Torsion-induced persistent current in a twisted quantum ring

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Abstract. We describe the effects of geometric torsion on the coherent motion of electrons along a thin twisted quantum ring. The geometric torsion inherent in the quantum ring triggers a quantum phase shift in the electrons' eigenstates, thereby resulting in a torsion-induced persistent current that flows along the twisted quantum ring. The physical conditions required for detecting the current flow are discussed.

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1. INTRODUCTION

Spatial confinement of particle's motion to low-dimensional space has an enormous influence on the quantum-mechanical properties of the particle. Of particular interests are systems in which a particle's motion is constrained to a thin curved layer by a strong confining force. Due to the confinement, excitation energies of the particle in a direction normal to the layer are significantly higher than those in a direction tangential to it; as a result, one can define an effective Hamiltonian that involves an anisotropic effective mass and a curvature-induced scalar potential [1, 2, 3]. This implies that the behavior of quantum particles that are confined to a thin curved layer is different from that of quantum particles on a flat plane, even in the absence of external field (except for the confining force). The effect of curvature was first suggested by Jensen and Koppe [1], and this was followed by subsequent studies that were conducted out of mathematical curiosity [4]. In recent years, the effect of curvature has been reconsidered from the viewpoints of condensed matter physics [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15], owing to technological progress that has enabled the fabrication of nanostructures with curved geometries [16, 17, 18, 19, 20, 21].

In addition to surface curvature, geometric *torsion* is another important parameter relevant to quantum mechanics in low-dimensional nanostructures. A torsion effect is manifested in quantum transport in a thin twisted nanowire with a finite cross section. When a quantum particle moves along a long thin twisted wire, it exhibits a quantum phase shift whose magnitude is proportional to the integral of the torsion along the wire [22, 23]. This torsion-induced phase shift is attributed to an effective vector potential that appears in the effective Hamiltonian defined for the movement of a particle in a twisted nanowire.

The mathematical mechanism for the occurrence of the effective vector potential was demonstrated by Takagi and Tanzawa [22], and independently by Magarill and Éntin [24]. Their results imply various intriguing phenomena purely originating from geometric torsion. For instance, the torsion-induced phase shift may give rise to a novel class of persistent current flow along a closed loop of a twisted wire; it is novel in the sense that no magnetic field need to penetrate inside the loop, which is in contrast with the ordinary persistent current [25, 26, 27, 28, 29, 30, 31, 32] observed in a non-twist quantum loop. However, optimal physical conditions as well as geometric parameters in order to measure those phenomena have been overlooked so far. Quantitative discussions as to what degree of torsion is necessary to make the phenomena be measurable in real experiments are important from both fundamental and practical viewpoints.

In this article, we have investigated the quantum state of electrons in a closed loop of a twisted wire, i.e. a twisted quantum ring. The wire consists of twisted atomic configuration, and its centroidal axis is embedded in a flat plane; these assumptions mean that the torsion in our system is defined with respect to a twisting crystalline reference frame. We have revealed that the magnitude of the torsion-induced persistent current I comes within a range of existing measurement techniques under appropriate conditions; this indicates the significance of torsion-induced quantum phase shift in the study of actual nanostructures, besides its theoretical interest. It should be emphasized that the persistent current I we have considered is free from a magnetic field penetrating through the ring, and thus differs inherently from the counterpart observed in untwisted rings.

2. QUANTUM STATE IN A TWISTED WIRE

In this section, we derive an explicit form of the effective vector potential in line with the discussions presented in reference [22]. Let us consider an electron propagating in a long thin curved cylinder with a weakly twisted atomic configuration (figure 1). For simplicity, the cylinder is assumed to have a circular cross section with constant diameter d. We introduce orthogonal curvilinear coordinates (q_0, q_1, q_2) such that q_0 parametrizes the centroidal axis C of the curved cylinder (i.e. the curve $q_1 = q_2 = 0$ coincides with C). We assume that C is embedded in a flat plane so that C *itself* has no torsion; therefore, the torsion of the present system is a consequence of the twisted atomic structure around the axis C of the conducting cylinder.

