Electronic States in Cylindrical Surfaces with Local Deformation

Hisao Taira and Hiroyuki Shima
Department of Applied Physics, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628 Japan
E-mail: taira@eng.hokudai.ac.jp

Abstract. Effects of the surface curvature on the electronic states of a cylindrical conducting surface with a variable diameter are theoretically investigated. The quantum confinement of electrons normal to the curved surface results in an effective potential energy that affects the electronic structures of the system at low energies. This suggests the possibility of controlling the electric conductivity of low-dimensional nanostructures by inducing a local geometric deformation.

1. Introduction
The rapid progress of nanotechnology has made it possible to fabricate quasi one- and two-dimensional nanostructures with novel geometrical shapes [1-8]. The successful manufacturing of such materials may pose questions concerning the effect of their geometry on their quantum properties. From the theoretical viewpoint, there have been several attempts to formulate the quantum mechanics of electrons confined within thin curved films [9-19]. These studies suggested that when the electron is strongly constrained to a smoothly curved surface, the quantization of the motion perpendicular to the surface results in an effective potential energy whose magnitude depends on the local curvatures along the surface. This implies that through an alteration in the local geometric curvature, one can control the quantum transport properties of the low-dimensional nanostructures which is an issue increasingly relevant to nanoscale device modelling.

In the present work, we theoretically investigate the quantum properties of electrons confined to a cylindrical surface with a variable diameter. The local deformation of the cylindrical surface significantly affects the electronic structures in the lowest-energy region. This indicates the occurrence of a curvature-induced alteration in the ballistic electron transport along nanoscale surfaces with cylindrical geometry.

2. Schrödinger Equation for Curved Surfaces
In what follows, we focus on a specific situation in which electrons are constrained to move along a curved surface. This is realized by introducing an infinite potential well that confines the electrons within a thin layer of constant thickness $d$. By taking the limit $d \to 0$, we obtain the Schrödinger equation for the electrons confined to the curved surface. This limiting procedure was initially suggested by da Costa [10], and has been successfully applied to quantum mechanical problems involving novel geometries [20-25].
Let \((x^1, x^2, x^3)\) be a three-dimensional curvilinear coordinate that allows the parameterization of a curved surface of interest by \(r = r(x^1, x^2)\). Then, a point \(p\) in this space can be determined through the relation

\[ p = r(x^1, x^2) + x^3 n(x^1, x^2), \]

where \(n(x^1, x^2)\) is the vector normal to the curved surface.

We now introduce a confining potential \(V(x^1, x^2, x^3)\). After a proper limiting procedure \([10]\), the potential becomes \(V = 0\) if \(x^3 = 0\) and \(V = \infty\) otherwise. This allows us to separate the \(x^3\) dependence in the Hamiltonian of the confined system and eventually provides the Schrödinger equation for curved surfaces:

\[-\frac{\hbar^2}{2m^*} \left[ \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left( \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} \right) - \left( H^2 - D \right) \right] \sigma = E \sigma. \tag{2}\]

Here, \(\sigma(x^1, x^2)\) is the wave function of the confined particles, \(g_{ij} = \partial r/\partial x^i \cdot \partial r/\partial x^j\) are the components of the metric tensor, \(g = \det [g_{ij}]\), \(g^{ij} = [g_{ij}]^{-1}\), and \(H(x^1, x^2)\) and \(D(x^1, x^2)\) are the mean and Gaussian curvatures of the surface, respectively \([26]\). The most striking feature is the occurrence of the non-trivial potential term, \(-(H^2 - D)\), in Eq. (2). This is a direct consequence of the quantization of the motion normal to the surface, and the resulting potential depends only on the local surface geometry and not on the mass or charge of the particle.

3. Model and Methods

Amongst the various geometries, we concern ourselves with the locally deformed cylindrical surfaces depicted in Figs. 1 (a) and 1 (b).\(^1\) These surfaces are parameterized by

\[ r = r(u, \phi) = [R(u) \cos \phi, R(u) \sin \phi, u], \tag{3}\]

where the radius of the cylinder is assumed to vary with \(u\) as

\[ R(u) = R_0 \left[ 1 + \beta \exp \left( \frac{-2u^2}{\alpha^2 R_0^2} \right) \right]. \tag{4}\]

Due to the rotational symmetry of the surfaces, the Schrödinger equation (2) can be further simplified by means of the variable-separation method. By substituting

\[ \sigma(u, \phi) = \frac{\eta(u)}{\sqrt{R(u)f(u)}} e^{im\phi}, \quad \text{with} \quad f(u) = \frac{1}{\sqrt{1 + (dR/du)^2}} \]

\(^1\) Similar cylindrical surfaces have been considered in Refs. [20] and [23].
into Eq. (2), we obtain the reduced Schrödinger equation for $\eta(u)$ as

$$-f(u)^2 \frac{d^2 \eta}{du^2} - V_d(u)\eta(u) = \epsilon \eta(u), \quad (6)$$

where

$$V_d(u) = f(u)^2 \left[ \frac{d\Gamma}{du} - \Gamma(u)^2 \right] + H(u)^2 - D(u) - \frac{m^2}{R(u)^2}. \quad (7)$$

and

$$\Gamma(u) = -\frac{1}{2R(u)f(u)} \frac{d(Rf)}{du}. \quad (8)$$

The potential $V_d(u)$ is referred to as the deformation-induced potential and exhibits a complicated dependence on $u$. We shall see that the presence of the term $V_d$ significantly affects the static and transport properties of the ground state of the confined electrons.

