Relativistic correction to the single-particle kinetic energy term
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tory, Washington DC — Evaluation of the relativistic kinetic energy, given by
$\sqrt{(p^2c^2 + m^2c^4)}$, is one strategy that may be promising from the standpoint of ap-
proximate scalar relativistic treatments. However the square root makes it cum-
bersome in quantum mechanical operator form. Chandra et al. [P. Chandra et al.,
Chem. Phys.**84**, 1 (1984)] have shown that it is possible to derive a simplified method
for evaluating the relativistic kinetic energy within a single-particle framework. In
this method a finite basis set of the p^2 operator is used to evaluate the expectation
values of the p^2 dependent operators. In our formulation, we use a complete basis
set of the p^2 operator to determine a variational expression for the above operator
that is useful for Gaussian-orbital-based calculations. We compare the results of the
corrections to the kinetic energy obtained by our formulation with other methods
such as the expansion of the kinetic energy operator method and an incomplete p^2
basis method. Comparison to the full Dirac equation is made for simple atoms and
the importance of the Darwin term will also be discussed.

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