

Abstract Submitted
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Compact wave function useful in educational physics ODIL YUSUPOV — In this abstract we want to submit for consideration compact wave function useful in study quantum mechanic. This is improved classical Guillemin-Zener[1] wave function for primary diatomic molecular system – molecular hydrogen ion. A study of this ion, where one electron moves in field two immovable nuclei, is important for molecular theory, chemical physics, theory of few particle coulomb systems, etc. Compact electronic wave function for ground state of molecular hydrogen ion is $\Psi = N * (\exp(-a1*\xi) + c * \exp(-a2*\xi)) * (\cosh(-b1*\eta) + d * \cosh(-b2*\eta))$ where N - normalization factor, ξ and η are spheroidal coordinates of electron, a1,a2,b1,b2 – nonlinear variational parameters, c and d - linear variational parameters. We found optimal values of this parameters for any internuclear distance R. For example, at R=2 a.u.: a1= 1.4345, a2= 1.9753, b1= 0.5399, b2= 1.3001, c= -0.332876, d= 0.592279 . 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. The calculations was shown that our wave function equivalent to 25- term standard mathematical expansion in spheroidal coordinates. This function can to use as good illustration of variational method in quantum mechanic.

[1]V.Guillemin, C.Zener. Proc. Natl.Acad. Sci. U.S., 15, 314, (1929)

[2]T.K.Rebane and O.N.Yusupov. Opt. and spectr . 72, 6, 1289 (1992)

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