



Dr Emmanuel Giner
Sorbonne Université
Laboratoire de Chimie Théorique
Paris, France

Telephone: + 33 14 27 70 88
Email: eginer@lct.jussieu.fr

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To the Editors of the Journal of Chemical Physics

Dear Editors,

Please find enclosed my manuscript entitled

“A new form of transcorrelated Hamiltonian inspired by range-separated DFT”,

which I would like you to consider as a full article in the *Journal of Chemical Physics*.

One of the most fundamental drawbacks of conventional wave function methods is the slow convergence of energies and properties with respect to the one-electron basis set. As proposed by Kutzelnigg more than thirty years ago, one can introduce a Jastrow factor explicitly depending on the interelectronic distance r_{12} to significantly speed up the convergence. In this framework, one can take into account the effect of such Jastrow factor directly into an effective Hamiltonian: the transcorrelated Hamiltonian. The generic form of such an effective Hamiltonian have been established in the late 60's by Boys and Handy, but a renewal of interest have emerged recently due to the fast convergence of its eigenvalues with respect to the basis set.

In the present work, I propose the analytical derivation and first numerical test of a new universal Jastrow factor specially designed for the transcorrelated framework. The equations leading to this new Jastrow factor are inspired by the range-separated DFT effective Hamiltonian. Such a Jastrow factor has several advantages: it is tuned by a unique parameter allowing to simply adapt to a typical scale-length, the explicit analytical form of the transcorrelated Hamiltonian is directly known and its eigenvalues converge extremely fast toward the complete basis set limit, all two-electron integrals can be easily performed analytically, the expensive three-body terms can be computed efficiently through a mixed numerical-analytical approach.

Because of its new results in the context of fundamental electronic structure theory, I expect this work to be of interest to a wide audience within the theoretical chemistry community. I suggest Seiichiro L. Ten-No, Ali Alavi, David Tew and Naoto Umezawa as potential referees. This contribution has never been submitted in total nor in parts to any other journal. I look forward to hearing from you soon.

Sincerely, Emmanuel Giner.