Selected Abstracts from Other Physical Review Journals

Abstracts of papers that are published in other Physical Review journals and may be of interest to Physical Review A readers are printed below.

Material equations for electromagnetism with toroidal polarizations V. M. Dubovik *Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, 141980, Dubna, Moscow region, Russia* M. A. Martsenyuk *Perm State University, Bukirev Street, 614600 Perm, Russia* Bijan Saha *The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34014 Trieste, Italy* (Received 7 September 1999)

With regard to the toroid contributions, a modified system of equations of electrodynamics moving continuous media has been obtained. Alternative formalisms to introduce the toroid moment contributions in the equations of electromagnetism has been worked out. The two four-potential formalism has been developed. Lorentz transformation laws for the toroid polarizations has been given. Covariant form of equations of electrodynamics of continuous media with toroid polarizations has been written.

Computational method for general multicenter electronic structure calculations P. F. Batcho *Department of Chemistry and Courant Institute of Mathematical Sciences, New York University, Room 1021, 31 Washington Place, New York, New York 10003 and Howard Hughes Medical Research Institute, New York, New York 10003* (Received 16 November 1999)

Here a three-dimensional fully numerical (i.e., chemical basis-set free) method [P. F. Batcho, Phys. Rev. A **57**, 6 (1998)], is formulated and applied to the calculation of the electronic structure of general multicenter Hamiltonian systems. The numerical method is presented and applied to the solution of Schrödinger-type operators, where a given number of nuclei point singularities is present in the potential field. The numerical method combines the rapid ''exponential'' convergence rates of modern spectral methods with the multiresolution flexibility of finite element methods, and can be viewed as an extension of the spectral element method. The approximation of cusps in the wave function and the formulation of multicenter nuclei singularities are efficiently dealt with by the combination of a coordinate transformation and a piecewise variational spectral approximation. The complete system can be efficiently inverted by established iterative methods for elliptical partial differential equations; an application of the method is presented for atomic, diatomic, and triatomic systems, and comparisons are made to the literature when possible. In particular, local density approximations are studied within the context of Kohn-Sham density functional theory, and are presented for selected subsets of atomic and diatomic molecules as well as the ozone molecule.