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Spheroidal geometry approach to fullerene molecules

R. Pincak [1]

Joint Institute for Nuclear Research, Bogoliubov Laboratory of Theoretical Physics, 141980 Dubna, Moscow region, Russia

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Abstract

Graphite is an example of a layered material that can be bent to form fullerenes which promise important applications in electronic nanodevices. The spheroidal geometry of a slightly elliptically deformed sphere was used as a possible approach to fullerenes. We assumed that for a small deformation the eccentricity of the spheroid $e \ll 1$. We are interested in the elliptically deformed fullerenes C_{70} as well as in C_{60} and its spherical generalizations like big C_{240} and C_{540} molecules. The low-lying electronic levels are described by the Dirac equation in $(2+1)$ dimensions. We show how a small deformation of spherical geometry evokes a shift of the electronic spectra compared to the sphere. The flux of a monopole field was included inside the surface to describe the fullerenes. Both the electronic spectrum of spherical and the shift of spheroidal fullerenes were derived.

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Keywords: Electronic spectrum; Fullerenes; Elliptic deformation; Dirac equation; Monopole field

1. Introduction

Fullerene molecules [1] are carbon cages which appear in the vaporization of graphite. One of their most beautiful features from a formal point of view is their geometric character and the exciting possibility of producing them in all sorts of geometric shapes having as building blocks sections of the honeycomb graphite lattice. The most abundant of them is the most spherical C_{60} molecule. The shape of the C_{60} molecule is that of a soccer ball, consisting of 12 pentagons and 20 hexagons. However, some fullerenes as C_{70} are slightly elliptically deformed with the shape being more similar to an American football. Fullerenes belong to a sort of carbon nanoparticles.

E-mail address: pincak@saske.sk (R. Pincak).

[1] On leave from Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 043 53 Kosice, Slovak Republic.

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Carbon nanoparticles, which are expected to have important implications for the development of electronic devices, flat panel displays, nanoswitches, etc., have recently received great attention of both experimentalists and theorists (see [2]). High flexibility of carbon allows one to produce variously shaped carbon nanoparticles: nanotubes, fullerenes, cones, toroids, graphitic onions and nanohorns. Particular attention was given to peculiar electronic states due to topological defects which were observed in different kinds of carbon nanoparticles by scanning tunneling microscopy (STM). For example, STM images with five-fold symmetry (due to pentagons in the hexagonal graphitic network) were obtained in the C_{60} fullerene molecule [3]. The peculiar electronic properties at the ends of carbon nanotubes (which include several pentagons) were probed experimentally in [4,5].

By its nature, the pentagon in a graphite sheet is a topological defect. Actually, as was mentioned in Ref. [6], fivefold coordinated particles are orientational disclination defects in the otherwise sixfold coordinated triangular lattice. The local density of states was found in the vicinity of a pentagonal defect for spherical fullerenes [7,8]. Moreover, disclinations are *generic* defects in closed carbon structures, fullerenes and nanotubes, because, in accordance with Euler's theorem, these microcrystals can only be formed by having a total disclination of 4π. According to the geometry of the hexagonal network, this implies the presence of twelve pentagons (60° disclinations) on the closed hexatic surface.

Investigation of the electronic structure requires formulating a theoretical model describing electrons on arbitrary curved surfaces with disclinations taken into account. An important ingredient of this model can be provided by the self-consistent effective-mass theory describing the electron dynamics in the vicinity of an impurity in graphite intercalation compounds [9]. The most important fact found in [9] is that the electronic spectrum of a single graphite plane linearized around the corners of the hexagonal Brillouin zone coincides with that of the Dirac equation in $(2+1)$ dimensions. This finding stimulated a formulation of some field-theory models for Dirac fermions on hexatic surfaces to describe electronic structure of variously shaped carbon materials: fullerenes [10,11] and nanotubes [12].

The Dirac equation for massless fermions in three-dimensional space–time in the presence of the magnetic field was found to yield $N-1$ zero modes in the N-vortex background field [13]. As was shown in Ref. [14], the problem of the local electronic structure of fullerene is closely related to Jackiw's analysis [13]. Notice that the field-theory models for Dirac fermions on a plane and on a sphere [15] were invoked to describe variously shaped carbon materials. Recently, the importance of the fermion zero modes was discussed in the context of high-temperature chiral superconductors and fullerene molecules.

