

Abstract Submitted
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Improved estimators for quantum Monte Carlo calculation of spherically averaged intracule densities¹ JULIEN TOULOUSE, Cornell University, ROLAND ASSARAF, Universite Pierre et Marie Curie, CYRUS UMRIGAR, Cornell University — System-averaged pair densities or “intracule densities” are important for qualitative and quantitative descriptions of electron correlation [1] In quantum Monte Carlo (QMC) simulations, spherically averaged intracule densities are usually calculated by means of the traditional histogram technique (i.e., by counting the number of times two electrons are found at a certain distance) that is very noisy at short electron-electron distances. We will show how previously-used improved estimators for the on-top pair density [2,3] can be generalized to the case of non-vanishing electron-electron distances, as an application of the “zero-variance” procedure [4]. The obtained estimators lead to noise several orders of magnitude smaller than the histogram technique, allowing unprecedented fast and accurate calculations of intracule densities in QMC. Illustrative calculations on simple atomic systems will be given. [1] J. M. Mercero, E. Valderrama and J. M. Ugalde, in “NATO-ASI Series in Metal-Ligand Interaction in Molecular-, Nano-, Micro, and Macro-systems in Complex Environments”, Ed.: N. Russo, D. R. Salahub and M. Witko, Kluwer Academic Publishers, Dordrecht (2003). [2] P. Langfelder, S. M. Rothstein and J. Vrbik, *J. Chem. Phys.* **107**, 8525 (1997). [3] A. Sarsa, F. J. Gálvez and E. Buendía, *J. Chem. Phys.* **109**, 7075 (1998). [4] R. Assaraf and M. Caffarel, *Phys. Rev. Lett.* **83**, 4682 (1999).

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