Abstract Submitted
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**Compact wave functions for variational calculations diatomic system**[1] ODIL YUSUPOV, Samarkand State Univercity — A study of diatomic quantum-mechanical systems is important for molecular theory, chemical physics, theory of few particle coulomb systems, etc. Early we propose [1,2] new type of variational wave function for quantum-mechanical two Coulomb center problem, where one light particle moves in field of two immovable particles. Our function, which is product of binomial combinations of exponential functions of spheroidal coordinates is very compact and accurate. We obtain that electronic energy of molecular hydrogen ion with this 4-term wave function equals -1.10263418 a. u. and very close to the "exact" value – 1.10263422 a.u. To improve the method we realize variational calculations of molecular hydrogen and some other diatomic two-electron ions with these compact exponential functions. To reduce calculations difficulties we apply uncorrelated one-electron approach and scaled basis wave functions. In these calculations we find electronic energies with accuracy about 0.005-0.01 percent. Our results show that improved exponential functions is physical valid, very compact and have acceptable accuracy. These functions can be used as molecular orbitals in quantum-mechanical calculations of diatomic molecules and in modeling few particle coulomb systems. T.K.Rebane and O.N.Yusupov. Opt. and spectr. 72, I6, 1289 (1992) T.K.Rebane and V.S.Zotev. Opt. and spectr. 77, N5, 730 ( 1994)

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Odil Yusupov
Samarkand State Univercity

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