The most spherical fullerene is the C_{60} molecule nicknamed a 'bucky ball'. Others are either slightly (as C_{70} whose shape is more like an elliptic deformation) or remarkably deformed. We are interested here in the C_{60} molecule as well as in its spherical generalizations like big C_{240} and C_{540} molecules with the symmetry group of the icosahedron, and also in the elliptically deformed fullerene C_{70} and its relatives. Big fullerenes are used to store radioactive material and inhibit enzymes related to different viruses [16,17].

2. The model

Almost all fullerenes are only slightly elliptically deformed spherical molecules, e.g., C_{70} and its relatives. We start with introducing spheroidal coordinates and writing down the Dirac operator for free massless fermions on the Riemann spheroid S^2. Pi-molecular orbitals in fullerenes as a free electron model (electron gas) bound on the surface of a sphere were used in [18]. We generalize that work to obtain an electronic spectrum for spherical and spheroidal geometries with and without the monopole field. The peculiarities of the electronic spectra for these two slightly different types of geometries are shown. To incorporate fermions on the curved background, we need a set of orthonormal frames $\{e_\alpha\}$, which yield the same metric, $g_{\mu\nu}$, related to each other by the local $SO(2)$ rotation,

$$e_\alpha \to e'_\alpha = \Lambda^\beta_\alpha e_\beta, \quad \Lambda^\beta_\alpha \in SO(2).$$

It then follows that $g_{\mu\nu} = e^{\alpha}_{\mu} e^{\beta}_{\nu} \delta_{\alpha\beta}$ where e^{μ}_{α} is the zweibein, with the orthonormal frame indices being $\alpha, \beta = \{1, 2\}$, and the coordinate indices $\mu, \nu = \{1, 2\}$. As usual, to ensure that physical observables are independent of a particular choice of the zweibein fields, a local $so(2)$ valued gauge field ω_{μ} is to be introduced. The gauge field of the local Lorentz group is known as a spin connection. For a theory to be self-consistent, the zweibein fields must be chosen to be covariantly constant [19]

$$\mathcal{D}_{\mu} e^{\alpha}_{\nu} := \partial_{\mu} e^{\alpha}_{\nu} - \Gamma^{\lambda}_{\mu\nu} e^{\alpha}_{\lambda} + (\omega_{\mu})^{\alpha}_{\beta} e^{\beta}_{\nu} = 0,$$

which determines the spin connection coefficients explicitly

$$(\omega_{\mu})^{\alpha\beta} = e^{\alpha}_{\nu} D_{\mu} e^{\beta\nu}. \tag{1}$$

Finally, the Dirac equation on a surface Σ in the presence of the magnetic monopole field A_{μ} is written as [20]

$$i\gamma^{\alpha} e_{\alpha}{}^{\mu} [\nabla_{\mu} - i A_{\mu}] \psi = E\psi, \tag{2}$$

where $\nabla_{\mu} = \partial_{\mu} + \Omega_{\mu}$ with

$$\Omega_{\mu} = \frac{1}{8} \omega^{\alpha}{}_{\mu}{}^{\beta} [\gamma_{\alpha}, \gamma_{\beta}], \tag{3}$$

being the spin connection term in the spinor representation.

The elliptically deformed sphere or a spheroid

$$\frac{x^2}{a^2} + \frac{y^2}{a^2} + \frac{z^2}{c^2} = 1, \tag{4}$$

may be parameterized by two spherical angles $q^1 = \theta$, $q^2 = \phi$ that are related to the Cartesian coordinates x, y, z as follows

$$x = a \sin\theta \cos\phi, \qquad y = a \sin\theta \sin\phi, \qquad z = c \cos\theta. \tag{5}$$

