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Electron-pair-density based approach to density functional theory[1] MARKUS DAENE, DONALD NICHOLSON, Oak Ridge National Laboratory — We propose a nonlocal density functional approximation motivated by consideration of the electron-pair-density. The fully interacting exchange correlation hole is approximated from the Slater electron-pair-density by utilizing coupling constant integration and the pair density as a function of coupling constant in the homogeneous electron gas. The electron-pair-density evaluated for closed shell configurations of spherical external potentials will be compared to exact results and approximate results from local density approximations. The electron-pair-density leads straightforwardly by integration to a density and its corresponding interaction energy. These quantities as a function of coupling constant allow us to discuss the quality of our approximation to the Hohenberg-Kohn functional at series of test densities drawn from spherical systems.

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