Regularization of coulomb potential for calculating electron density in quantum mechanical systems

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Abstrak

ABSTRAK
In this paper we show a simple and effective method for regularizing the Coulomb potential for numerical calculations of quantum mechanical problems, such as, for example, the solution of the Schrodinger equation, the expansion of charge density and others. The introduction explains why the regularization of the Coulomb potential is important. In the second part, the regularization method itself as well as its advantages and disadvantages will be described in detail. The third part demonstrates some numerical calculations for the Sulfur plus Hydrogen system using the proposed method. In the final part, the obtained results are summed up.