PHYSICAL REVIEW A VOLUME

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the long-range correlations present in the electron
gas cannot occur. They proposed using LSD only
for antiparallel-spin correlation
Eanti-II ELsD
c c [n n]

-z,'"[n,,o] -E:"[n„o],
a scheme which also effectively subtracts out the self-correlation.

"

Both the SIC and antiparallel-spin approxima-tions give accurate (within 20%) correlation ener-
gies for neutral atoms with Z 18.'"~'

In order

to predict the results for larger atoms and for ions, we have constructed a simple analytic model for the correlation energy as a function of nuclear-charge Z and electron number N. The model shows that all three electron-gas approximations for the correlation energy are qualitatively wrong when Z —~

DENSITY-FUNCTIONAL THEORY OF THE CORRELATION... 2787

0.00 I I I I I I I I I
o EXPERIMENT
~ NUMERICAL SIC

L NUMERICAL LSD

NALYTIC ANTI —

DENSITY-FUNCTIONAL THEORY OF THE CORRELATION.