Geometric effects of a quarter of corrugated torus

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In the spirit of the thin-layer quantization scheme, we give the effective Shrödinger equation for a particle confined to a corrugated torus, in which the geometric potential is substantially changed by corrugation. We find the attractive wells reconstructed by the corrugation being not identical depths, which is strikingly different from that of corrugated nanotube, especially in the inner side of the torus. By using transfer matrix technique, we numerically calculate the transmission probability of electron confined to the inner side of a quarter corrugated torus, and find that the resonant tunneling peaks and the transmission gaps are merged and broadened by corrugation. These results provide a relatively simple method to design curvature-tunable filter.

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With the rapid development of nanotechnology, a variety of nanostructures with complex geometries are successfully fabricated, and then the related geometric effects attract both theoretical and experimental researchers to study. Specifically, the geometric effects are shown by the geometric potential$^{1,2}$, geometric momentum$^{3,4}$, geometric orbital angular momentum$^5$, geometric gauge potential$^{2,6,7}$, geometric magnetic moment$^6,8$ and so on. One of the most important geometric effects is the geometric potential that has been investigated widely. Researchers found that the geometric potential can be used to change the band-structure of the geometrically deformed systems$^{9,10,11}$, to generate localized surface states$^{12,13}$, and prompt energy shifts$^{14,15}$ for an electron confined to a curved surface and to affect the transport properties of electron confined to a curved surface or a space curve$^{16,17}$. Experimentally, the geometric potential$^{18}$, and the geometric momentum$^{19}$ are observed. These results provide evidences to the validity of the confining potential method.

Nanotube has nonvanishing curvature that contributes a attractive scalar potential for a particle moving on the tube. When the nanotube is deformed$^{12,25,26}$, the geometric potential will be substantially reconstructed by the deformation. In other words, the deformation plays an important role in the effective quantum dynamics, like Dirac comb$^{26}$, with attractive wells. Particularly, a corrugation is a deformation. Semiconductor films reconstructed by corrugation$^{29–32}$ have been investigated widely. The corrugation extremely affects the geometric potential, and further influences the corresponding electronic transport. Usually, corrugations appear in the bend of a tube. Using a bend tube to connect two tubes with different radiuses smoothly, we have to consider a part torus with corrugation, a quarter corrugated torus particularly in the present letter.

A torus reconstructed by corrugation (see Fig. 1(b)) that is parametrized by

\[ r = (x, y, z), \]

where \( x, y \) and \( z \) are

\[ r_x = r_{x0} + r_x', \quad r_y = r_{y0} + r_y', \quad r_z = r_{z0} + r_z', \]

respectively, with

\[ r_{x0} = (R + r \cos \theta) \cos \phi, \quad r_x' = \frac{\varepsilon}{2}(1 - \cos n\phi) \cos \theta \cos \phi, \]

\[ r_{y0} = (R + r \cos \theta) \sin \phi, \quad r_y' = \frac{\varepsilon}{2}(1 - \cos n\phi) \cos \theta \sin \phi, \]

\[ r_{z0} = r \sin \phi, \quad r_z' = \frac{\varepsilon}{2}(1 - \cos n\phi) \sin \phi, \]

wherein \( R \) and \( \phi \) are the large radius and azimuthal angle, \( r \) and \( \theta \) are the small radius and polar angle of a torus (see Fig. 1(a)), respectively, \( \varepsilon \) is the amplitude of corrugation and \( n \) denotes the period number of corrugation. The position vector \( r_0 = (r_{x0}, r_{y0}, r_{z0}) \) describes a torus, \( r = (x, y, z) \) describes the torus with corrugation shown in Fig. 1(a) and (b), respectively. And the vector \( r' = (r_x', r_y', r_z') \) describes corrugation.

From the corrugated torus Eq. (1), the two tangent unit basis vectors \( e_n, e_\xi \) and the normal unit basis vector \( e_n \) are obtained as

\[ e_n = (-\cos \phi \sin \theta, -\sin \theta \sin \phi, \cos \phi), \]

\[ e_\xi = \frac{1}{U}(-T \sin \phi + S \cos \theta \cos \phi, \quad T \cos \phi + S \cos \theta \sin \phi, S \sin \theta), \]

\[ e_n = -\frac{1}{U}(T \cos \theta \cos \phi + S \sin \phi, \quad T \cos \theta \sin \phi - S \cos \phi, T \sin \theta) \]
where
\[ Q = 2r + \varepsilon - \varepsilon \cos n\phi, \]
\[ S = \varepsilon n \sin n\phi, \]
\[ T = 2R + Q \cos \theta, \]
\[ U = \sqrt{S^2 + T^2}. \]

And the position vector \( \mathbf{R} \) of a point close to the deformed torus is then described by
\[ \mathbf{R} = \mathbf{r} + q_3 \mathbf{e}_n. \] (4)

where \( q_3 \) is the curvilinear coordinate variable along \( \mathbf{e}_n \).

