Effects of hydrostatic strain on eigenstates of Möbius strips

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***Abstract*—In this paper we theoretically investigate the allowed energies and associate wave-functions for Möbius strips with varying thicknesses. We show that the induced strain in fabricating these Möbius strips will have an pronounced impact on the energies and wave-functions for thick strips, while for thin strips the impact of strain is negligible. We furthermore, show that a simpler strain free approximate theory base on differential geometry is in excellent agreement with detailed finite element calculations.**

I. Introduction

It is nowadays possible to fabricate geometrically complex nanostructures. For example, in the 2002 nature paper by Tanda et al. [1] a crystalline nanoscale Möbius strip has been fabricated. It is well-known that shape and size of nanostructures have pronounced consequences for the electrical and optical properties. Furthermore, deformations of these structures markedly change these properties. These changes can be utilized to design new and novel devices such as sensors, optoelectronic devices and nanogenerators [2]. There is, therefore, a need to investigate the consequences of changing the shape and size of nanostructures and the effect of deformations on optoelectronic properties.

While the underlying theory for these kind of systems is well established, there is still ample opportunity to develop simple and more tractable models able to accurately describe these systems. One such approach is to utilize differential geometric techniques to put the governing equations on a more generic form enabling new approximate approaches [3]. In this work, this approximate approach is compared to more detailed finite element calculation.

II. Theory

In this section we outline the theory behind the calculation of allowed energies and associate wave-functions for Möbius strips based on the one-band model. For a more detailed description consult the paper by Gravesen and Willatzen [3].

The parametrization of the Möbius strip is given by

$$\vec{x}(u^1,u^2,u^3) = \vec{r}(u^1) + u^2\left(\vec{b}(u^1) + \Psi(u^1)\vec{t}(u^1)\right) - u^3\vec{n}(u^1), \quad (1)$$

where $\vec{r}(u^1)$ is the parametrization of the median given in equation (6), $\vec{t}$ is the unit tangent vector, $\vec{n}$ is the normal vector, $\vec{b}$ is the binormal vector, $\Psi = \frac{\tau}{\kappa}$, and $\psi = \frac{\mathrm{d}\Psi}{\mathrm{d}s}$ (s is the arc-length). The coefficients c_1, c_2, and c_3 have been found by minimizing the bending energy while keeping the length fixed.

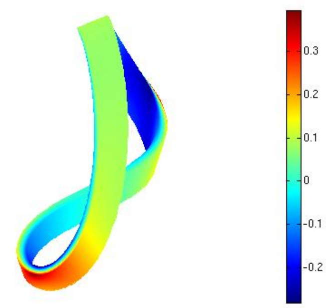

Fig. 1. The hydrostatic strain on the surface of a Möbius stripe with $w = 3.333$ nm, $L = 200$ nm, and $t = 2.25$ nm

In order to determine the electron eigenvalues and eigenstate including strain we solve the one-band Schröndinger equation, in cartesian coordinates given by

$$-\frac{\hbar^2}{2m_{eff}}\Delta\chi + a_c\mathrm{Tr}(\varepsilon)\chi = E\chi, \quad (2)$$

where m_{eff} is the effective mass, Δ is the Laplacian, a_c is the deformation potential, ε is the strain tensor, and $\mathrm{Tr}(\varepsilon)$ is the hydrostatic strain component. The strain tensor is given by

$$\varepsilon_{ij} = \frac{1}{2}\left(\delta_{ij} - \frac{\partial\vec{R}}{\partial v_i}\frac{\partial\vec{R}}{\partial v_j}\right) = \frac{1}{2}\left(\delta_{ij} - \sum_{k,l=1}^{3}\frac{\partial u_k}{\partial v_i}\frac{\partial\vec{x}}{\partial u_k}\frac{\partial u_l}{\partial v_j}\frac{\partial\vec{x}}{\partial u_l}\right). \quad (3)$$

where $\vec{R}(v_1,v_2,v_3) = \vec{x}(u^1(v_1,v_2),v_2,v_3)$ and

$$v_1 = \int_0^{u^1}|\vec{r}'(s)|ds + u^2\Psi, \quad v_2 = u^2, \text{ and } v_3 = u^3. \quad (4)$$

The coordinates (v_1,v_2,v_3) have been introduced to model a Möbius strip which median has not been stretched during fabrication. In figure 1 we show the hydrostatic strain component on the surface of the Möbius strip.

