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Variational solution of the Schrödinger equation in an inhomogeneous central field as applied to emission problems.

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The present work is devoted to the supercomputer modelling of the emission processes from the surface of nanostructures that are perspective for modern applications. Within the subject emission processes from single-wall nanotubes with diameters of nanometre range are of particular interest. These devices can be successfully used in nanolithography and non-destructive sounding of nanomaterials. However, for their practical realization the emission processes are needed a detailed study, considering quantum effects. One of essential elements of such analysis is studying the properties of the nanotube surface at the atomic level. In the present paper, we use the fact that the fragment of the nanotube surface is a layer of graphene. A hydrogen-like atom model is used for a detailed consideration of the properties of this object. Earlier, we solved this problem without taking into account the inhomogeneity of the ion field. This research was made with considering the influence of the inhomogeneity of the ion field on the solution of the ground state of a weakly bound electron of a hydrogen-like carbon atom in a graphene lattice. It is shown that the use of the virial theorem in an inhomogeneous field essentially affects the variational solution of the Schrödinger equation.

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