Erratum: Hückel versus Möbius aromaticity: The particle in a cylinder versus a Möbius strip [Phys. Rev. A **82**, 062118 (2010)]

Evangelos Miliordos

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In the titled article the single particle constrained in a Möbius strip was studied from the quantum-mechanical viewpoint. Unfortunately, the transformation of the Hamiltonian operator in Cartesian coordinates (x , y , and z) to the internal coordinates (s , ϕ) is incorrect. C. C. Bastos, A. C. Pavão, E. S. G. Leandro have recently published the quantum mechanical problem of a particle in generalized cylinders and referred to this issue [1]. The proof provided in the Appendix of the original article is based on the expression of s , ϕ in terms of x , y , and z . Instead, the correct Laplacian is given by the Laplace-Beltrami operator,

$$\nabla^2 = |g|^{-1/2} \sum_{a,b=1}^2 \frac{\partial}{\partial \sigma_a} |g|^{1/2} g_{ab} \frac{\partial}{\partial \sigma_b}, \quad (\text{E1})$$

where $\sigma_1 = s$, $\sigma_2 = \phi$, and $|g|$ is the determinant of the g matrix given by

$$(dx)^2 + (dy)^2 + (dz)^2 = \sum_{a,b=1}^2 g_{ab} d\sigma_a d\sigma_b. \quad (\text{E2})$$

Next, we use that $dw = (\partial w/\partial s)ds + (\partial w/\partial \phi)d\phi$, where $w = x, y, z$. Exploiting Eq. (4) of the original article we come up with $(dx)^2 + (dy)^2 + (dz)^2 = (ds)^2 + \tau^2(d\phi)^2$, where

$$\tau^2 = [R + s \cos(\phi/2)]^2 + s^2/4 = r^2 + s^2/4. \quad (\text{E3})$$

Finally going back to the above Eq. (E1) we obtain

$$\nabla^2 = \frac{1}{\tau} \frac{\partial}{\partial s} \tau \frac{\partial}{\partial s} + \frac{1}{\tau} \frac{\partial}{\partial \phi} \frac{1}{\tau} \frac{\partial}{\partial \phi}. \quad (\text{E4})$$

Consequently, the variable r of Eq. (5) of the original article must be replaced by τ , which goes to r , at first approximation, and finally to R when $r \sim R \gg L > |s|$. Therefore the conclusions drawn in the original article are not affected. However, Eqs. (17)–(21) must be changed as follows:

$$a_{p,q} = \frac{1}{\delta^2} + \frac{4r_{p,q} \cos(\phi_q/2) + s_p}{8\tau_{p,q}^2 \delta}, \quad (17)$$

$$b_{p,q} = \frac{1}{\delta^2} - \frac{4r_{p,q} \cos(\phi_q/2) + s_p}{8\tau_{p,q}^2 \delta}, \quad (18)$$

$$c_{p,q} = \frac{1}{\tau_{p,q}^2 \epsilon^2} + \frac{r_{p,q} s_p \sin(\phi_q/2)}{4\tau_{p,q}^4 \epsilon}, \quad (19)$$

$$d_{p,q} = \frac{1}{\tau_{p,q}^2 \epsilon^2} - \frac{r_{p,q} s_p \sin(\phi_q/2)}{4\tau_{p,q}^4 \epsilon}, \quad (20)$$

$$e_{p,q} = -2 \left[\frac{1}{\delta^2} + \frac{1}{\tau_{p,q}^2 \epsilon^2} \right]. \quad (21)$$

Finally, the numerical results of Table I change slightly as shown in the new Table I.

TABLE I. Energy levels E (a.u.) of an electron confined to a Möbius strip with $R = 5.67$ and $L = 3.78$ a.u. The approximate energies $E_{n,m}$ (a.u.) as calculated from Eq. (8) are also given.

State(s)	E		$E_{n,m}$	n	m
1	0.345411		0.345371	1	0
2,3	0.361414	0.361335	0.360924	1	± 1
4,5	0.408739	0.408739	0.407582	1	± 2
6,7	0.487445	0.487445	0.485345	1	± 3
8,9	0.597063	0.597063	0.594213	1	± 4
10,11	0.737028	0.737028	0.734187	1	± 5
12,13	0.906640	0.906640	0.905266	1	± 6
14,15	1.105089	1.105089	1.107450	1	± 7
16,17	1.331494	1.331494	1.340740	1	± 8
18,19	1.384986	1.384986	1.385373	2	$\pm 1/2$
20,21	1.418194	1.418194	1.416478	2	$\pm 3/2$
22,23	1.482914	1.482914	1.478689	2	$\pm 5/2$
24,25	1.580113	1.580113	1.572005	2	$\pm 7/2$
26,27	1.584945	1.584945	1.605134	1	± 9
28,29	1.709906	1.709906	1.696426	2	$\pm 9/2$
30,31	1.864554	1.864554	1.851952	2	$\pm 11/2$
32,33	1.872426	1.872426	1.900634	1	± 10
34,35	2.067780	2.067780	2.038584	2	$\pm 13/2$

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[1] C. C. Bastos, A. C. Pavão, and E. S. G. Leandro, *J. Math. Chem.* **1** (2016), doi:[10.1007/s10910-016-0652-5](https://doi.org/10.1007/s10910-016-0652-5).