We have assumed that the eccentricity of the spheroid is $e \ll 1$ which in the case $c < a$ gives expressions $e = \sqrt{1 - (\frac{c}{a})^2} \ll 1$. The metric tensor and the natural diagonal zweibein different from zero on the spheroid are

$$g_{\phi\phi} = a^2 \sin^2\theta, \qquad g_{\theta\theta} = a^2 \cos^2\theta + c^2 \sin^2\theta, \tag{6}$$

where $a, c \geqslant 0$, $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \phi < 2\pi$ and

$$e^2_{\phi} = \frac{1}{a \sin\theta}, \qquad e^1_{\theta} = \frac{1}{\sqrt{a^2 \cos^2\theta + c^2 \sin^2\theta}}, \tag{7}$$

which, in view of Eq. (1) gives the spin connection coefficients

$$\omega^{12}_{\phi} = -\omega^{21}_{\phi} = \frac{a}{\sqrt{a^2 + c^2 \tan^2\theta}} =: 2\omega. \tag{8}$$

In 2D the Dirac matrices can be chosen to be the Pauli matrices, $\gamma^1 = -\sigma^2$, $\gamma^2 = \sigma^1$; Eq. (3) then reduces to

$$\Omega_{\phi} = i\omega\sigma^3. \tag{9}$$

We have assumed that $A_{\theta} = 0$ and only the monopole field A_{ϕ} is different from zero.

The eigenfunctions of the Dirac operator are two-component spinors that satisfy the eigenvalue equation

$$-i\hat{\nabla} \begin{pmatrix} \alpha_{\lambda}(\theta, \phi) \\ \beta_{\lambda}(\theta, \phi) \end{pmatrix} = \lambda \begin{pmatrix} \alpha_{\lambda}(\theta, \phi) \\ \beta_{\lambda}(\theta, \phi) \end{pmatrix}. \tag{10}$$

This system of first order partial differential equations in α and β allows separation of variables therefore we can isolate the ϕ-dependence by expanding the spinors into the Fourier series

$$\Psi(\theta,\phi)=\begin{pmatrix}\alpha_\lambda(\theta,\phi)\\ \beta_\lambda(\theta,\phi)\end{pmatrix}=\sum_m \frac{\exp(im\phi)}{\sqrt{2\pi}}\begin{pmatrix}\alpha_{\lambda m}(\theta)\\ \beta_{\lambda m}(\theta)\end{pmatrix},\quad m=\pm\frac{1}{2},\pm\frac{3}{2},\ldots, \tag{11}$$

where m are half-integers since we work with the spin $\frac{1}{2}$ field. Then the general form of the Dirac equation, Eq. (2), on the spheroid becomes

$$\begin{aligned}&\left[\partial_\theta+\sqrt{\cot^2\theta+\left(\frac{c}{a}\right)^2}m+\left(1-2A_\phi\sqrt{1+\left(\frac{c}{a}\right)^2\tan^2\theta}\right)\frac{\cot\theta}{2}\right]\beta_{\lambda m}(\theta)\\ &\quad=-\sqrt{a^2\cos^2\theta+c^2\sin^2\theta}\,E\alpha_{\lambda m}(\theta),\\ &\left[\partial_\theta-\sqrt{\cot^2\theta+\left(\frac{c}{a}\right)^2}m+\left(1+2A_\phi\sqrt{1+\left(\frac{c}{a}\right)^2\tan^2\theta}\right)\frac{\cot\theta}{2}\right]\alpha_{\lambda m}(\theta)\\ &\quad=\sqrt{a^2\cos^2\theta+c^2\sin^2\theta}\,E\beta_{\lambda m}(\theta).\end{aligned} \tag{12}$$

The number m may be called the projection of angular momentum onto the polar axis. If $a=c=R$, where R is the radius of a sphere, Eq. (12) becomes the Dirac equation for sphere geometry.

