Eigenstates of Möbius nanostructures including curvature effects

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Möbius-shell structures and their physical properties have recently received considerable attention experimentally and theoretically. In this work, eigenstates and associated eigenenergies are determined for a quantum-mechanical particle bounded to a Möbius shell including curvature contributions to the kinetic-energy operator. This is done using a parametrization of the Möbius shell–found by minimizing the elastic energy of the full structure–and employing differential-geometry methods. It is shown that inclusion of curvature contributions to the kinetic energy leads to splitting of the otherwise doubly degenerate groundstate and significantly alters the form of the groundstate and excited-state wavefunctions. Hence, we anticipate qualitative changes in the physical properties of Möbius-shell structures due to surface confinement and curvature effects.

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I. INTRODUCTION

The present state of nanotechnology [4] allows in principle any structure to be grown experimentally and provides insight into understanding the relation between the global geometry of a structure and associated physical properties [5–10]. Moreover, studies of geometry effects and quantum-mechanical wave functions may lead to identification of new types of states and novel applications [2]. Recently, $NbSe_3$ Möbius-shell structures have been fabricated [1]. In this work, the problem of a quantum-mechanical particle confined to a Möbius-shell structure is considered. Special emphasis is given to the understanding of elastic energy and surface-curvature effects on eigenstates and eigenvalues employing differential-geometry methods. In particular, comparison with the flat-cylinder and flat-Möbius structure problems [3] (where elastic energy and curvature contributions to the kinetic energy are neglected) shows that surface-curvature effects lead to splitting of the otherwise degenerate ground-state energy and significant alterations of the ground- and excited-state wave functions. Hence, qualitative changes to the physical properties of Möbius quantum nanostructures are expected due to surface-curvature effects. We assume in this work that the quantum-confined particle obeys fermion or boson statistics such that wave functions are single valued, hence disregarding fractional spin-particle systems characterized by multivalued wave functions (anyon systems [11]).

II. THE SCHRÖDINGER EQUATION IN GENERALIZED COORDINATES

The Schrödinger equation for a quantum-mechanical particle bounded to a surface Σ reads

$$-\frac{\hbar^2}{2m}(\Delta_0+\partial_3^2)\chi(u^1,u^2)+V(u^1,u^2,u^3)\chi(u^1,u^2)=E\chi(u^1,u^2), \tag{1}$$

where m is the particle mass and E its energy. The surface Σ is defined as the surface for which the third coordinate u^3 is zero and the potential V is a completely confining potential, i.e.,

$$V(u^1,u^2,u^3)=\begin{cases}0 & \text{if } u^3=0,\\ \infty & \text{else}.\end{cases} \tag{2}$$

The operators Δ_0 and ∂_i in Eq. (1) are [12]

$$\Delta_0=\Delta_\Sigma+M^2-K, \tag{3}$$

$$\partial_i=\frac{\partial}{\partial u^i},\quad i=1,2,3, \tag{4}$$

where Δ_Σ is the Laplace-Beltrami operator on Σ and M and K are the mean and Gaussian curvatures [in our case, M is nonzero but K is zero; see Eq. (11)].

III. THE PARAMETRIZATION AND SHAPE OF THE MÖBIUS-SHELL STRUCTURE

Now consider a Möbius surface. We can parametrize it by coordinates $(u^1,u^2)\in[0;L]\times[-w;w]$, where L is the length (one turn) and $2w$ is the width of the strip. Since M is not a separable function of u^1 and u^2 for the Möbius surface parametrized, it is not possible to separate χ in Eq. (1) in functions of u^1 and u^2. Hence, we solve Eq. (1) by employing a simple two-dimensional finite-difference scheme so as to obtain energy eigenvalues E and associated eigenstates χ. Boundary conditions for the Möbius surface are as follows:

$$\chi(u^1,u^2=-w)=\chi(u^1,u^2=w)=0 \tag{5}$$

and

$$\chi(u^1=0,u^2)=\chi(u^1=L,-u^2). \tag{6}$$

For comparison, we also compute analytically eigenstates and eigenvalues for the flat-cylinder problem case with boundary conditions

