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Title:	Exact separation of radial and angular correlation energies in two-electron atoms
Authors:	Kammath, Anjana R. (/jspui/browse?type=author&value=Kammath%2C+Anjana+R.)
Keywords:	Schroedinger equation Hylleraas Correlation energy Variational principle
Issue Date:	2019
Publisher:	Elsevier
Citation:	Chemical Physics Letters, 720, pp. 93-96.
Abstract:	Partitioning of helium atom's correlation energy into radial and angular contributions, although of fundamental interest, has eluded critical scrutiny. Conventionally, radial and angular correlation energies of helium atom are defined for its ground state as deviations, from Hartree-Fock and exact values, of the energy obtained using a purely radial wavefunction devoid of any explicit dependence on the interelectronic distance. Here, we show this rationale to associate the contribution from radial-angular coupling entirely to the angular part underestimating the radial one, thereby also incorrectly predict non-vanishing residual radial probability densities. We derive analytic matrix elements for the high-precision Hylleraas basis set framework to seamlessly uncouple the angular correlation energy from its radial counterpart. The resulting formula agrees with numerical cubature yielding precise purely angular correlation energies for the ground as well as excited states. Our calculations indicate 60.2% of helium's correlation energy to arise from strictly radial interactions; when excluding the contribution from the radial-angular coupling, this value drops to 41.3%.
Description:	Only IISERM authors are available in the record.
URI:	https://www.sciencedirect.com/science/article/pii/S0009261419301010 (https://www.sciencedirect.com/science/article/pii/S0009261419301010) http://hdl.handle.net/123456789/2142 (http://hdl.handle.net/123456789/2142)
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