Now we want to find an electronic spectrum for the sphere and spheroid analytically and numerically, respectively; therefore, we firstly assume that pentagon defects represented in this model by the monopole field $A_\phi=0$. Next, we want to separate the equations for the spinor components α and β. This can be done by taking the square Δ (Laplace operator) of the Dirac operator $\hat{\nabla}$ for spheroidal geometry. Finally, we find the equations

$$\begin{aligned}&\left[-\frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta+\left(\cot^2\theta+\left(\frac{c}{a}\right)^2\right)m^2-\sigma^3\frac{\cot\theta}{\sqrt{\cot^2\theta+(c/a)^2}}\frac{m}{\sin^2\theta}+\frac{1}{4\sin^2\theta}\right]\begin{pmatrix}\alpha_{\lambda m}(\theta)\\ \beta_{\lambda m}(\theta)\end{pmatrix}\\ &\quad=\left[\left(a^2\cos^2\theta+c^2\sin^2\theta\right)E^2-\frac{1}{4}\right]\begin{pmatrix}\alpha_{\lambda m}(\theta)\\ \beta_{\lambda m}(\theta)\end{pmatrix}.\end{aligned} \tag{13}$$

Further simplifications come from the change of variables $x=\cos\theta$, $x\in[-1,1]$, which converts Eq. (13) into the generalized hypergeometric equations

$$\begin{aligned}&\left[\frac{d}{dx}\left(1-x^2\right)\frac{d}{dx}-\left(\frac{x^2}{1-x^2}+\left(\frac{c}{a}\right)^2\right)m^2+\sigma^3\frac{x}{\sqrt{x^2+(c/a)^2(1-x^2)}}\frac{m}{1-x^2}-\frac{1}{4(1-x^2)}\right]\begin{pmatrix}\alpha_{\lambda m}(x)\\ \beta_{\lambda m}(x)\end{pmatrix}\\ &\quad=-\left[\left(a^2x^2+c^2\left(1-x^2\right)\right)E^2-\frac{1}{4}\right]\begin{pmatrix}\alpha_{\lambda m}(x)\\ \beta_{\lambda m}(x)\end{pmatrix}.\end{aligned} \tag{14}$$

The replacement $x\to -x$ (or $m\to -m$) is equivalent to changing α for β. Thus, the upper and lower spinor components are conjugate with respect to mirror reflection. Eq. (14) is singular at the poles of the spheroid $x=\pm1$. We redefine the unknowns

$$\begin{pmatrix}\alpha_{\lambda m}(x)\\ \beta_{\lambda m}(x)\end{pmatrix}=\begin{pmatrix}(1-x)^{1/2|m-1/2|}(1+x)^{1/2|m+1/2|}\xi_{\lambda m}(x)\\ (1-x)^{1/2|m+1/2|}(1+x)^{1/2|m-1/2|}\eta_{\lambda m}(x)\end{pmatrix}, \tag{15}$$

and use that in our model of a slightly deformed sphere $c\sim a$; hence $\frac{c}{a}\doteq 1\pm\delta$, where $\delta\ll 1$ is small deformation of the sphere. Neglecting the second and higher order powers of δ we solve Eq. (14) to the first order in δ and by using redefinition (15) we arrive at the separate equations of hypergeometric type in $\xi_{\lambda m}$ and $\eta_{\lambda m}$

$$\left\{\left(1-x^2\right)\frac{d^2}{dx^2}-\left(1-2(m-1)x\right)\frac{d}{dx}-m(m-1)+\lambda^2-\frac{1}{4}+f(x)\right\}\xi_{\lambda m}(x)=0, \tag{16}$$

where

$$f(x) = \delta\left(\mp 2m^2 \pm 2a^2E^2 \mp mx \mp 2a^2E^2x^2\right), \qquad \lambda = Ea.$$

For the above calculations we have assumed that $m - 1/2 \leqslant 0$. A similar solution can be also found for the case $m - 1/2 \geqslant 0$. Following the calculations above we can get also the equation for function $\eta_{\lambda m}(x)$. The function $f(x)$ is the deviation of the solution for a spheroid from that for a sphere, see [21], and can be perceived as next energy part, i.e., the energy shift for a spheroid compared to a sphere geometry. Thus the expression $f(x)$ can also be called as a perturbation part of Eq. (16).