According to the two position vectors \( \mathbf{r} \) and \( \mathbf{R} \), with the definitions of two matric tensors \( g_{ab} = \partial_a \mathbf{r} \cdot \partial_b \mathbf{r} \) \((a, b = 1, 2)\) and \( G_{ij} = \partial_i \mathbf{R} \cdot \partial_j \mathbf{R} \) \((i, j = 1, 2, 3)\), we obtain their covariant elements as
\[ g_{11} = 1, \quad g_{22} = 1, \quad g_{12} = g_{21} = 0, \] (5)
and
\[ G_{11} = (1 - \frac{2T}{QU} q_3)^2 + \frac{4S^2 \sin^2 \theta}{U^4} q_3^2, \]
\[ G_{12} = G_{21} = \frac{4S \sin \theta}{U^2} q_3 - \left[ \frac{T}{QU^3} \right] \left[ \frac{(S^2 + U^2) \cos \theta - \varepsilon n^2 T \cos n\phi}{U^5} \right] 4S \sin \theta q_3^2, \]
\[ G_{22} = [1 - \frac{(S^2 + U^2) \cos \theta - \varepsilon n^2 T \cos n\phi}{U^3} 2q_3]^2 \]
\[ + \frac{4S^2 \sin^2 \theta}{U^4} q_3^2, \]
\[ G_{33} = 1, \quad G_{13} = G_{31} = G_{23} = G_{32} = 0, \] (6)
respectively. It is straightforward to check the relationship between \( g \) and \( G \) as
\[ G = f^2 g, \] (7)
where \( g \) and \( G \) are the determinants of \( g_{ab} \) and \( G_{ij} \), respectively, and \( f \) is the rescaling factor, that is
\[ f = 1 - \frac{Q(S^2 + U^2) \cos \theta - n^2 \varepsilon QT \cos n\phi + U^2 T}{QU^3} 2q_3 \]
\[ + \frac{(S^2 + U^2) T \cos \theta - n^2 \varepsilon T^2 \cos n\phi - QS^2 \sin^2 \theta}{QU^4} 4q_3^2. \] (8)

For a particle confined to the corrugated torus (see Fig.1(b)), we deduce the effective Schrödinger equation by the confining potential approach\(^{2,6,33}\) (i.e. the thin-layer quantization scheme\(^{1,5,34}\)), that is
\[ - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial q^2} + \frac{\partial^2}{\partial \xi^2} q_2 + V_g \psi = E \psi, \] (9)
where \( \hbar \) is the Plank constant divided by \( 2\pi \), \( m^* \) is the effective mass of electron, \( \eta \) and \( \xi \) are two tangent coordinate variables of the deformed torus, \( \psi \) is the wave function describing the motion of the confined particle, \( E \) is the energy with respect to \( \psi \), and \( V_g \) is the geometric potential induced by curvature, that is
\[ V_g = \frac{\hbar^2}{2m^*} \left\{ \frac{4S^2 \sin^2 \theta}{U^4} \right\} \]
\[ + \left[ \frac{(S^2 + U^2) \cos \theta - T(U^2 + n^2 \varepsilon T \cos n\phi)}{QU^3} \right]^2. \] (10)

The geometric potential Eq. (10) is still valid to a part deformed torus with \( \phi \) ranging from \( \phi_0 \) to \( \phi_1 \) \((0 < \phi_0 < \phi_1 < 2\pi)\). In practical terms, we consider two models, one is a quarter corrugated torus with \( n = 6 \) and the other with \( n = 12 \), (see Fig.2(c) and (d)). For the sake of expressing convenience, a deformed tube and a quarter torus are also sketched (Fig.2 (a) and (b)). The deformation of tube generates the geometric potential, like
Dirac comb, attractive wells with identical depths. The Dirac comb can used to filter particles with particular incident energies. It is obvious that the quarter torus can connect two tubes with identical radius in different direction. The rest two quarter deformed toruses own the two features simultaneously. In what follows, we will discuss the properties of geometric potential of the quarter corrugated torus.