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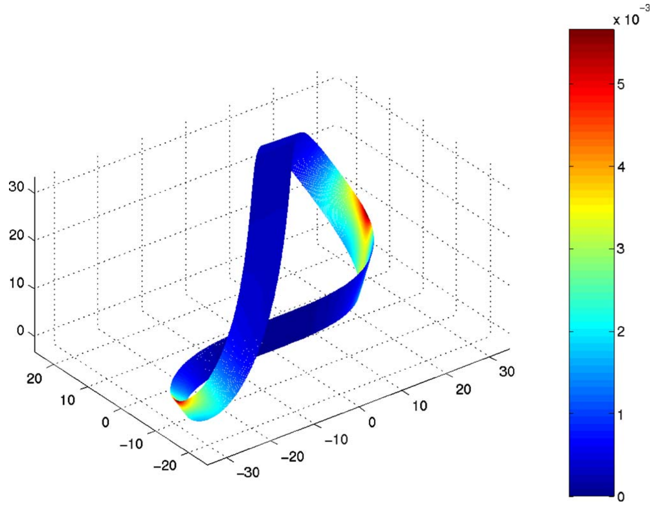

FIG. 1. (Color online) The Möbius structure color coded with the value of M^2 (in Å^{-2}), the square of the mean curvature. The units on the axes are in ångstroms.

$$\chi(u^1,u^2=-w)=\chi(u^1,u^2=w)=0 \tag{7}$$

and

$$\chi(u^1=0,u^2)=\chi(u^1=L,u^2), \tag{8}$$

and similar for the flat-Möbius problem. Both latter-mentioned problems (cylinder flat and Möbius flat) imply solving the Schrödinger problem and discarding the M^2 kinetic-energy contributions. In this way, we can verify our numerical results against analytical results and identify the importance of the Möbius topology versus the cylinder topology as well as surface-curvature effects.

Consider a rectangular strip of paper. Applying a half twist and gluing the ends together leads to the formation of a Möbius-shell structure. We can push and pull the paper so the exact shape is not determined; however, disregarding external forces including gravity implies that the resulting shape minimizes the elastic energy. The problem of determining this shape goes back to 1930 and the exact mathematical description of the shape is still not known [13–18].

In the case of a Möbius-shell structure made out of paper it is reasonable to assume that the shape is the result of pure bending, and the same is probably true for the nanostructures [1]. Then the shape is developable and is completely determined by the median or center curve of the Möbius structure. If $\mathbf{r}(u)$ is a parametrization of the median then the parametrization of the Möbius structure is given by

$$\mathbf{x}(u,v)=\mathbf{r}(u)+v\left(\mathbf{b}(u)+\frac{\tau(u)}{\kappa(u)}\mathbf{t}(u)\right), \tag{9}$$

where $\mathbf{t}$ is the tangent vector, $\mathbf{b}$ is the binormal vector, κ is the curvature, and τ is the torsion [15–17]. If we let s denote the arclength on the median and put

$$\Psi=\frac{\tau}{\kappa} \quad \text{and} \quad \psi=\frac{d\Psi}{ds}, \tag{10}$$

then the mean and Gaussian curvatures are

$$M=-\frac{\kappa}{2}\frac{1+\Psi}{1+v\psi} \quad \text{and} \quad K=0, \tag{11}$$

respectively. The elastic energy is

$$E=\frac{1}{2}\int M^2 dA=\frac{1}{2}\int_0^L\int_{-w}^{w}\frac{\kappa^2}{4}\frac{(1+\Psi^2)^2}{(1+v\psi)^2}dv\,ds$$
$$=\frac{1}{8}\int_0^L\frac{\kappa^2(1+\Psi^2)^2}{\psi}\ln\left(\frac{1+w\psi}{1-w\psi}\right)ds, \tag{12}$$

