Scattering in nanotubes: a position-dependent effective mass approach

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The discovery of carbon-based materials as nanotubes, fullerenes and graphene with their novel mechanical, thermal and electrical properties aroused great interest in the scientific community in recent years. The experimental realization of quasi-two dimensional curved nanostructures in desired shapes, inspired the study of electronic phenomena induced by the geometry of the structure. For example, surface curvature can create p-n junctions in bilayer graphene [PRB 80 (2009)153405] or induce a Hall-like effect in helicoidal ribbons [PRB 79(2009)033404]. In a recent work [Nanotechnology 27(2016)135302], our group showed how to use geometry to manipulate electronic properties on deformed nanotubes. For example, energy gaps may be created and tuned by suitably choosing the shape of the nanotube. In the present work we extend this study to include a spatially varying electronic effective mass. It is well-know that the effective electronic mass in a carbon nanotube depends on its radius. So, this adds a new property which can also be geometrically controlled. We then study the transmittance of charge carriers in nanotubes with specific geometries, taking into account the position-dependent effective mass. This is done in the da Costa approach to the quantum motion of particles constrained to curved surfaces [PRA 23(1981)1982] in combination with the position-dependent effective mass Hamiltonian model proposed by two of us [J. Math. Phys. 53(2012)072101] and coworkers. We numerically solve the Schrödinger equation and find the transmittance for nanotubes with different shapes. In comparison with our previous work, where only geometry is responsible for the emergence of a band gap, the da Costa geometric potential now becomes more intense making the effects on the transmittance more effective. Including the position-dependent effective mass also enhances the effects like generation of band gaps allowing for the use of simpler surfaces than in the previous study. Our results indicate that geometric manipulation of electronic properties can used in the design of nanotube-based electronic devices.