A point on C is given by the position vector $\boldsymbol{r} \equiv \boldsymbol{r}(q_0)$. Similarly, a point in the vicinity of C is represented by

$$\boldsymbol{R} = \boldsymbol{r}(q_0) + q_1\boldsymbol{e}_1(q_0) + q_2\boldsymbol{e}_2(q_0), \tag{1}$$

where the set $(\boldsymbol{e}_0, \boldsymbol{e}_1, \boldsymbol{e}_2)$ with $\boldsymbol{e}_0 \equiv \partial_0 \boldsymbol{R}$ and $|\boldsymbol{e}_1| = |\boldsymbol{e}_2| = 1$ forms a right-handed orthogonal triad; we use the notation $\partial_a \equiv \partial/\partial q_a$ $(a = 0, 1, 2)$ throughout the paper. Here, the unit vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ span the cross section normal to C, and they rotate along C with the same rotation rate as that of the atomic configuration. To be precise, the q_0-dependences of $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ are chosen such that the torsion τ defined by

$$\tau = \boldsymbol{e}_2 \cdot \partial_0 \boldsymbol{e}_1 \tag{2}$$

conforms to that of the twisted atomic structure. Using continuum approximation, we obtain the Schrödinger equation for the twisted quantum cylinder as

$$-\frac{\hbar^2}{2m^*}\sum_{a,b=0}^{2}\frac{1}{\sqrt{g}}\partial_a\left(\sqrt{g}g^{ab}\partial_b\right)\phi + V\phi = E\phi. \tag{3}$$

Here, m^* is the effective mass of the electron, and $V = V(q)$ with $q \equiv (q_1^2 + q_2^2)^{1/2}$ is a strong confining potential that confines the electron's motion to the vicinity of C. g^{ab} are elements of the matrix $[g^{ab}]$, which is the inverse of $[g_{ab}]$ whose elements are $g_{ab} = \partial_a \boldsymbol{R} \cdot \partial_b \boldsymbol{R}$ and $g = \det[g_{ab}]$ [33]. From equation(1), we obtain the following explicit forms of g^{ab}:

$$g^{00} = \gamma^{-4},\ g^{0a} = \gamma^{-4}\tau\epsilon_{0ab}q_b,$$
$$g^{ab} = \delta_{ab} + \gamma^{-4}\tau^2\left(|q|^2\delta_{ab} - q_a q_b\right),\ [a, b = 1, 2] \tag{4}$$

where $\gamma = (1 - \kappa_a q_a)^{1/2}$ and $\kappa_a = \boldsymbol{e}_0 \cdot \partial_0 \boldsymbol{e}_a$; the summation convention was used in equation (4). The quantity $\kappa \equiv (\kappa_1^2 + \kappa_2^2)^{1/2}$ represents the local curvature of C. Note that both τ and κ are functions only of q_0.

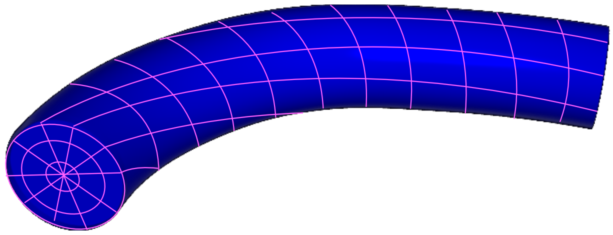

Figure 1. Sketch of a twisted quasi-one dimensional wire with a circular cross section. The mesh indicates the curvilinear coordinate (q_0, q_1, q_2) used in this study. Geometric torsion of the atomic configuration along the cylindrical axis is represented by the rotation of the reference frame in cross section (see text).

Hereafter, we assume that the geometric modulation of the cylinder (i.e. torsion and curvature) is sufficiently smooth and small so that the relations $\kappa d \ll 1$ and $\tau d \ll 1$ are satisfied. Under these conditions, equation(3) is reduced to [22]

$$\mu \left[\left(\partial_1^2 + \partial_2^2 \right) + \left(\partial_0 - \frac{i\tau L}{\hbar} \right)^2 + \frac{\kappa^2}{4} \right] \phi + V\phi = E\phi, \tag{5}$$

where $\mu \equiv -\hbar^2/(2m^*)$ and $L \equiv -i\hbar(q_1\partial_2 - q_2\partial_1)$ is the angular momentum operator in the cross section. The solution for equation(5) is assumed to have the form