To find the spectrum for spherical geometry $a = c = R$, we have to put the expression $f(x) = 0$, so the case if $\delta = 0$. The spectrum can be found in the form

$$\lambda^2_{\text{sphere}} = \left(n + |m| + \frac{1}{2}\right)^2, \tag{17}$$

with non-negative integer $n \geqslant 0$, with n being the order of Jacobi polynomials, see [21]. The eigenvalues λ for the sphere of the unit radius S^2 are non-zero integers

$$\lambda_{\text{sphere}} = \pm 1, \pm 2, \ldots, \tag{18}$$

and indeed the Dirac operator has no zero-modes. The spectra of the spherical geometry as the numerical calculations of Eq. (12) with $A_\phi = 0$ and for $a = c$ are illustrated in Fig. 1 and fit the analytical results in (18).

To find the electronic spectrum also in the case of spheroidal geometry when $f(x) \neq 0$, we solve Eq. (12) for two cases, when $a < c$ and $a > c$, i.e., for two different types of an elliptically deformed sphere. The numerical results are shown in Fig. 2.

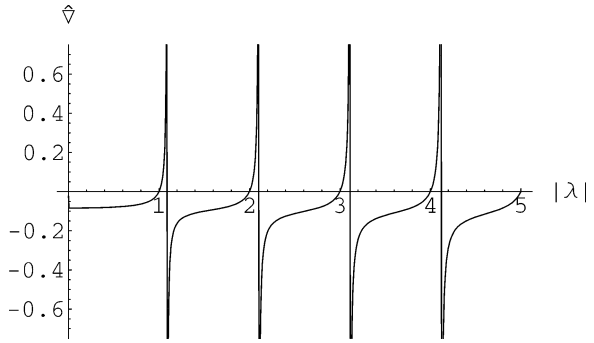

Fig. 1. The electronic spectra of spherical geometry $|\lambda|_{\text{sphere}}$, where $a = c$.

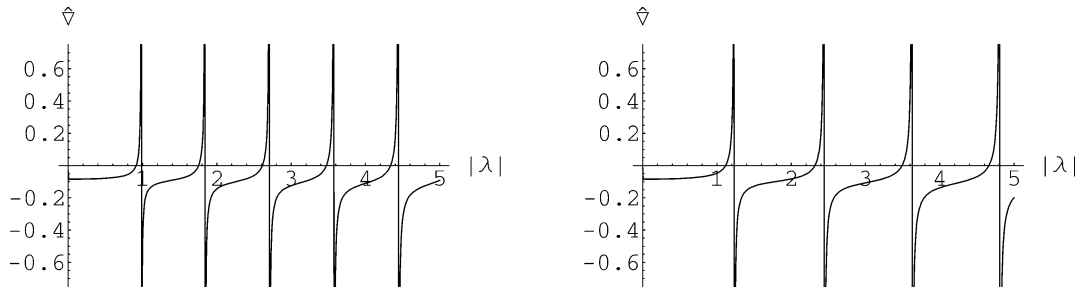

Fig. 2. The electronic spectra of spheroidal geometry $|\lambda|_{\text{spheroid}}$ where, $a < c$ and $a > c$ (going from left to right).

As can be seen from Fig. 2, the spectra display the energetic shifts compared to the spectra of the sphere in Fig. 1. The shift increases or reduces the initial electronic spectrum of sphere depending on the type of elliptic deformation. The shift is bigger with increasing value of the modes of the electronic spectra, which can be also seen from the structure of $f(x)$ in Eq. (16). The perturbation parameter $\delta = 0.3$ was used to obtain the electronic spectra of the Dirac equation for the spheroidal geometry. The angular momentum $m = 1/2$ was used in the calculations. All the spectra are mirror symmetric with respect to the y-axis.

3. Dirac equations for spheroid with monopole field

We assume that the parameter of perturbation and the eccentricity of the spheroid $e \ll 1$, so we can use the magnetic monopole field inside the surface to obtain C_{70} fullerene or bigger fullerene molecules like C_{240} and C_{540} also with a small elliptical deformation. The area of surface for a small elliptically deformed sphere, spheroid, e.g., for oblate spheroid ($a = b$) can be formulated as, see [22]

