Adiabatic approximation within time-dependent density functional theory using inversion of the ground-state spin-density Kohn-Sham formalism

Ingo Dreissigacker*, Manfred Lein

Institut für Theoretische Physik and Centre for Quantum Engineering and Space-Time Research (QUEST),
Leibniz Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany

Abstract

It has recently been shown by Thiele *et al.* [Phys. Rev. Lett. 100 (2008), 153004] that the exact adiabatic approximation in time-dependent density functional theory gives a good description of non-sequential double ionization in the one-dimensional helium atom. In this paper, we propose an adiabatic approximation based on the inversion of ground-state spin-density functional theory and apply it to several model systems. We demonstrate that our approach reproduces the derivative discontinuity and yields correlation potentials close to the exact correlation potentials for a strong-field ionization process as well as for the 1D H_2 and LiH molecules at large internuclear distance.

Keywords: time-dependent density functional theory, adiabatic approximation, strong-field ionization, inversion problem, derivative discontinuity

In the last decade, experimental research on atoms and molecules in ultra-short laser pulses has made rapid progress [1]. Although the computation power has increased in this time as well, only slow progress has been made in the non-perturbative simulation of atoms and molecules with more than one electron. The problem arises from the exponential increase of computation time and memory need with increasing particle number in the direct solution of the time-dependent Schrödinger equation (TDSE). Therefore, present-day simulations rely heavily on methods such as the (multi-configurational) Hartree-Fock theory [2–4] or time-dependent density functional theory (TDDFT) [5, 6]. Exceptions are super-computer studies of helium [7, 8], calculations on H_2 using the B-spline method [9], and the R-matrix Floquet theory for multiphoton processes [10].

TDDFT is in principle exact, but relies in practice on approximations for the exchange-correlation (xc) potential. Though application of TDDFT to the linear-response regime is very succesful [11–14], many problems are encountered in the regime of non-linear response. The most prominent example is the failure of the "standard" TDDFT approximations in predicting the non-sequential double ionization (NSDI) of atoms by strong laser fields correctly [15]. It has been shown that this failure is closely connected to the lack of a derivative discontinuity in present approximations [16]. The derivative discontinuity is known from static density functional theory [17]

and refers to the jump of the xc potential as the particle number passes through an integer. Also certain types of ground-state problems, such as molecules at large internuclear distances, cause severe problems [18, 19].

By calculating the exact adiabatic xc potential, Thiele *et al.* have recently demonstrated that the correlation effects in the double ionization of helium are well described by an adiabatic approximation [20]. However, obtaining the exact adiabatic xc potential is demanding since it requires finding the potential that reproduces a given density as its ground-state density. In this paper, we present a new adiabatic approximation for the exchange-correlation potential in TDDFT that uses inversion of static spin-density functional theory (SDFT). The method gives correlation contributions very close to the exact adiabatic approximation in several model systems that we investigate. At the same time, the computational effort required in the SDFT inversion is much less than in the exact static inversion.

We consider 1D systems containing two particles in a (time-dependent) external potential $v_{ext}(z, t)$. Instead of the time-dependent Schrödinger equation

$$i\frac{\mathrm{d}\psi(z_1, z_2, t)}{\mathrm{d}t} = H\psi(z_1, z_2, t) \tag{1}$$

with
$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z_2^2} + v_{ext}(z_1, t) \\ + v_{ext}(z_2, t) + w(z_1 - z_2) \tag{2}$$

(atomic units are used throughout), in TDDFT we have the time-dependent Kohn-Sham (KS) equation [21]

$$i\frac{\mathrm{d}\varphi(z, t)}{\mathrm{d}t} = \left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + v_s[n](z, t)\right)\varphi(z, t). \tag{3}$$

*Corresponding author
Email address:* `ingo.dreissigacker@itp.uni-hannover.de`
(Ingo Dreissigacker)

Here, $\varphi(z,t)$ is the KS orbital, $n(z,t) = 2|\varphi(z,t)|^2 = 2\int \mathrm{d}z' \, |\psi(z,z',t)|^2$ is the density, and $v_s[n](z,t)$ is the KS potential

$$v_s[n](z,t) = v_{\text{ext}}(z,t) + v_h[n](z,t) + v_{\text{xc}}[n](z,t). \quad (4)$$

