Erratum: Demonstration of initial-state dependence in time-dependent density functional theory [Phys. Rev. A. 63, 042501 (2001)]

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The illustration of initial-state dependence for two non-interacting electrons in one dimension in Fig. 1 was incorrect because the orbitals $\tilde{\phi}_1$ and $\tilde{\phi}_2$ were not chosen to be orthogonal.

A simpler example is provided here. An orthonormal choice, satisfying the conditions that Φ and $\widetilde{\Phi}$ have equal density and equal first time-derivative of the density, is

$$\begin{aligned}\widetilde{\phi}_1(x) &= \sqrt{1+f(x)\phi_2^2(x)}\phi_1(x)\\ \widetilde{\phi}_2(x) &= \sqrt{1-f(x)\phi_1^2(x)}\phi_2(x)\end{aligned} \tag{1}$$

where ϕ_1 and ϕ_2 are the lowest and first excited states of the harmonic oscillator of $k = 1$ and $f(x) = c(256x^4 - 192x^2 + 12)e^{-2x^2}$. The parameter c may be arbitrarily chosen between about -0.172 and 0.147. In the figure below we take $c = -0.1$. The top panel of the figure shows the orbitals and the density while the lower panel shows the initial potentials which keep the densities constant and equal.

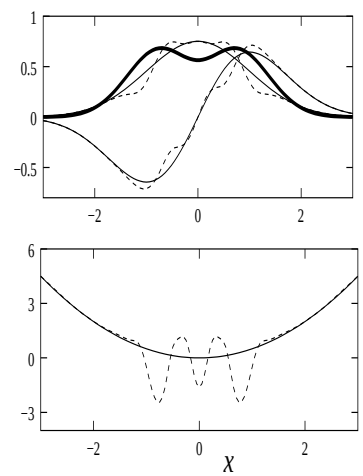

FIG. 1. The top panel shows the lowest and first excited state orbitals ϕ_1 and ϕ_2 (solid) for the harmonic potential, the alternative orbitals $\tilde{\phi}_1$ and $\tilde{\phi}_2$ (dashed), and the density, n (thick solid) which is the same for Φ and $\widetilde{\Phi}$. In the lower panel are the initial potentials v (solid) and $\tilde{v}$ (dashed) in which Φ and $\widetilde{\Phi}$ respectively, evolve with the same density.