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Spheroidal geometry approach to fullerene molecules

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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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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.

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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,

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

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