Centre for Research in Molecular Modeling
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Wavefunctions for strong correlation drawn from exactly solvable models

The established methods of quantum chemistry are built upon the orbital picture: electrons interact only with the average field produced by the other electrons. The wavefunction is a Slater determinant of the occupied orbitals. Such an approach is expedient when it is possible to unambiguously label each orbital as occupied or unoccupied. These types of systems are *weakly-correlated* and are generally well treated by existing methods. On the other hand, when it is difficult to label orbitals as occupied or unoccupied, the wavefunction is not a single Slater determinant, and further, the number of important determinants grows exponentially with the system size. These types of systems are *strongly-correlated*. Our goal is to develop accurate and affordable techniques for strongly-correlated systems. We employ the eigenvectors of exactly solvable models as a starting point to expand the physical wavefunction. We will outline our approach with a simple model built upon pairs of electrons.

Paul Johnson was a Vanier Canada Graduate Scholar under the supervision of Paul Ayers at McMaster, and Dimitri Van Neck and Patrick Bultinck in Ghent. He was a postdoc with Gustavo Scuseria before starting as an assistant professor at Université Laval.