

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Improved Guillemin-Zener wave function useful in molecular and chemical physics.** ODIL YUSUPOV — Classical Guillemin-Zener[1] wave function for primary diatomic molecular system – molecular hydrogen ion have shown high accuracy and quality of exponential functions basis. We want to submit improved compact wave function useful in study quantum mechanic. Compact electronic wave function for ground state of molecular hydrogen ion is  $\Psi = N * (\exp(-a_1 * \xi) + c * \exp(-a_2 * \xi)) * (\cosh(-b_1 * \eta) + d * \cosh(-b_2 * \eta))$  where N - normalization factor,  $\xi$  and  $\eta$  are spheroidal coordinates of electron,  $a_1, a_2, b_1, b_2$  – nonlinear variational parameters, c and d - linear variational parameters. By optimization of energy functional we found optimal values of this parameters for any internuclear distance R. For example, at R=2 a.u.:  $a_1 = 1.4345$ ,  $a_2 = 1.9753$ ,  $b_1 = 0.5399$ ,  $b_2 = 1.3001$ ,  $c = -0.332876$ ,  $d = 0.592279$ . 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 comparison was shown that our improved wave function equivalent to about 25- term standard mathematical expansion in spheroidal coordinates. This function can be used in educational physics as well as for molecular theory, chemical physics, theory of few particle coulomb systems, etc.

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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Date submitted: 30 Nov 2005

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