The study of energy states in the Thomson problem

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One of the most important contemporary problems experimental physicists face is calculation of coordinates of an optimal nanostructure. An example is the problem of coating of carbon nanotubes by a suitable fullerene. A nontrivial character of the problem is provided by an exponentially increasing number of suitable halves of the molecule among which an optimal configuration must be chosen guided by the stability of the chemical bond between carbon atoms [1].

The well-known Thomson problem has received unexpected development in the context of this problem. It was noted that through the transition to the so-called dual lattice, the problem of finding a suitable fullerene is reduced to solving the problem similar to the Thomson problem on a hemispherical surface [2].

The main difficulty in solving the problem is not the search for optimal solutions, but their classification. The generally accepted approach is that the configurations are considered equivalent if their potential energies coincide with the specified accuracy [3, 4]. The correct way of classification is to check overlaying solutions using rotations and reflections.

The task was set: to develop a method that allows us to classify the solutions of the Thomson problem depending on the position of point charges on a sphere. To solve the problem, a complete weighted graph was constructed. As vertices of the graph are chosen point charges. In this case, the compatibility of configurations reduces to the isomorphism problem for complete weighted graphs.

The result of the study is a method that allows to undertake research of the solutions of the Thomson problem. In addition, an auxiliary software product was written that allows to quickly generate Thomson problem solutions, as well as to check the emerging solutions for compatibility.

References

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