On some applications of pseudo-differential calculus in quantum mechanic

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e study a new approach to determine the asymptotic behaviour of quantum many-particle systems near coalescence points of particles which interact via singular Coulomb potentials. This problem is of fundamental interest in electronic structure theory in order to establish accurate and efficient models for numerical simulations. Within our approach, coalescence points of particles are treated as embedded geometric singularities in the configuration space of electrons. Based on a general singular pseudo-differential calculus, we provide a recursive scheme for the calculation of the parametrix and corresponding Green operator of a nonrelativistic Hamiltonian. In our singular calculus, the Green operator encodes all the asymptotic information of the eigenfunctions. Explicit calculations and an asymptotic representation for the Green operator of the hydrogen atom and isoelectronic ions are presented.

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