In this equation, $v_{\text{xc}}[n](z,t)$ is the xc potential and $v_h[n](z,t)$ the instantaneous Hartree potential

$$v_h[n](z,t) = \int \mathrm{d}z' \, n(z',t)w(z-z'). \quad (5)$$

In writing Eq. (4), we have assumed the system to be initially in the ground state, which is why we can omit the initial-state dependence of $v_s[n](z,t)$ and $v_{\text{xc}}[n](z,t)$ by virtue of the Hohenberg-Kohn theorem [22]. Since in our case the external potential $v_{\text{ext}}(z,t)$ does not include any spin-dependent interaction, we have made in Eq. (3) the assumption that spin symmetry holds for all times, *i.e.* $\varphi_\uparrow(z,t) = \varphi_\downarrow(z,t) = \varphi(z,t)$. The exchange potential is therefore given by $v_x[n](z,t) = -v_h[n](z,t)/2$. In case of an adiabatic approximation, the xc potential $v_{\text{xc}}[n](z,t)$ depends only on the density at time t and does not have memory of times earlier than t. This can be interpreted as inserting the instantaneous density into a functional without explicit time dependence, denoted as $v_{\text{xc}}^{\text{adia}}[n](z)$.

The exact adiabatic approximation for this system reads [20]

$$v_{\text{xc}}^{\text{adia}}[n](z) = v_s^{\text{adia}}[n](z) - v_h[n](z) - v_{\text{ext}}^{\text{adia}}[n](z) \quad (6)$$

where $v_s^{\text{adia}}[n](z)$ is the adiabatic KS potential corresponding to the density $n(z)$, *i.e.* the potential for which the orbital $\phi(z) = \sqrt{n(z)/2}$ is the ground state of the static KS equation

$$-\frac{1}{2}\frac{\mathrm{d}^2\phi(z)}{\mathrm{d}z^2} + v_s^{\text{adia}}[n](z)\phi(z) = \epsilon\phi(z). \quad (7)$$

Therefore, $v_s^{\text{adia}}[n](z)$ takes the simple form

$$v_s^{\text{adia}}[n](z) = \frac{1}{2\phi(z)}\frac{\mathrm{d}^2\phi(z)}{\mathrm{d}z^2} + \text{const.} \quad (8)$$

In Eq. (6), $v_{\text{ext}}^{\text{adia}}[n](z)$ denotes, in analogy to the potential $v_s^{\text{adia}}[n](z)$, the external potential that yields the density $n(z)$ as a ground-state density of the interacting system, *i.e.* as the density of the ground-state solution of the static two-particle Schrödinger equation

$$E\psi(z_1,z_2,t) = H^{\text{adia}}\psi(z_1,z_2,t) \quad (9)$$

$$\text{with} \quad H^{\text{adia}} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z_1^2} - \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z_2^2} + v_{\text{ext}}^{\text{adia}}[n](z_1)$$
$$+ v_{\text{ext}}^{\text{adia}}[n](z_2) + w(z_1-z_2). \quad (10)$$

From Eq. (6) we now develop an adiabatic approximation that does not require inversion of the static two-particle Schrödinger equation to obtain $v_{\text{ext}}^{\text{adia}}[n](z)$, but instead only an SDFT system to obtain an approximate external potential $\tilde{v}_{\text{ext}}^{\text{adia}}[n](z)$. Thus, an approximate adiabatic xc-potential

$$\tilde{v}_{\text{xc}}^{\text{adia}}[n](z) = v_s^{\text{adia}}[n](z) - v_h[n](z) - \tilde{v}_{\text{ext}}^{\text{adia}}[n](z) \quad (11)$$

is obtained. For this, we use a set of KS equations

$$-\frac{1}{2}\frac{\mathrm{d}^2\phi_\sigma(z)}{\mathrm{d}z^2} + v_{s,\sigma}^{\text{adia}}[n_\uparrow, n_\downarrow](z)\phi_\sigma(z) = \epsilon_\sigma\phi_\sigma(z), \ \sigma = \uparrow, \downarrow \quad (12)$$

for the spin orbitals $\phi_\sigma(z)$ with spin densities $n_\sigma(z) = |\phi_\sigma(z)|^2$ and $n_\uparrow(z) + n_\downarrow(z) = n(z,t)$. In Eq. (12), the potentials $v_{s,\sigma}^{\text{adia}}[n_\uparrow, n_\downarrow](z)$ are given by

$$v_{s,\sigma}^{\text{adia}}[n_\uparrow, n_\downarrow](z) = \tilde{v}_{\text{ext}}^{\text{adia}}[n](z) + v_{\text{hx},\sigma}[n_\uparrow, n_\downarrow](z)$$
$$+ v_{c,\sigma}[n_\uparrow, n_\downarrow](z), \quad (13)$$

$$v_{\text{hx},\uparrow}[n_\uparrow, n_\downarrow](z) = \int \mathrm{d}z' \, n_\downarrow(z')w(z-z'), \quad (14)$$

$$v_{\text{hx},\downarrow}[n_\uparrow, n_\downarrow](z) = \int \mathrm{d}z' \, n_\uparrow(z')w(z-z'). \quad (15)$$