For a corrugated tube (see Fig.2 (a)), the geometric potential is determined by the radius of tube, the periodic length and the amplitude of corrugation together. As the periodic length fixed, it is easy to check that the amplitude is larger, the attractive wells are deeper. When the amplitude of corrugation is fixed, it is easy to confirm that the periodic length is longer, the wells are shallower. The corrugation can create a Dirac comb for the particle passing the deformed torus. In order to learn the differences in the four cases described in Fig. 2 (a), (b), (c) and (d), the corresponding four geometric potentials are sketched in Fig. 3 (a), (b), (c) and (d), respectively. In the case of a quarter torus, the geometric potential well is minimal at $\theta = \pi$, and it does not change by varying the azimuthal angle $\phi$. This result means that the inner side of the quarter torus is more capable of attracting particles. According to the figures of the geometric potential versus $\theta$ and $\phi$ shown in Fig.3 (c) and (d), it is easy to find that the geometric potentials take their minima at $\theta = \pi$, $\phi = (i + 1/2)\pi$ and $\phi = (i + 1/2)\pi$ with $(i = 0, 1, 2, \cdots)$ for $n = 6, 12$, respectively. The minima of the geometric potential can be in general expressed by

$$V_{\text{min}} = -\frac{\hbar^2}{8m^*} \left(\frac{1}{r - r - \varepsilon} + \frac{1}{r + \varepsilon} - \frac{n^2\varepsilon}{2(R - r - \varepsilon)^2}\right)^2. \tag{11}$$

It is obvious that the minima depends on curvature. For the quarter torus with corrugation, the geometric potential looks like the Dirac comb that can affect the transport of the electron confined to the particular quarter torus. When the variable $\theta$ is far away from $\pi$, the wells sharply become shallow. These results are useful to control the electronic transport by designing geometry. In next subsection, we will investigate the geometric effects of the quarter corrugated torus on transmission probability.

In terms of the quarter corrugated torus, from left to right, the head skirt can be taken as a free electron beam source, the first connection between the head skirt and the deformed torus plays the role of a barrier, the central part is a quarter corrugated torus that can provides a geometric potential, the second connection between the central part and the foot skirt can be taken as the other barrier, the foot skirt plays the role of a drain. This system in the $\phi$ direction can be simplified as a model that has the form as (see Fig. 4) which consists of two leads, two barriers and a geometric potential.

In a simplified case by vanishing the geometric potential, the present model becomes a simple model with double barriers. The double barriers resonant tunneling structure is a typical microstructure attracted various investigations. If a quarter corrugated torus is introduced, the geometric potential induced by curvature will substantially affect the resonant peaks created by the double barriers. For transport properties, the resonant peaks correspond to quasibound states, which are associated with geometric quantum wells. The electrons are primarily confined to a curved surface, and tend to stay in the attractive wells, but the electron has a certain probability to tunnel the corrugation, if the energy of the electron is nearly the energy eigenvalue of the quasibound state. Physically, when the spatial dimension is reduced to a scale being comparable with the de Broglie wavelength of electron in the vicinity of Fermi energy, the wave nature of electron is expected to play an important role in transport properties. In this section, we will investigate four generic cases: a periodically corrugated nanotube with 1.5 periods, a quarter of a nanotorus, a quarter nanotorus with 1.5 corrugations and a quarter nanotorus with 3 corrugations.
For the effective quantum equation Eq. (9), when \( \theta \) is fixed with constant, the equation can be simplified as

\[
-\frac{\hbar^2}{2m^*} \frac{d^2}{d\xi^2} \psi(\xi) + V(\xi)\psi(\xi) = E\psi(\xi),
\]

(12)

where \( m^* \) is the effective mass of electron, \( \hbar \) is the Planck constant divided by \( 2\pi \), \( \psi \) is a wave function describing the motion of electron confined to the surface with \( \theta \) being a constant, \( E \) is the energy with respect to \( \psi \), and the potential \( V(\xi) \) has the general form as

\[
V(\xi) = \begin{cases} 
0 \text{meV}, & \xi \in R_1, \\
20 \text{meV}, & \xi \in R_2, \\
V_g(\xi), & \xi \in R_3, \\
20 \text{meV}, & \xi \in R_4, \\
0 \text{meV}, & \xi \in R_5,
\end{cases}
\]

wherein \( V_g(\xi) \) denotes the geometric potential that is specifically expressed in Eq. (10) and \( \text{meV} \) stands for milli electron volts.