$$\phi(q_0, q_1, q_2) = \psi(q_0) \sum_{j=1}^{N} c_j u_j(q_1, q_2). \tag{6}$$

Here $u_j(q_1, q_2)$ is an N-fold degenerate eigenfunction of the operator of $H_\perp \equiv \mu \left(\partial_1^2 + \partial_2^2 \right) + V(q)$ that is invariant to the rotation of the coordinates q_1, q_2. This means that $u_j(q_1, q_2)$ is an eigenfunction of L such that

$$L u_j(q_1, q_2) = \hbar m_j u_j(q_1, q_2), \tag{7}$$

where m_j is an integer. Thus, we multiply both sides of equation(5) with $\sum_j c_j^* u_j^*(q_1, q_2)$ and integrate with respect to q_1 and q_2 in order to obtain an effective one-dimensional equation,

$$\mu \left[\left(\partial_0 - \frac{i\tau \langle L \rangle}{\hbar} \right)^2 + \frac{\kappa^2}{4} - \frac{\tau^2}{\hbar^2} \left(\langle L^2 \rangle - \langle L \rangle^2 \right) \right] \psi(q_0) = \epsilon \psi(q_0), \tag{8}$$

where $\langle L \rangle = \hbar \sum_j |c_j|^2 m_j$ and ϵ is the eigenenergy of an electron moving in the axial direction. The product $\tau \langle L \rangle$ in parentheses is identified to the effective vector potential mentioned earlier.

3. TORSION-INDUCED PERSISTENT CURRENT

We now consider a closed loop of a twisted quantum wire with a circular cross section of constant radius R_2, which we call a twisted quantum ring. For simplicity, the centroidal axis C of the ring is set to be a circle of radius $R_1 \gg R_2$, which results in a constant curvature $\kappa \ll 1/R_2$ (i.e. q_0-independent). In addition, we assume that the torsion τ

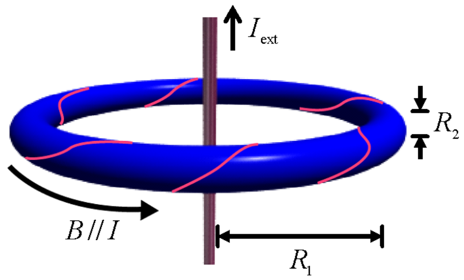

Figure 2. Twisted quantum ring encircling external current flow I_{ext}. A magnetic field B induced along the ring breaks the time reversal symmetry of the system, thus resulting in a torsion-induced persistent current I parallel to B.

of the atomic configuration around C is constant throughout the ring and satisfies the condition $\tau R_2 \ll 1$ (generalization to the case in which κ and/or τ are q_0-dependent is straightforward). Hence, an electron's motion in the twisted ring is described by equation(8), from which we obtain

$$\psi(q_0) = \psi_{\text{unt}}(q_0) \exp\left(-i\frac{\tau}{\hbar}\int_0^{q_0} \langle L\rangle dq_0'\right), \tag{9}$$

where $\psi_{\text{unt}} \propto \exp(-ikq_0)$ is the eigenfunction of an untwisted ring (i.e. $\tau \equiv 0$). An additional quantum phase proportional to τ implies the presence of a torsion-induced persistent current throughout the ring, as will be proved below.

Equation(9) shows that the condition $\langle L\rangle \neq 0$ is necessary for the presence of a torsion-induced persistent current. The condition can be realized by applying an external current I_{ext} that penetrates through the center of the ring, as shown in figure 2. Using the polar coordinate system (r,θ) with respect to the circular cross section, L in equation(5) is rewritten as

$$L_B = -i\hbar\frac{\partial}{\partial\theta} - \frac{eBr^2}{2}, \tag{10}$$

where $B = \mu_0 I_{\text{ext}}/\ell$, $\ell = 2\pi R_1$ and μ_0 is the permeability constant. The confining potential $V(r)$ is set to be a parabolic well centered at $r=0$, $V(r) = m^*\omega_p^2 r^2/2$, where ω_p characterizes the steepness of the potential. Hence, the lowest energy eigenstate u_0 in the cross section is given by [34, 35]

$$u_0(r) = \sqrt{\frac{m^*\Omega}{\pi\hbar}} \exp\left(-\frac{m^*\Omega}{2\hbar}r^2\right), \tag{11}$$

where $\Omega = \sqrt{\omega_p^2 + (\omega_c/2)^2}$ and $\omega_c = eB/m^*$ is the cycrotron frequency. As a consequence, the expectation value of L_B with respect to u_0 reads

$$\langle L_B\rangle = \int_0^\infty rdr \int_0^{2\pi} d\theta u_0^* L_B u_0 = -\frac{\hbar eB}{2m^*\Omega}, \tag{12}$$

or equivalently,

$$\langle L_B\rangle = -\frac{e\mu_0\hbar}{2\ell m^*\left[\omega_p^2 + \left(\frac{e\mu_0}{2\ell m^*}I_{\text{ext}}\right)^2\right]^{1/2}} I_{\text{ext}}. \tag{13}$$

From equation(13), we see that $\langle L_B \rangle \neq 0$ if $I_{\rm ext} \neq 0$.