In Eq. (13), $v_{c,\sigma}[n_\uparrow, n_\downarrow](z)$ includes only correlation effects, since the exact exchange in a two electron system is already included in the Hartree-exchange potentials in Eqs. (14) and (15). Note that the orbitals $\phi_\sigma(z)$ correspond to the time-dependent orbital $\varphi(z,t)$ only via the requirement that $n_\uparrow(z) + n_\downarrow(z) = n(z,t) = 2|\varphi(z,t)|^2$.

In contrast to the time-dependent orbital, which is filled with two electrons due to spin-symmetry, the orbitals $\phi_\sigma(z)$ are explicitly allowed to break the spin symmetry, *i.e.* $\phi_\uparrow(z) \neq \phi_\downarrow(z)$ in general. If the ground state of Eq. (12) leads to the symmetric case $\phi_\uparrow(z) = \phi_\downarrow(z)$, then $v_{s,\sigma}^{\text{adia}}[n_\uparrow, n_\downarrow](z) = v_s^{\text{adia}}[n](z)$ will hold and therefore the resulting adiabatic xc potential will simply be the xc potential applied in the ground-state KS equations (Eq. (12)):

$$\tilde{v}_{\text{xc}}^{\text{adia}}[n](z) = -\frac{1}{2}v_h[n](z) + v_{c,\sigma}[n/2, n/2](z), \quad (16)$$

if $v_{c,\uparrow}[n/2, n/2](z) = v_{c,\downarrow}[n/2, n/2](z)$, which is true for physical functionals. However, in the asymmetric case $\phi_\uparrow(z) \neq \phi_\downarrow(z)$, which is likely to occur when the electron density $n(z,t)$ is strongly delocalized, the xc potential $\tilde{v}_{\text{xc}}^{\text{adia}}[n](z)$ includes more complicated correlation effects.

For simplicity, we apply exchange-only SDFT for the ground-state inversion, *i.e.* $v_{c,\sigma}[n_\uparrow, n_\downarrow](z) = 0$ throughout the paper. Note that exchange-only SDFT will lead to correlation contributions in $\tilde{v}_{\text{xc}}^{\text{adia}}[n](z)$ once the spin symmetry is broken.

Unlike the exact adiabatic approximation, our approach can lead to a practically applicable approximation, as a performance increase compared to the Schrödinger equation is gained by excluding all multi-particle functions. However, even the inversion of the SDFT KS equations is a demanding task that requires an iterative algorithm. We make use of an algorithm suggested by Peirs *et al.* [23], which has been slightly modified to account for electron density spread widely around the nucleus. Starting with an initial potential $v^{(0)}(z)$, a new guess $v^{(1)}(z)$ to the potential $\tilde{v}_{\text{ext}}^{\text{adia}}[n](z)$ is calculated according to

$$v^{(k+1)}(z) = v^{(k)}(z) + \alpha \frac{n^{(k)}(z) - n(z)}{|n^{(k)}(z) - n(z)|^\beta}. \quad (17)$$

Here, $n^{(k)}(z)$ is the ground-state density for the potential $v^{(k)}(z)$, calculated via Eq. (12) with $\tilde{v}_{\text{ext}}^{\text{adia}}[n](z)$ replaced by $v^{(k)}(z)$. We compare the densities $n(z)$ and $n^{(k)}(z)$ by the integral

$$\Delta_k = \int dz \left| n^{(k)}(z) - n(z) \right| \qquad (18)$$

and iterate until Δ_k is smaller than a given number Δ. For all calculations in this paper, we chose $\Delta = 10^{-4}$. The parameters α and β in Eq. (17) have to be chosen carefully in order to achieve fast convergence. Usually, $\alpha \approx 0.1$ and $\beta \approx 0.5$ give a reasonable convergence behaviour.