It is assumed that the electron is completely confined to the Möbius strip and, as consequence, Dirichlet boundary

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conditions are imposed on the surface of the structure. As the Möbius strip is rotated 180° we impose anti-periodic boundary conditions on the end surfaces

$$\chi(u^1 = 0, u^2, u^3) = \chi(u^1 = 2\pi, -u^2, -u^3). \qquad (5)$$

In the paper [3] Gravesen and Willatzen have shown that for a thin curved structure the Schröndinger equation without strain can be approximated by a the separable equation

$$-\frac{\hbar^2}{2m_e}\left(\Delta_\Sigma + \left(\frac{\partial}{\partial u^3}\right)^2 + M^2 - K\right)\chi = E\chi, \qquad (6)$$

where Δ_Σ is the Laplace-Beltrami operator on Σ, M and K are the mean and Gaussian curvatures, respectively.

III. Result

In this section we present results for a $L = 200$ nm long, $w = 3.333$ nm wide Möbius strip with thicknesses of $t = 0.75$ nm and $t = 2.25$ nm. The coefficients are in this case given by $c_1 = 32.25$ nm, $c_2 = 19.05$ nm, and $c_3 = 6.26$ nm. We assume that the material of the Möbius strip is InAs and use the values $m_{eff} = 0.022m_0$ and $a_c = -5.08$ eV for the effective mass and the deformation potential respectively, where m_0 is the free electron mass.

In table I we list the first three allowed energies found using the approximate (separable) model, the full model without strain, and the full model taking into account strain. We observe that the effect of strain is negligible for the 0.75 nm thick strip, while the strain gives a significant contribution for the 2.25 nm thick strip. The reason for this is that the main contribution to the strain is coming from bending and as the thickness is increased the bending strain increases as is the case for a normal bend beam in classical mechanics. In figure 2 we show the groundstate wave-function along the center of the Möbius strip for the two thicknesses. In the left column we show the groundstate without strain and in the right the groundstate taking into account strain. Again we see that for the thin strip, strain has a negligible effect, while for the thick strip, there is a pronounced change in the wave-function. We notice that the wave-function in the thick structure is highly localized at two small areas of the strip. These two areas corresponds to places in the strip with high hydrostatic strain, see figure 1.

This shows that for thick bend nanostructures, strain effects are important, and needs to be taken into account.

IV. Conclusion

We have investigated the effect of strain on electronic states in Möbius strips. We have shown that the approximate theory based on differential geometry and disregarding strain is very accurate for thin Möbius strips while for thick Möbius strips strain effects become important resulting in large discrepancies between the approximate and exact solutions.

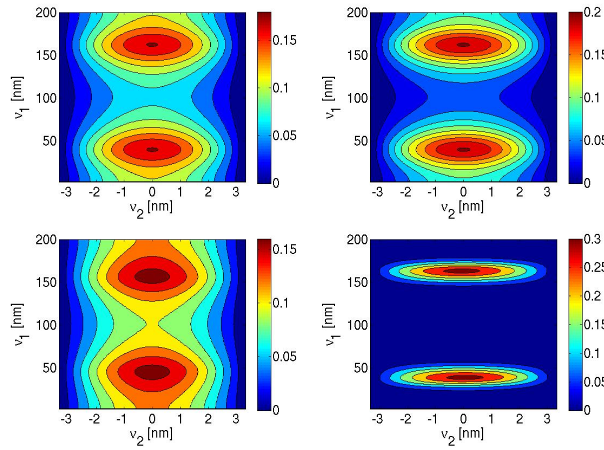

Fig. 2. Groundstates for Möbius stripe with $w = 3.333$ nm, $L = 200$ nm, $t = 0.75$ nm (upper row), and $t = 2.25$ nm (lower row). The left plots are eignestates without taking into account strain and the right plots with strain. See Equation (4) for the definition of ν_1 and ν_2.

References

[1] S. Tanda, T. Tsuneta, Y. Okajima, K. Inagaki, K. Yamaya, and N. Hatekenaka, Nature (London) 417, 397 (2002).

[2] X. Wang, J. Song, J. Liu, and L. Wang, Science, 316, 102 (2007).

[3] J. Gravesen and M. Willatzen, Phys. Rev. A 72, 032108 (2005).

TABLE I

The first three allowed energies both with and without strain and using the approximative zeroth-order expansion in u^3.

	E(1)		
	approx.	no strain	strain
$t = 0.75$ nm	7.9790	7.9793	7.9776
$t = 2.25$ nm	1.2265	1.2275	1.1408
	E(2)		
	approx.	no strain	strain
$t = 0.75$ nm	7.9802	7.9803	7.9783
$t = 2.25$ nm	1.2277	1.2287	1.1408
	E(3)		
	approx.	no strain	strain
$t = 0.75$ nm	7.9818	7.9822	7.9817
$t = 2.25$ nm	1.2293	1.2300	1.1871

$$\vec{r}(u^1) = \left(c_1 \sin(u^1), c_2\left(\sin(u^1) - \frac{1}{2}\sin(2u^1)\right), c_3\left(\frac{5}{3} - \frac{5}{2}\cos(u^1) + \cos(2u^1) - \frac{1}{6}\cos(3u^1)\right)\right), \qquad (6)$$