where we recall that $ds=|\mathbf{r}'(u)|du$. We do not attempt to determine the exact shape as we only want to determine a reasonable shape. Hence, we consider curves of the form

$$\mathbf{r}(u)=(c_1\sin u, c_2\sin 2u, c_3\cos 3u), \tag{13}$$

representing the general form of the median of a Möbius structure. The case $c_1=c_2=1$ and $c_3=3/2$ is the parametrization given by Schwarz [16,17]. We now consider the optimization problem

$$\text{minimize} \quad \int_0^{2\pi}\frac{\kappa^2(1+\Psi^2)^2}{\psi}\ln\left(\frac{1+w\psi}{1-w\psi}\right)|\mathbf{r}'|du, \tag{14}$$

$$\text{such that} \quad \int_0^{2\pi}|\mathbf{r}'|du=L=200\ \text{Å}, \tag{15}$$

$$\text{and} \quad |\psi(u)|<w^{-1}=0.3\ \text{Å}^{-1}, \quad u\in[0,2\pi]. \tag{16}$$

Using the optimization toolbox in MATLAB we find the numerical solution

$$c_1=32.252\ \text{Å}, \quad c_2=19.051\ \text{Å}, \quad c_3=6.264\ \text{Å}. \tag{17}$$

The resulting Möbius structure is shown in Fig. 1.

The Möbius structure can be developed into a rectangle with rectangular coordinates $(u^1,u^2)\in[0;L]\times[-w;w]$ given by

$$u^1=s(u)+v\Psi(u)=\int_0^u|\mathbf{r}'(u)|du+v\frac{\tau(u)}{\kappa(u)} \quad \text{and} \quad u^2=v. \tag{18}$$

Using these coordinates, Δ_Σ is the usual Laplacian in the plane and Eq. (3) becomes

$$\Delta_0=\partial_1^2+\partial_2^2+M^2. \tag{19}$$

IV. NUMERICAL RESULTS AND DISCUSSION

In Fig. 2, the M^2 contribution to the Laplacian is plotted in contour in the (u^1,u^2) plane as computed according to Eq. (11) for the parameter values $L=200$ Å and $2w=6.67$ Å. Obviously, the relatively complicated geometry of the Möbius structure makes the M^2 contribution a complicated function of (u^1,u^2) coordinates. The observed lack of symmetry leads to splitting of states which are degenerate in the flat-Möbius case [i.e., states with quantum numbers $+m$ and $-m$ as defined in Eq. (20)]. In Table I, we give the first ten values of

