Origin of static and dynamic steps in exact Kohn-Sham potentials (Supplemental Material)

M. J. P. Hodgson, J. D. Ramsden, and R. W. Godby
Department of Physics, University of York and European Theoretical Spectroscopy Facility, Heslington, York YO10 5DD, United Kingdom
(Dated: April 7, 2016)

THE ALMBLADH-VON BARTH THOUGHT EXPERIMENT

The external potential is (we use Hartree atomic units)

$$v_{\text{ext}} = -\tfrac{6}{5} e^{-\frac{1}{125}(x-a)^4} - \tfrac{9}{10} e^{-\frac{1}{10}(x+a)^2}, \tag{1}$$

where $a = 10$ a.u. For this system converged results are obtained with $\delta x = 0.1$ a.u.

SYSTEM 1 (TWO SPINLESS ELECTRONS IN AN ASYMMETRIC DOUBLE WELL)

The external potential is the same as the Almbladh-von Barth thought experiment, with a grid spacing $\delta x = 0.1$ a.u.

SYSTEM 2 (MOLECULE)

The external potential is of the same form as Eq. 1 with $a = 4$ a.u. The wells are brought together so that the second crossover of the single-particle KS densities occurs while the density is within machine precision. The grid spacing $\delta x = \frac{4}{30}$ a.u.

SYSTEM 3 (DYNAMIC DOUBLE-WELL)

The ground-state external potential is

$$v_{\text{ext}} = -\tfrac{13}{20} e^{-\frac{1}{2}(x-3)^2} - \tfrac{1}{2} e^{-\frac{1}{10}(x+3)^2}. \tag{2}$$

For $t \geq 0$ a perturbing field ($0.1\,|x|$) pushes the electrons together. The grid spacings are $\delta x = 0.1$ a.u. and $\delta t = 1 \times 10^{-4}$ a.u.

SYSTEM 4

The external potential was optimized in order to give a non-interacting density where the integer electron point and density minimum are distinctly different, and hence has no analytical form.

SYSTEM 5

The external potential was optimized in order to give an interacting density where the integer electron point and density minimum are distinctly different, and hence has no analytical form.

SYSTEM 6

The first system (System 6) has an external potential of the form of Eq. 1 with $a = 5$ a.u. The second system (System 6′) has an external potential of the form of Eq. 1 with $a = 3.5$ a.u. The wells have been brought closer together so that the electrons are more delocalized in the region of the step.

SYSTEMS 7A, 7B AND 7C (GROUND-STATE)

The external potential of 7A is of the same form as Eq. 1, with $a = 5$ a.u. The external potential of 7B is the mirror of 7A, i.e. $a \to -a$. And the third system's (System 7C) external potential is given by $v_{\text{ext}}^{C} = \frac{1}{2}\left(v_{\text{ext}}^{A} + v_{\text{ext}}^{B}\right)$. For these three systems converged results were found with $\delta x = 0.05$ a.u.

SYSTEMS 8A, 8B AND 8C (TIME-DEPENDENT)

The ground-state of System 8A ($t < 0$) has an external potential of the form

$$v_{\text{ext}} = -\tfrac{1}{2}e^{-\frac{1}{5}(x+3)^2} - \tfrac{1}{2}e^{-\frac{1}{5}(x-3)^2}. \tag{3}$$

For $t \geq 0$ the external potential is

$$v_{\text{ext}}(t \geq 0) = -e^{-\frac{1}{5}(x+3)^2} - \tfrac{1}{2}e^{-\frac{1}{5}(x-3)^2}. \tag{4}$$

Hence the left well is reduced in depth. This causes the left electron to explore excited energy states.

System 8B is the mirror of System 8A, and again System 8C's external potential is given by $v_{\text{ext}}^{C}(t) = \frac{1}{2}\left(v_{\text{ext}}^{A}(t) + v_{\text{ext}}^{B}(t)\right)$. For these three systems converged results were found with $\delta x = 0.05$ a.u. and $\delta t = 5 \times 10^{-5}$ a.u.