$$S \approx 2\pi\left(a^2 + c^2\frac{\operatorname{arctanh}(e)}{e}\right).$$

In the case of small eccentricity the surface area of a spheroid becomes the surface area of a sphere $S \approx 2\pi a^2$. It means that we can include the existence of a fictitious magnetic monopole charge g inside the surface of the spheroid with the structure as in Ref. [15]. The values of g, e.g., for tetrahedron and icosahedron structures required $1/2$ and $3/2$, respectively. With the monopole field taken as $A_\theta = 0$ and $A_\phi = \frac{j}{2}\cos\theta$, where $j/2 = g$ (for structures above $j = 1, 3$), the resulting Dirac equation (12) for the spheroid with the monopole field reads

$$\begin{aligned}
&\left[\partial_\theta + \sqrt{\cot^2\theta + \left(\frac{c}{a}\right)^2}m + \left(1 - \frac{j}{a}\sqrt{a^2\cos^2\theta + c^2\sin^2\theta}\right)\frac{\cot\theta}{2}\right]\beta_{\lambda m}(\theta)\\
&\quad = -\sqrt{a^2\cos^2\theta + c^2\sin^2\theta}\,E\alpha_{\lambda m}(\theta),\\
&\left[\partial_\theta - \sqrt{\cot^2\theta + \left(\frac{c}{a}\right)^2}m + \left(1 + \frac{j}{a}\sqrt{a^2\cos^2\theta + c^2\sin^2\theta}\right)\frac{\cot\theta}{2}\right]\alpha_{\lambda m}(\theta)\\
&\quad = \sqrt{a^2\cos^2\theta + c^2\sin^2\theta}\,E\beta_{\lambda m}(\theta).
\end{aligned} \tag{19}$$

Unfortunately, general solutions to Eq. (19) are not available yet for spherical and spheroidal fullerenes, so we do not have initial conditions for numerical calculations which are very sensitive to them. However, we will present some analytical predictions of the electronic spectra for spherical and spheroidal fullerenes from the square of Dirac operator in Eq. (19).

To find an analytical expression for the shift of the spheroidal fullerenes, we put for simplicity in Eq. (19) the value of the angular momentum $m = 0$. For elliptically deformed fullerenes in the special case where $m = 0$ with using the model of a slightly deformed sphere where $\frac{c}{a} \doteq 1 \pm \delta$, the square of Dirac operator (19) was found in the form

$$\begin{aligned}
&\left[-\frac{1}{\sin\theta}\partial_\theta\sin\theta\partial_\theta + \frac{(j\sqrt{(1 \pm 2\delta\sin^2\theta)} - \sigma^3)^2}{4\sin^2\theta} + \sigma^3\frac{\pm j\delta\cos^2\theta}{\sqrt{(1 \pm 2\delta\sin^2\theta)}}\right]\begin{pmatrix}\alpha_{\lambda m}(\theta)\\ \beta_{\lambda m}(\theta)\end{pmatrix}\\
&\quad = \left[\left(\lambda^2 + \left(\frac{j}{2}\right)^2\right)(1 \pm 2\delta\sin^2\theta) - \frac{1}{4}\right]\begin{pmatrix}\alpha_{\lambda m}(\theta)\\ \beta_{\lambda m}(\theta)\end{pmatrix},
\end{aligned} \tag{20}$$

where $\delta \ll 1$ is small deformation of the sphere. We neglect the second and higher order powers of δ in the calculations.

If the perturbation parameter $\delta = 0$, we get the square of Dirac operator for spherical fullerenes with the electronic spectrum as in Ref. [11]. To get connection with Section 2, the spectrum with the monopole field for the spherical fullerenes can be rewrite from the right-hand side of Eq. (20) to the form

$$\lambda_{\text{field}}^2 = \left(|\lambda|_{\text{sphere}} - \frac{1}{2}\right)^2 - g^2, \tag{21}$$

with $|\lambda|_{\text{sphere}} - 1/2 = n + |m|$, see [21]. The value of the electronic spectrum λ_{field} is shifted (decreases) by the value of the charge g of the monopole field. Moreover, the presence of the monopole restricts possible values of the angular momentum [15], so that $m \geqslant ||j| - 1|/2$ and, therefore, the values of m change contrary to structures without a monopole field inside, as in Section 2. It means that for fullerenes the angular momentum m can get the values $m = 0, 1, \ldots$. The spectra of fullerenes are appended by the monopole charge compared to Eq. (13) for spherical geometry. So the spectra of fullerenes are greatly dependent on the value of the monopole field. In the case of tetrahedron and icosahedron structures expression (21) can predict the existence of zero modes where $\lambda_{\text{field}} = 0$.