On the basis of the above results, we will calculate the transmission probability in the special situations considered in the present paper by using transfer matrix method \(^{32,43}\). For calculating convenience, we split \( R_3 \) up into segments instead of continuous variations of \( V(\xi) \), in each segment \( V_g(\xi) \) can be taken as a constant. And then let us assume \( R_3 \) consists of a sequence \( N_3 \) small segments, \( R_2 \) one segment \( (N_2 = 1) \) and \( R_4 \) one segment \( (N_4 = 1) \). It is straightforward to obtain that the total number of segments is \( N = N_2 + N_3 + N_4 \), that of boundaries is \( N + 1 \). In the numerical calculating procedure, it is worthwhile to notice that the tangent variable \( \xi \) in the \( j \)-th segment of \( R_3 \) should be replaced by \( \xi_j \), which can be described by

\[
\xi_j = \frac{1}{2} \int_{\phi_{j-1}}^{\phi_j} \sqrt{T^2 + S^2} d\phi,
\]

(14)

with \( T = 2R + (2r + \varepsilon - \varepsilon \cos n\phi) \cos \theta \) and \( S = \varepsilon n \sin n\phi \).

Subsequently, the transmission probability can be calculated for electron moving on the particular torus.

The transmission probabilities of the electron confined to the four curved surfaces described in Fig.2 (a)-(d) are shown in Fig.5 (a)-(d), respectively. In these cases, the substrate is graphene in which the effective mass of electron is \( m^* = 0.173m_0 \) with \( m_0 \) being the static mass of an electron. The figure Fig.5 shows that the geometric potential makes the strips of resonant tunneling peaks curved tend to the lower energy. And the corrugation of nanotube and nanotorus deepens the geometric potential wells extremely, the energy levels of the quasibound states shift downward that means a shift of the resonant peaks to lower energy. As a result, there are more the resonant peak strips shown in Fig.5. Comparing Fig 5 (c) with Fig 5 (a), we find that the bent corrugated nanotube can create more the resonant peak strips than the straight one. And it is apparent that the resonant peak strips are deformed by corrugation. The deformation becomes more important when the number of corrugations is increased. As a consequence, the quarter corrugated nanotorus can be not only employed to connect different nanotubes, but also to control the electronic transport. These results become more straightforward when
the two-dimensional (2D) figures describing the transmission probabilities versus the incident energy given by Fig. 6. The transmission gaps  are deepened and emerged and the tunneling peaks  are emerged and broadened (see Fig. 6 (d)).

![Figure 7](image7.png)

**FIG. 7.** (Color online) Surface plot of the transmission probability as a function of and for in and regions and in (a) with and , (b) with and , (c) with and and (d) with and and . Those resonant peaks are generated by the boundaries constructed by different materials in which electron has different effective masses. Comparing (c) and (d) with (a) and (b) in Fig. 7, we find that the deeper wells are more capable of emerging multiple resonant peaks into one. In other words, the geometric potential can broaden the width of the resonant peaks and the transmission gaps.

For GaAs substrate with and graphene , the transmission probability depending on the incident energy is described in the Fig. 8, (a) , (b) , (c) , (d) . It is obvious that the above mentioned results are more manifest in graphene than in GaAs substrate. Generally, the geometric potential can influence the electronic transport of various materials. Specifically, for different materials the geometric effects have certain difference.

In the present paper, the main investigation is to illustrate how geometry can be employed to affect the electronic transport of nanotubes and a quarter of nanotorus with corrugations. By researching four examples, a periodically corrugated nanotube, a quarter torus, a quarter torus with  corrugations and a quarter torus with corrugations, we found that the corrugations can extremely deepen the geometric potential wells. It is worthwhile to point out that the integer values of the number of corrugations for an usual torus would be broken when the investigated models are taken as a quarter torus. Subsequently, a part of corrugated torus can be selected to include any number of corrugations, and it can be used to connect two nanotubes with different radiiuses in different directions.

The corrugations of the deformed nanotube and nanotorus can deepen the attractive wells, and can emerge the resonant peaks and valleys to broaden them. In the resonant peaks electron can easily pass, in the particular transmission gaps electron is almost reflected. Practically, we can adjust the widths of the resonant peaks and the transmission gaps by designing corrugation, which may be used to design some quantum electronic and photonic nanodevices. In the present models, the interactions between electrons are neglected. A model including interactions of particles is still an interesting project that needs a further investigation.

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