

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

The structure of the second-order non-Born-Oppenheimer density matrix D_2 :¹ EDUARDO LUDENA, CIDNA-ESPOL, Guayaquil, Ecuador, PETER IZA, Department of Physics, ESPOL, Guayaquil, Ecuador, YOSSLEN ARAY, MAURICIO CORNEJO, CIDNA-ESPOL, Guayaquil, Ecuador, DIK ZAMBRANO, Department of Physics, ESPOL, Guayaquil, Ecuador — Properties of the non-Born-Oppenheimer 2-matrix are examined. Using a coordinate system formed by internal translationally invariant plus the total center-of-mass coordinates it is shown that regardless of the point of reference selected, the operator for the reduced second order density matrix, 2-RDM, solely depends upon the translationally invariant internal coordinates. We apply this result to examine the nature of the 2-RDM extracted from the exact analytical solutions for model non-Born-Oppenheimer four-particle systems of the Coulomb-Hooke and Moshinsky types. We obtain for both these models explicit closed-form analytic expressions for the electron and nuclear 2-RDM. An explicit expression is also obtained for the electron-nuclear 2-RDM in the Moshinsky case, which shows coupling between the electron and nuclear coordinates.

¹EVL and YA acknowledge support of SENESCYT's Prometheus Program

Eduardo Ludena
CIDNA-ESPOL, Guayaquil, Ecuador

Date submitted: 05 Nov 2015

Electronic form version 1.4