The first system under investigation is a 1D model H_2 molecule with nuclear positions R_1, $R_2 = -R_1$ and a potential

$$v_{\text{ext}}(z) = -\frac{1}{\sqrt{(z-R_1)^2 + 1}} - \frac{1}{\sqrt{(z-R_2)^2 + 1}}. \qquad (19)$$

Here and in all following calculations, we use the interaction potential

$$w(z_1, z_2) = \frac{1}{\sqrt{(z_1 - z_2)^2 + s}}. \qquad (20)$$

For the 1D H_2 system, we use the softcore parameter $s = 1$. We compute the exact density by solving the static Schrödinger equation for different internuclear distances $d = |R_1 - R_2|$. With this density as input, we evaluate the approximate adiabatic correlation potential

$$\tilde{v}_c^{\text{adia}}[n](z) = \tilde{v}_{\text{xc}}^{\text{adia}}[n](z) + \frac{1}{2} v_h[n](z) \qquad (21)$$

for various distances d, as well as the exact correlation potentials $v_c^{\text{ex}}[n](z)$, which can be obtained from Eq. (21) and Eq. (11) by replacing $\tilde{v}_{\text{ext}}^{\text{adia}}[n](z)$ with the known external potential $v_{\text{ext}}(z)$. For an internuclear distance of $d = 2$, the two spin orbitals in the ground-state inversion are equal (not shown) and therefore the correlation potential $\tilde{v}_c^{\text{adia}}[n](z)$ is zero because of Eq. (16), see Fig. 1(a). For a critical distance d_{crit}, however, the symmetry in the ground-state inversion breaks and the spin orbitals become different [24, 25]. For $d > d_{\text{crit}}$, the correlation potential is found to be close to the exact one, see Figs. 1(b)-(d), even in the problematic region between the nuclei.

Additionally, we test our xc functional in an LiH model molecule, described by the potential [18]

$$v_{\text{ext}}(z) = -\frac{1}{\sqrt{(z-R_1)^2 + 0.7}} - \frac{1}{\sqrt{(z-R_2)^2 + 2.25}} \qquad (22)$$

to investigate if not only the peak between the nuclei is well described, but also the potential shift between the two atoms [18]. For LiH, we chose the softcore parameter $s = 0.6$. As in the case of H_2, we evaluate the exact density for different internuclear distances $d = |R_1 - R_2|$ by solving the static Schrödinger equation and use this density as input for calculation of the approximate adiabatic
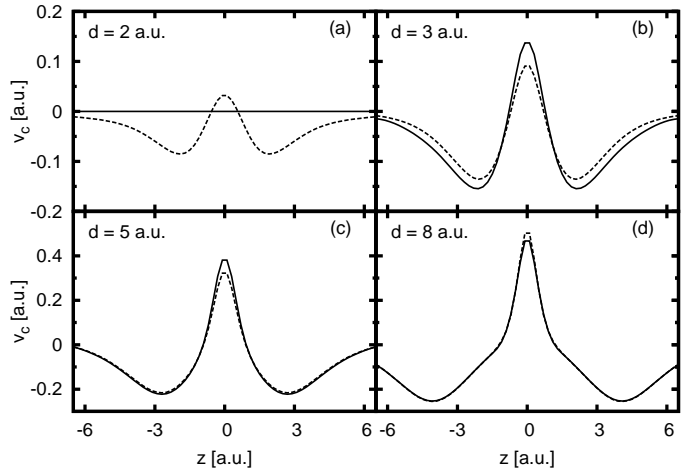

Figure 1: Comparison of the approximate adiabatic correlation potential $\tilde{v}_c^{\text{adia}}(z)$ (solid curves) with the exact correlation potential $v_c^{\text{ex}}(z)$ (dashed curves) in 1D H_2 with different internuclear distances d, as indicated.

correlation potential $\tilde{v}_c^{\text{adia}}[n](z)$ and the exact correlation potential $v_c^{\text{ex}}[n](z)$. Again, for large enough internuclear distance d, the spin orbitals in the ground-state inversion differ from each other and therefore a non-zero correlation contribution is obtained. The step that occurs for large internuclear distance is reproduced very well by our approximation, see Fig. 2(b). For smaller distances d, the correlation potential $\tilde{v}_c^{\text{adia}}[n](z)$ still gives a good approximation to the exact correlation potential, see Fig. 2(a). For even smaller internuclear distances d, the spin orbitals become equal at a critical distance d_{crit} and the approximate correlation potential vanishes (not shown). We have done preliminary studies indicating that a peak at $z = 0$ remains in the approximate adiabatic potential when an approximate density, e.g. from a linear combination of atomic orbitals [19] is used.
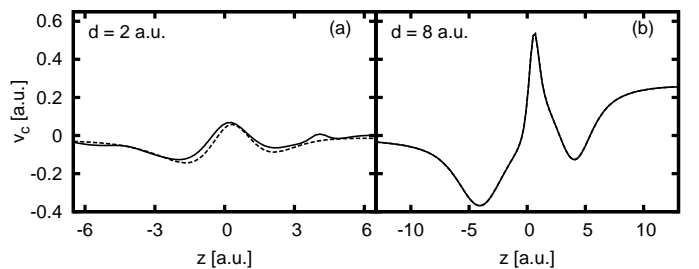