If $\delta \neq 0$, the shift of the spheroidal fullerenes from the spherical ones in Eq. (20) were found. Moreover, when we use the substitution $x = \cos\theta$ as in Section 2, we can rewrite the shift on the right-hand side of Eq. (20) in the following form

$$f(x) = 2\delta\left(\lambda^2 + g^2\right)\left(\pm 1 \mp x^2\right), \quad \lambda = aE. \tag{22}$$

The electronic spectrum will be shifted by the value $\pm 2\delta(\lambda^2 + g^2)$. The function $f(x)$ is the deviation of spheroidal from spherical fullerenes, similarly to the previous section, and can also be perceived as the energy shift to spheroidal fullerenes compared to spherical ones. Moreover, the perturbation function $f(x)$ is in the case when $m = 0$ and $g = 0$ the same as the shift in Eq. (16) for spheroidal geometry. So we can expect a similar behavior (shifts) of the spectra of spheroidal fullerenes (decreases by the value of the monopole charge g) as in the case of spheroidal geometry without a monopole field, see Fig. 2.

4. Conclusion

To find the electronic spectra of the C_{70} fullerene and its relatives, we have used the model of a slightly elliptically deformed sphere, the spheroidal geometry ($\delta \neq 0$), as distinct from the C_{60} fullerene where the spherical geometry ($\delta = 0$) was used. The Dirac equation in $(2 + 1)$ dimensions for slightly elliptically deformed fullerenes with monopole field inside the surface was evaluated, Eq. (19). The discrete spectrum of energy for both types of geometries was found. The electronic spectrum and the shift of the spheroidal geometry in Eq. (16) contrary to the sphere was calculated both analytically and numerically. Fig. 2 shows the shift of the spectra for spheroidal geometry. From the square of Dirac operator for spheroidal fullerenes valid at first order perturbation in the eccentricity, Eq. (20), the electronic spectrum of spherical and the shift of spheroidal fullerenes were derived analytically. The spectra of spherical and spheroidal fullerenes decreasing by the value of monopole charge g were found. The expression $f(x)$ for deviation of the solution for a spheroid from that for a sphere in Eq. (16) was found the same as for the deviation between spheroidal and spherical fullerenes in expression (22). So we can expect a similar shift of the spectra for real elliptically deformed fullerenes when the magnetic monopole field has to be included inside the surface to simulate pentagon defects and create fullerenes. Zero energy modes dictated by the charge g were found for fullerenes contrary to spherical geometry without the monopole field inside. The shift of the electronic spectra of spheroidal, in contrast to spherical fullerenes, gives rise to reduction or increase in the conduction bandwidth depending on the type of elliptical deformation ($a < c$, $a > c$). Due to this, the crystals made of these deformed fullerene molecules, when doped should be poorer or better conductors than the spherical ones. Moreover, the spherical fullerenes as C_{60} are stable towards fragmentation than the other bigger fullerenes [23], following our

analysis, also with small elliptical deformations and with a shift of the electronic spectra. The presence of the magnetic monopole field with the charge leads to a decrease in the electronic spectra and shifts for spherical and spheroidal molecules, respectively. The decrease is smaller with increasing value of the modes of the electronic spectra and, therefore, for low-lying electronic levels the spectra of the spheroidal fullerenes C_{70} or C_{240} and C_{540} could be shifted to a lower magnitude. The very big structures like C_{960} and C_{1500} become more deformed, faceted and can no longer form a free-electron model like the electronic shell [18], which was the assumption for this model. For these structures the deviation from the sphericity is larger when the pentagon defects are localized at the opposite poles. In the case when the poles are far away from each other we obtain the structure of nanotubes, and for the exact description some new model related to that proposed here should be used. We hope that the knowledge of the shifts of the electronic spectra of spheroids could be useful for experimentalists for choosing the optimal energetic scale for different types of fullerenes. Finally, we think that the spheroidal geometry approach could also be related to other physical problems with slightly deformed spherical structures that are common in the nature.

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