The persistent current I driven by τ is evaluated by considering the periodic boundary condition $\psi(q_0+\ell) = \psi(q_0)$ that holds for the twisted ring. Since $\psi_{\rm unt}(q_0) \propto \exp(-ikq_0)$, it follows from equation(9) that

$$\exp(-ik\ell)\exp\left(-\frac{i}{\hbar}\tau\langle L_B\rangle\ell\right) = 1, \tag{14}$$

or equivalently,

$$k = \frac{2\pi}{\ell}\alpha - \frac{\tau\langle L_B\rangle}{\hbar} \equiv k_\alpha, \ \ (\alpha = 0, \pm1, \pm2\cdots). \tag{15}$$

The current carried by a single electron in the αth eigenstate is $I_\alpha = ev_\alpha/\ell = e\hbar k_\alpha/(m^*\ell)$ [36]. The total persistent current I in a ring containing N electrons at zero temperature is obtained by summing the contributions from all eigenstates with energies less than E_F. It is known that I for odd N, denoted by $I_{\rm odd}$, differs from that for even N, denoted by $I_{\rm even}$ [36]‡. In fact, straightforward calculation yields

$$\begin{aligned} I_{\rm odd} &= 2\times\sum_{\alpha=-(N-1)/2}^{(N-1)/2} I_\alpha = 2\times\sum_{\alpha=-(N-1)/2}^{(N-1)/2}\frac{e\hbar}{m^*\ell}\left(\frac{2\pi}{\ell}\alpha - \frac{\tau\langle L_B\rangle}{\hbar}\right) \\ &= -\frac{ev_F}{\ell}p, \quad \text{for} \quad -2 \le p < 2 \end{aligned} \tag{16}$$

and

$$I_{\rm even} = 2\times\sum_{\alpha=-N/2+1}^{N/2} I_\alpha = \frac{ev_F}{\ell}\left(2-p\right), \quad \text{for} \quad 0 \le p < 4 \tag{17}$$

where $v_F \equiv \pi\hbar N/(m^*\ell)$ and $p = 4\tau\langle L_B\rangle\ell/h$. We note that $I_{\rm odd}(p) = I_{\rm odd}(p+4)$ and $I_{\rm even}(p) = I_{\rm even}(p+4)$. The periodicities of $I_{\rm odd}$ and $I_{\rm even}$ stem from the fact that only the states $|k_\alpha| \le \sqrt{2m^*E_F}/\hbar$ contribute to the current; if $|k_\alpha|$ for a given α exceeds $\sqrt{2m^*E_F}/\hbar$ by imposing a sufficiently large (or small) $\langle L_B\rangle$, the state k_α becomes vacant and instead the state $k_\alpha - 2\pi/\ell$ is occupied (See reference [36] for details).

Since precise control of N is difficult experimentally, we assume an ensemble average over many experimental realizations of isolated twisted rings to obtain $(I_{\rm odd}+I_{\rm even})/2$, namely,

$$I = I(p) = \begin{cases} 0 & \text{for} \quad p = 0, \\ \frac{ev_F}{\ell}(1-p) & \text{for} \quad 0 < p < 2, \end{cases} \tag{18}$$

where $I(p) = I(p+2)$.

4. ESTIMATION OF THE INDUCED CURRENT

In order to estimate the magnitude of I observed in experiments, we consider a twisted silver quantum ring. Successful syntheses of ultrathin crystalline silver

‡ It is noteworthy that a complete description of the sign and magnitude of the persistent current for non-twisted rings has been recently proposed in reference [37] by considering the role of electron-electron interactions.