Figure 2: Comparison of the approximate adiabatic correlation potential $\tilde{v}_c^{\text{adia}}(z)$ (solid curves) with the exact correlation potential $v_c^{\text{ex}}(z)$ (dashed curves) in 1D LiH with different internuclear distances d, as indicated. The two curves in panel (b) are in perfect agreement.

In order to correctly describe ionization processes in TDDFT, the xc potential must reproduce the signatures of the derivative discontinuity at integer particle numbers, even though the particle number stays constant [26]. For this reason, the next test of our approximation is its application to a system with fractional particle number

$N = 1 + \varepsilon$, $0 \le \varepsilon < 1$. We use a one-dimensional soft-core helium atom given by the potential

$$v_{\text{ext}}(z) = -\frac{2}{\sqrt{z^2 + 1}} \qquad (23)$$

and softcore parameter $s = 1$. For this system, the ground state density $n_{1+\varepsilon}(z)$ reads

$$n_{1+\varepsilon}(z) = (1 - \varepsilon)n_1(z) + \varepsilon n_2(z) \qquad (24)$$

where $n_1(z)$ and $n_2(z)$ are the ground-state densities of the single- and two-electron system. These densities are calculated exactly by solving the single- and two-particle Schrödinger equation, respectively. With these densities as input, we compute the correlation potential according to Eq. (21) for different values of ε (Fig. 3). The fractional particle number is accounted for by occupying the more weakly bound orbital with only ε electrons, i.e. $n_\uparrow(z) = \varepsilon|\phi_\uparrow(z)|^2$ and $n_\downarrow(z) = |\phi_\downarrow(z)|^2$ or vice versa. We keep the form $v_x[n](z) = -v_h[n](z)/2$ for the exchange potential in analogy to the time-dependent case with $N = 2$. For comparison, we calculate also the corresponding exact correlation potential [16] by using the known external potential $v_{\text{ext}}(z)$ in Eq. (11). For $\varepsilon = 1$, the correlation potential from our approach is again zero (not shown), whereas the exact correlation is small, but nonzero [16]. However, the agreement between our approach and the exact correlation potential improves with decreasing ε. For $\varepsilon \to 0$ and thus approaching the derivative discontinuity, the agreement becomes perfect, see Fig. 3. The excellent agreement can simply be explained by the fact that the exchange-only two-orbital SDFT turns for $\varepsilon \to 0$ into the single-particle Schrödinger equation, because one of the spin-densities approaches zero and thus the SDFT Hartree-exchange potential vanishes. Note that all examples we have investigated so far are ground-state problems, so there is no distinction between the exact adiabatic correlation potential and the exact correlation potential.

Finally, we test the new approximation in a strong-field process using the model helium atom with $N = 2$. For simplicity, we use a DC electric field ramped up linearly during the first 27 a.u. of propagation and held constant at $E_0 = 0.141$ a.u. afterwards, as in [16, 20]. The interaction with the field is cut off at a distance of 35 a.u. from the nucleus to avoid numerical problems due to strongly accelerated electrons. For this system, we solve the time-dependent Schrödinger equation numerically and use the exact densities at different times to calculate the correlation potentials $\tilde{v}_c^{\text{adia}}[n](z)$. The results are shown in Figs. 4(b)-(d). As a reference, the exact time-dependent Kohn-Sham potential is computed by inversion of the time-dependent KS propagator [16]. To be able to compare the results to those in the system with fractional particle number we calculate for each density the number of bound electrons N_b as