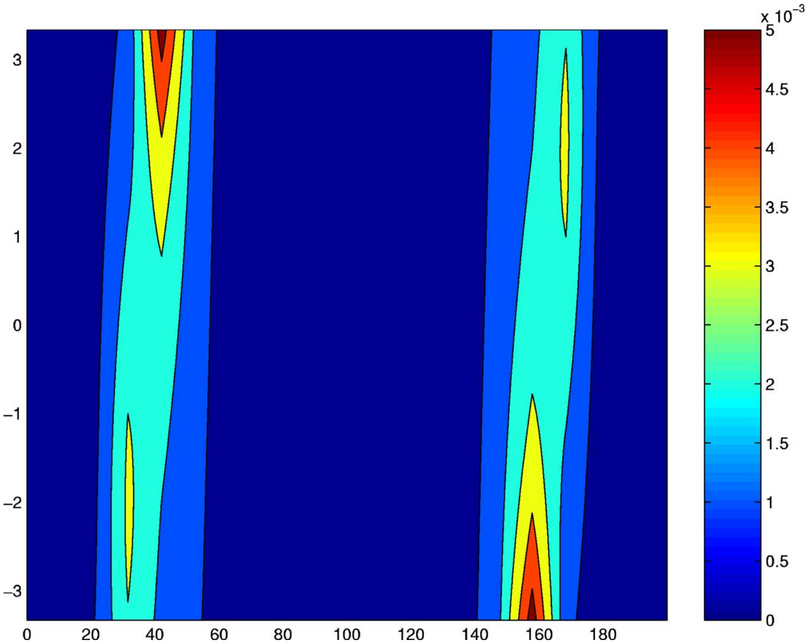

FIG. 2. (Color online) Plot of the M^2 contribution to the kinetic energy versus coordinates u^1 and u^2 in the domain $(u^1,u^2)=[0;L]\times[-w;w]$. Parameter values for L and w are as in Table I. The maximum value of the M^2 contribution is approximately 5.6×10^{-3} Å^{-2} (dark red) corresponding to [in energy, i.e., $(\hbar^2/2m)M^2$] a maximum value of approximately 21 meV.

the eigenenergy E corresponding to the flat-cylinder problem case. These values can be found analytically using separation of variables as will be next explained. Assuming a separable solution $\chi(u^1,u^2)=\chi_1(u^1)\chi_2(u^2)$ and imposing the cylinder boundary conditions in Eqs. (7) and (8) leads to the following eigenstates by solving Eq. (1) for $M=0$:

$$\chi_1(u^1) = \sin\left(\frac{m\pi}{L}u^1 + \phi\right), \tag{20}$$

with ϕ an arbitrary phase, and

$$\chi_2(u^2) = \sin\left(\frac{n\pi}{w}u^2\right), \tag{21}$$

or

$$\chi_2(u^2) = \cos\left(\frac{(2n+1)\pi}{2w}u^2\right), \tag{22}$$

where n is an integer $(0,\pm1,\pm2,\pm3,\ldots)$ and m is an even number $(0,\pm2,\pm4,\pm6,\ldots)$. The corresponding energy eigenvalues are

TABLE I. Computed first three eigenenergy values E in meV for a particle with mass $m=9.11\times10^{-31}$ kg confined to [in case (a)] a flat-cylinder (or flat-Möbius) structure, and [in case (b)] a Möbius-shell structure including M^2 contributions. Geometrical parameters are $L=200$ Å and width $2w=6.67$ Å and Planck's constant is $\hbar=1.0545\times10^{-34}$ J s. Note that due to the small width $(2w)$, the first several eigenenergies and eigenstates for the flat-cylinder and flat-Möbius structure problems are the same.

Parameter values	$E(1)$	$E(2)$	$E(3)$
Case (a)	845.8	849.7	860.7
Case (b)	841.5	843.6	847.9

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{m\pi}{L}\right)^2 + \left(\frac{n\pi}{w}\right)^2\right], \tag{23}$$

if χ_2 is one of the functions in Eq. (21), or

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{m\pi}{L}\right)^2 + \left(\frac{(2n+1)\pi}{2w}\right)^2\right], \tag{24}$$

if χ_2 is one of the functions in Eq. (22).

We may obtain the eigenstates for the flat-Möbius problem by use of the flat-cylinder problem eigenstates just found. Note that flat-Möbius strip eigenstates on the domain $(u^1,u^2)=[0;L]\times[-w;w]$ are also solutions to the flat-cylinder problem on the (double) domain $(u^1,u^2)=[0;2L]\times[-w;w]$ restricted to the domain $(u^1,u^2)=[0;L]\times[-w;w]$. This fact allows us to identify the flat-Möbius structure eigenstates as

$$\chi(u^1,u^2) = \chi_1(u^1)\chi_2(u^2) = \sin\left(\frac{m\pi}{2L}u^1 + \phi\right)\cos\left(\frac{(2n+1)\pi}{2w}u^2\right), \tag{25}$$