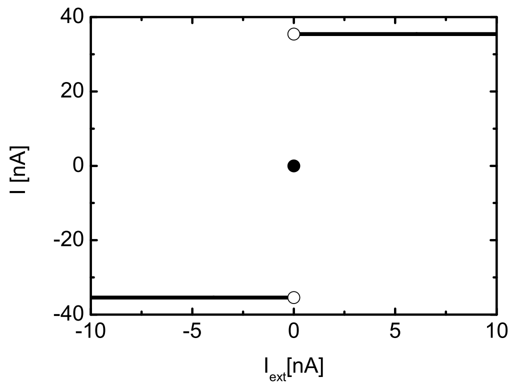

Figure 3. Stepwise behavior of I for the twisted ring with $R_1 = 1.0\mu$m, $R_2 = 1.0$nm and $\tau = 1/\ell$. Except at $I_{\rm ext} = 0$, the magnitude of I is almost invariant to the changes in $I_{\rm ext}$ and τ.

nanowires of nanometer scale width and micrometer scale length have been reported [38, 39, 40], followed by theoretical studies on their structural and transport properties [41, 42, 43, 44]. Such nanowires with high aspect ratios (i.e. the ratio of length to width) may be candidates for fabricating a twisted quantum ring. It should be borne in mind, however, that the applicability of our theory is not limited to a specific material but to general mesoscopic rings with twisted geometries.

Figure 3 is a plot of I as a function of $I_{\rm ext}$ as given in equation(18). We have set $R_1 = 1\mu$m, $R_2 = 1$nm by referring to an actual length and radius of the silver nanowires presented in references [38, 39, 40], and $\tau = 1/\ell$ (*i.e.,* one twist for one round) for simplicity. The Fermi velocity in silver is $v_F = 1.39 \times 10^6$m/s [45] , and the characteristic energy scale $\hbar\omega_p$ that corresponds to the cross-sectional radius $R_2 = 1$nm is estimated by $\hbar\omega_p = 0.1$ eV from the relation $\hbar\omega_p \sim m^*\omega_p^2 R_2^2/2$ and $m^* = 9 \times 10^{-31}$ kg for silver. In figure 3, we observe a stepwise increase in I that jumps from $I = -35.4$nA (for $I_{\rm ext} < 0$) to $I = +35.4$nA (for $I_{\rm ext} > 0$). Except at $I_{\rm ext} = 0$, the magnitude of I is almost invariant to the changes in $I_{\rm ext}$ and τ. This constant behavior of I is attributed to the fact that under the present conditions, p is much less than unity; as a result, $I \sim \dfrac{ev_F}{\ell}$ for $I_{\rm ext} > 0$ and $I \sim -\dfrac{ev_F}{\ell}$ for $I_{\rm ext} < 0$, respectively, as seen from equation(18).

The most important observation is the amplitude of I being 35.4nA that is comparable with the values obtained by using conventional measurement techniques [25, 26, 27, 28, 29, 30, 31]. This result indicates the physical significance of the torsion-induced quantum phase shift in actual nanostructures with twisted geometries. We emphasize that the mechanism by which a persistent current is induced in our system differs inherently from its counterpart in an untwisted ring, in the latter of which quantum phase shift occurs as the result of the application of an external magnetic field that threads the center of the ring.

5. CONCLUDING REMARKS

It deserves comments on other possible apparatus that exhibit torsion-induced current flow. In the present work, an external current I_{ext} was assumed to thread the center of the ring in order to obtain a non-zero expectation value of the angular momentum of the cross-sectional wave function. Differing from the manner, we may directly apply an external magnetic field in a direction *tangential* to a twisted structure. For instance, let us consider a twisted wire (not ring) both ends of which are connected by a lead, and apply a magnetic field of the order of one gauss in a direction tangential to the wire. Such an apparatus functions in a way similar to that considered in Section 3, and therefore, it causes torsion-induced current flow in the loop composed of the wire and lead. To date, many attempts have been done to synthesize [46, 47] and simulate [48, 49] a various kind of twisted nanowires. Their results may give a clue to build a set-up toward experimental test of our theoretical predictions.

In conclusion, we have demonstrated that a novel type of persistent current is induced in a quantum coherent ring formed by a long thin twisted quantum ring. This persistent current is a result of the geometric torsion of the ring that causes a quantum phase shift in the eigenstates of the electrons moving in the ring. The magnitude of the persistent current is within a realm of the results obtained from laboratory experiments; this indicates the importance of torsion-induced phenomena in influencing the physical properties of actual nanostructures with twisted geometries.

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