$$N_b = \int_{-5\,\text{a.u.}}^{+5\,\text{a.u.}} dz\, n(z). \qquad (25)$$
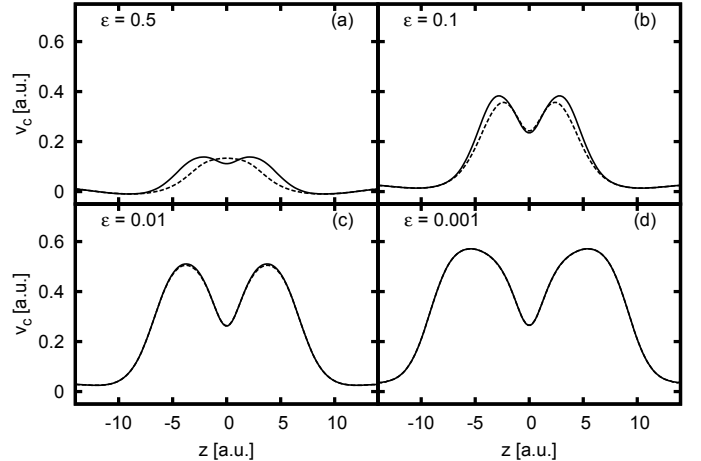
Figure 3: Correlation potentials for the 1D model helium atom with different particle numbers $N = 1 + \varepsilon$. Solid curves: approximate adiabatic correlation potential $\tilde{v}_c^{\text{adia}}[n](z)$. Dashed curves: exact correlation potential $v_c^{\text{ex}}[n](z)$.

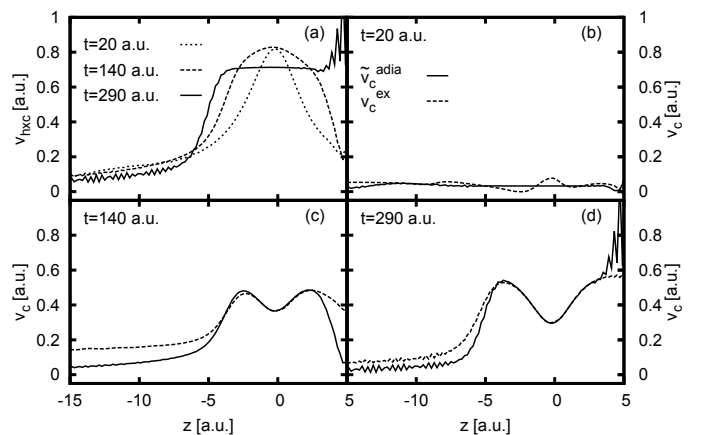The integration limits ± 5 a.u. are chosen arbitrarily. In

Figure 4: (a) Comparison of the Hartree-exchange-correlation potentials $\tilde{v}_{\text{hxc}}^{\text{adia}}(z)$ at the three different times $t = 20$, 140 and 290 a.u., with the number of bound electrons N_b being 1.996, 1.129, and 1.008, respectively. (b)-(d) The corresponding correlation potentials $\tilde{v}_c^{\text{adia}}(z)$ in comparison to the exact correlation potentials $v_c^{\text{ex}}(z)$.

addition, in Fig. 4(a), the complete interaction potentials $\tilde{v}_{\text{hxc}}^{\text{adia}}[n](z) = v_h[n](z,t) + \tilde{v}_{\text{xc}}^{\text{adia}}[n](z)$ are shown for different instants during propagation. The development of a plateau and a step-like structure is clearly visible for increasing ionization, similar to the exact adiabatic potential [20]. As long as the system is only weakly perturbed from its ground state, the correlation potential is practically zero, see Fig. 4(b). With increasing ionization, however, the correlation potential becomes more significant, and our approximation comes close to the exact correlation potentials, see Figs. 4(c) and (d). The only difference is a slight overestimation of the step that decreases with increasing ionization. The dip at the nucleus and the step-like structure in the correlation potential are very similar to those of the atom with fractional particle number, which confirms the importance of the derivative discontinuity in

ionization processes.

We observe that essential correlation effects are introduced in TDDFT by using an adiabatic approximation based on accurate mapping from densities to potentials. In strong-field ionization of a two-electron system, it is enough to allow the spin symmetry in the ground-state inversion to break in order to achieve correlation potentials close to the exact ones. We expect that our approach yields similar results when generalized to $N > 2$ particles. Moreover, the quality of the adiabatic correlation potential can be further enhanced by applying more elaborate functionals than the exchange-only approximation in the ground-state inversion process. In this respect, TDDFT can directly profit from the great knowledge of functionals in static density functional theory. In the future, we plan to implement the approximate adiabatic potential in full TDDFT calculations.

Acknowledgements

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