Erratum: Entanglement and density-functional theory: Testing approximations on Hooke's atom [Phys. Rev. B 77, 205122 (2008)]

J. P. Coe, A. Sudbery, and I. D'Amico (Received 2 August 2010; published 23 August 2010)

DOI: 10.1103/PhysRevB.82.089902

PACS number(s): 03.67.-a, 71.15.Mb, 99.10.Cd

In the subsection "Comparison to standard perturbation theory" the expression for the total energy of Hooke's atom to first order should read

$$E = E^{(0)} + E^{(1)} = 3\omega + \sqrt{\frac{2\omega}{\pi}}$$
.

Consequently results for the error in energy from standard first-order perturbation [dotted curve in Fig. 13 (see Fig. 1 below)] are modified.

Standard first-order perturbation still has the lowest accuracy and no other results are affected.

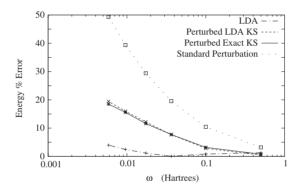


FIG. 1. Relative error of the approximate energy from LDA, first-order perturbation of the LDA KS equations, first-order perturbation of the exact KS equations and standard first-order perturbation, compared to the exact energy plotted against ω .

In addition:

- (i) In the last equation of the subsection "Position-space information entropy" the constant term in the expression for S when neglecting off-diagonal terms should read $\ln N/\ln 2$ instead of $1/\ln 2$;
 - (ii) The y-axis in Fig. 5 and Fig. 12 should be labeled $S_n/\ln 2$;
 - (iii) In the sixth paragraph of the section "Overview and Conclusions" it should be $\omega \ge 0.03$, instead of $\omega \ge 0.003$.

The results and conclusions of the paper remain unaffected.