with $m=0,\pm4,\pm8,\pm12,\ldots$ and $n=0,\pm1,\pm2,\pm3,\ldots$, or

$$\chi(u^1,u^2) = \chi_1(u^1)\chi_2(u^2) = \sin\left(\frac{m\pi}{2L}u^1 + \phi\right)\sin\left(\frac{n\pi}{w}u^2\right), \tag{26}$$

with $m=\pm2,\pm6,\pm10,\ldots$ and $n=0,\pm1,\pm2,\pm3,\ldots$. The corresponding energy eigenvalues are

$$E = \frac{\hbar^2}{2m}\left[\left(\frac{m\pi}{2L}\right)^2 + \left(\frac{(2n+1)\pi}{2w}\right)^2\right], \tag{27}$$

if χ is one of the functions in Eq. (25), or

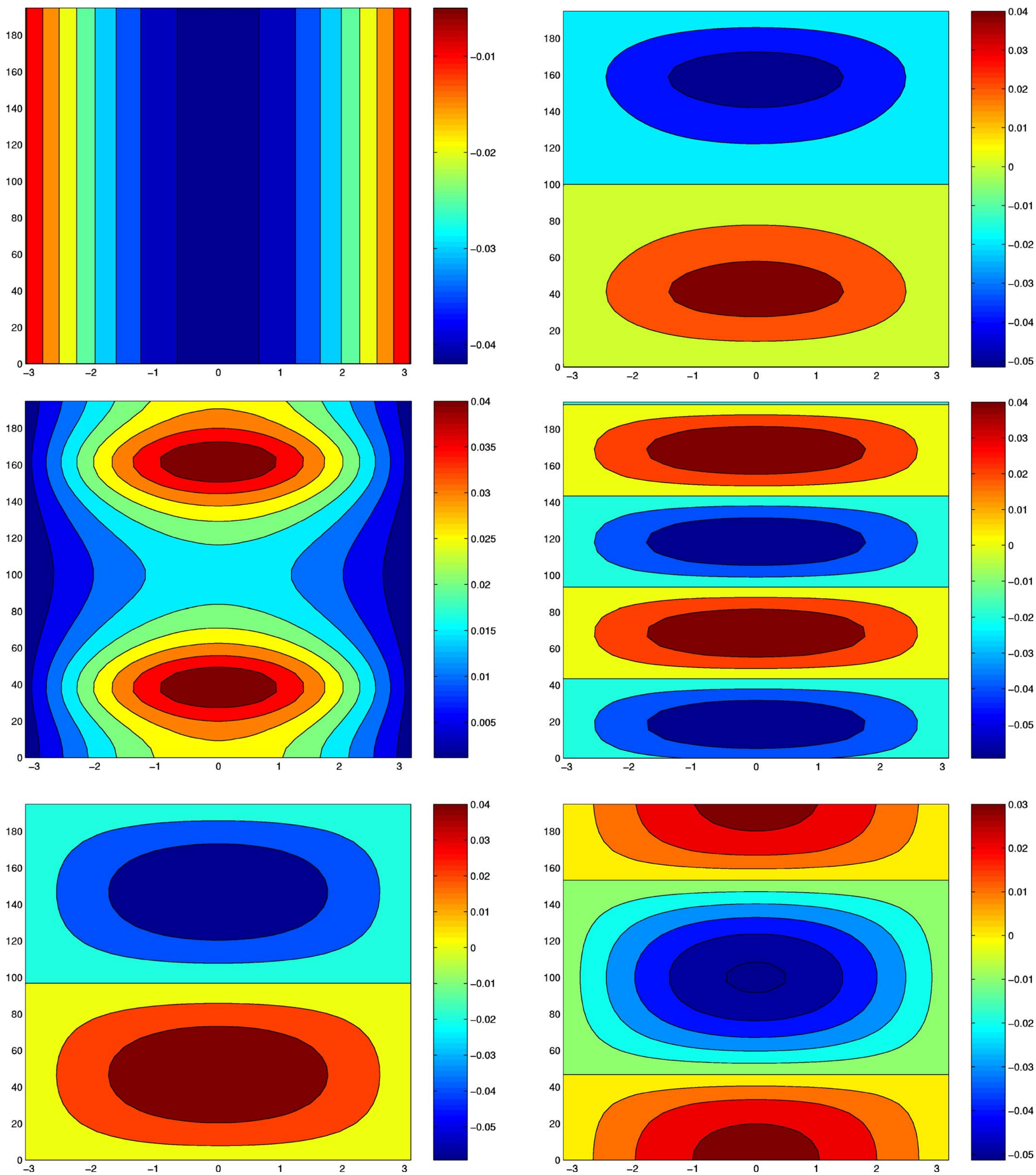

FIG. 3. (Color online) Contour plots of the first three eigenstates for the flat-Möbius structure case (upper left, middle left, and lower left plots) and the Möbius-structure case including the M^2 contributions (upper right, middle right, and lower right plots). Eigenstates are plotted versus coordinates u^1 and u^2 in the domain $(u^1,u^2)=[0;L]\times[-w;w]$. Parameter values for L and w are as in Table I.

$$E=\frac{\hbar^2}{2m}\left[\left(\frac{m\pi}{2L}\right)^2+\left(\frac{n\pi}{w}\right)^2\right], \tag{28}$$

if χ is one of the functions in Eq. (26).

In Fig. 3, we show the first three eigenstates (contour plots) for the flat-Möbius structure case (upper left, middle left, and lower left plots) and the Möbius structure case including the M^2 contributions (upper right, middle right, and lower right plots). Apparently, as is found analytically for the flat-Möbius problem, the ground state has no nodes, the first excited state two nodes, and the second excited state four nodes. Note also that all states are doubly degenerate for the flat-Möbius structure problem. The effect of the M^2 contribution to the Möbius problem is most significant for the ground state (compare upper left with upper right plots). In actual fact, due to the strongest effect of the potential at u^1 values near 0.4 and 1.6, the slopes of the ground state are highest near the same u^1 values. Since the $-(\hbar^2/2m)M^2$ contribution is a negative kinetic-energy contribution, the $-(\hbar^2/2m)(\partial_1^2+\partial_2^2)$ contribution to the kinetic energy must compensate, hence being more positive where M^2 is high since the potential energy is constant (zero) everywhere inside the Möbius shell and eigenstates have a definite energy. The above assertion is easily observed in Fig. 3, upper right plot, since the ground state is a concave function of u^1 and u^2, i.e., $\partial_1^2\chi$ and $\partial_2^2\chi$ are negative. Note, in particular, that with the small value of the Möbius width $(2w)$ as compared to the length (L), the first several eigenstates in the flat-cylinder problem case are also eigenstates in the flat-Möbius problem case.

The effect of the M^2 on energies is to shift ground-state energy by −4.3 meV. Similarly, the first excited and second excited states are shifted downward in energy by −6.1 and −12.8 meV, respectively. It must be noted here that the ground state and first excited states in the Möbius-structure case (with M^2 contribution) are nondegenerate solely due to the M^2 constribution stemming from curvature effects to the kinetic energy.

V. CONCLUSIONS

The problem of a quantum-mechanical particle bounded to a Möbius-shell structure is analyzed using differential-geometry methods. The geometry of the Möbius-shell structure is found by minimizing the elastic energy for a given structure of parametrizations. In particular, eigenstates and associated eigenvalues are determined accounting for contributions from Möbius-shell confinement to the kinetic-energy operator in the Schrödinger problem. A comparison with the corresponding eigenstates and eigenvalues for the flat-Möbius structure is given and it is shown that the ground-state double degeneracy found in the flat-Möbius structure case is lifted when including surface-curvature effects in the kinetic-energy operator of the Schrödinger problem. Moreover, the forms of the ground-state and excited-state wave functions are significantly altered due to surface-curvature effects.

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