but their values of $(p_1 - p_2)|_{\mathrm{mod}3}$ are different.

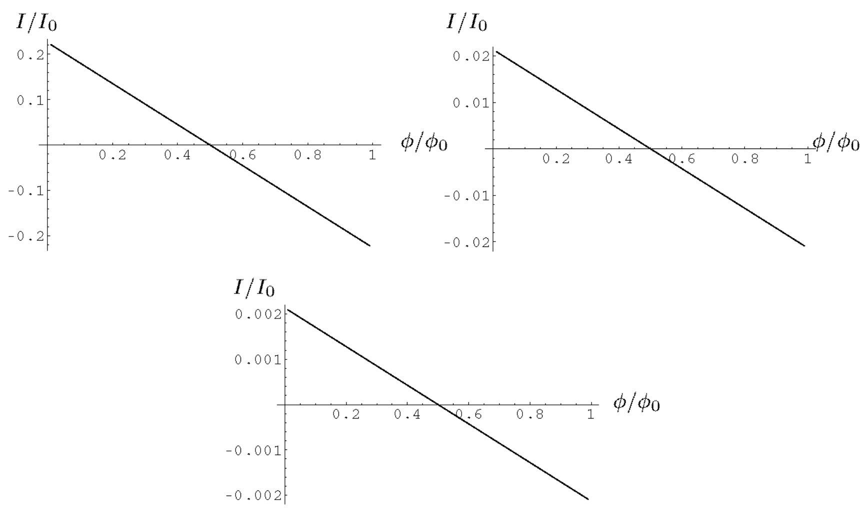

Fig. 7. The persistent current I/I_0 for the tori $(4,1)\times(-30,60)$, $(4,1)\times(-300,600)$ and $(4,1) \times (-3000,6000)$. They all have the same chirality and twist, while their circumference varies by a factor of 10 and 100.

the tube is not metallic, Fermi points lie far from the allowed momentum states, so even when quite many of them cross the edge of the Brillouin zone, the effect is not big.

4. Conclusions

We have shown that at the half-filling, *i.e.* when the number of free electrons in the nanotorus is equal to the number of its atoms, the main factor determining the strength of the persistent currents is the chirality of the constituent nanotube. The condition for the enhancement of the current coincides with the criterion for the metalicity of the nanotube, $(m_1 - m_2)|_{\rm mod3} = 0$. Within this condition, if in addition the twist parameters obey $(p_1 - p_2)|_{\rm mod3} = 0$, the currents are paramagnetic for small ϕ/ϕ_0 and have sawtooth-shaped plots like in a single metallic ring with odd number of electrons. Otherwise, for $(p_1 - p_2)|_{\rm mod3} \neq 0$ the amplitude remains similar, but the currents are diamagnetic for small ϕ/ϕ_0 and behave like the currents in a single ring with odd number of electrons. Instead of one, two jumps of the current occur, at $\phi/\phi_0 = 1/3$ and $\phi/\phi_0 = 2/3$. When varying the circumference of the torus while keeping the chirality and twist unchanged we observe inverse proportionality of the current to the circumference. In case when the constituent nanotube is not metallic, the amplitude of the current drops significantly and no jumps are observed any more. It becomes sinusoidal with the applied field and both paramagnetic and diamagnetic currents are observed for small ϕ/ϕ_0. The twist of the torus, when $(p_1 - p_2)|_{\rm mod3}$ is fixed, seems to have no significant influence on the currents.

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