The actual calculations of Eq. (6) are performed by using the tight-binding approach wherein the continuous variable $u$ is discretized. In keeping with the general practice, the lattice constant and the hopping energy are assumed to be of unit length and unit energy, respectively. The radius $R_0$ of an undeformed part of the surface is fixed at $R_0 = 50$, and the length $L$ of the cylinder is assumed as $L = 1000$. The eigenenergies and eigenfunctions of Eq. (6) are evaluated by a direct diagonalization scheme.

4. Results and Discussions

Figures 2 (a) and (b) depict the spatial profile of $V_d(u)$ and that of the square amplitude of the ground-state eigenfunction $|\eta|^2$ with $m = 0$. The parameters are $\alpha = 1.0$ for (a) and $\alpha = 1.5$ for (b), and $\beta = 1.0$ for both the figures. Figure 2 (a) shows that $V_d$ may provide a steep potential well in which the ground-state wavefunction is strongly bounded (see Fig. 2 (a)). The occurrence of the potential well is attributed to the fact that for certain values of $\alpha$ and $\beta$, the term $f^2(d\Gamma/du - \Gamma^2)$ involved in $V_d$ (see Eq. (7)) assumes a considerably large positive value at $u=0$. The magnitude of this potential well decreases with increasing $\alpha$; in fact, when $\alpha > 1.5$, slight contributions from $V_d$ are no longer sufficient to bound the ground eigenstates of $m = 0$, as shown in Fig. 2 (b).
Interestingly, the spatial profiles of $|\eta(u)|^2$ (as well as $V_d(u)$) change considerably depending on the values of $\alpha$ and $\beta$, and also the quantum number of the angular momentum $m$. This is illustrated by Figs. 3 (a) and 3 (b); these are contour plots of the localization length $\xi = \left(\sum_{i=1}^{L} \eta_i^4\right)^{-1}$ of the lowest-energy eigenstate with $m = 0$ (a) and $m = 1$ (b). Here, $i$ is the site index of the tight-binding Hamiltonian we have considered. The localization length $\xi$ provides a measure of the spatial extent of the wavefunction in question; $\xi << L$ if the eigenfunction is spatially localized, while $\xi \sim L$ if it extends over the whole system. Hence, by examining the dependence of $\xi$ on the geometric parameters $\alpha$ and $\beta$, we obtain an understanding of the geometric effect on the electron system on cylindrical surfaces. Figures 3 (a) and (b) show that the ground-state eigenfunction may be strongly bounded (the dark region) or may extend over the entire system (the light region) depending on the values of $\alpha$ and $\beta$.

Importantly, in both the cases $m = 0$ and $m = 1$, the $\alpha$-dependence of $\xi$ is completely different between the regions $\beta > 0$ (bulgy deformation) and $\beta < 0$ (constricted deformation). With $m = 0$, for instance, $\xi$ for $\beta > 0$ tends to increase with $\alpha$, and eventually becomes equal to the system length $L$ at $\alpha \sim 1.5$ (followed by a slight decrease at $\alpha > 2.0$). This indicates that the ground-state becomes extended ($\xi \sim L$) when reforming the bulgy part to be more stretched in the direction of $u$-axis. On the other hand, $\xi$ for $\beta < 0$ is almost invariant with regard to changes in $\alpha$, and its value is always smaller than $L$. In short, (i) the crossover behaviour of $\xi$ from bound to extended states is observed only in the case of bulgy deformation ($\beta > 0$), and in that case, (ii) the magnitude of $\xi$ for a fixed $\beta$ rapidly increases at $\alpha \sim 1.5$. These two findings suggest the possibility of controlling the ballistic electron transport in cylindrical nanostructures by introducing a subtle geometric deformation.

It is to be noted that a similar crossover behaviour of $\xi$ was observed in the case of $m = 1$ where, in contrast to the case of $m = 0$, the crossover occurs for negative $\beta$. In fact, we have confirmed that when $m \geq 1$, the extended low-energy states occur only at $\beta < 0$ which is in contrast to the case of $m = 0$ where the extended states occur only at $\beta > 0$. This difference as well as the global behaviour of $\xi(\alpha, \beta)$ depicted in Figs. 3 (a) and (b) can be accounted for by considering the contribution from each term in the expression for $V_d(u)$ (see (7)); detailed analyses will be presented elsewhere [27].
5. Conclusion
In the present study, we have investigated the effect of local geometric deformation on the electronic states strongly confined to a thin cylindrical surface with a variable rotational radius. The spatial profile of the deformation-induced potential and that of the square amplitude of the lowest-energy eigenstates were numerically evaluated by using the tight-binding approach. The localization length of the eigenstate was calculated as a function of the geometric parameters $\alpha$ and $\beta$; the results indicate that a subtle geometric deformation could induce a drastic change in the ballistic electron transport along nanoscale cylindrical surfaces. We hope that our findings prove to be a fundamental basis for further fruitful studies on the development of quantum devices based on low-dimensional nanostructures.

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