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Construction of Exchange-Correlation Potentials for Strongly Interacting One-Dimensional Systems

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Abstract One-dimensional (1D) systems are useful laboratories aiming further improvement of electronic structure calculations. In order to simulate electron-electron interactions, two types of expressions are commonly considered: soft-Coulomb and exponential. For both cases, in the context of density-functional theory (DFT), 1D systems can be employed to gain insight into the ingredients accurate exchange-correlation (XC) density functionals must incorporate. A question of major interest is the treatment of strongly interacting situations, one of the main modern challenges for DFT. In this manuscript, we propose a generalization of preexisting XC potentials which can be applied to investigate the transition from weak to strong interactions. Specifically, we employ the intriguing behavior of electrons confined in one dimension: the spin-charge separation, for which spin and charge are decoupled to form two independent quasiparticles, spinons, and chargons. By means of Friedel oscillations, our results indicate it is possible to reproduce the weak-strong interaction transition by using a simple strategy we name, from previous works, spin-charge separation correction (SCSC). In addition, SCSC also yields good results in reproducing the constancy of the highest occupied Kohn-Sham eigenvalues upon fractional electron charges.

Keywords Density functional theory · Strong interactions · One-dimensional systems · Soft-Coulomb · Exponential

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1 Introduction

The Kohn-Sham (KS) formalism of density-functional theory (DFT) [1, 2] considers *noninteracting* particles subject to an effective potential which is able to include all electron-electron interaction effects. Nevertheless, even though the KS equations are formally exact, there is a tremendous difficulty in finding an effective potential which accurately describes strongly interacting electrons, and this feature is commonly considered as one of the main modern challenges for DFT [3].

One-dimensional (1D) systems have emerged as very instructive laboratories to the development of DFT. First, by considering the simplicity of computational implementation (in comparison with 3D systems). Second, in spite of the simplicity, they allow the verification of exact constraints to be satisfied by exchange-correlation (XC) density functionals, in order to gain insight into the ingredients they must incorporate. In addition, it is important to note that electronic confinement in one dimension can be even considered in experimental realizations, for example, in applications to $SrCuO_2$ [4] and Sr_2CuO_3 [5].

In the context of 1D systems, recent manuscripts [6–8] have employed two types of electron-electron interaction models: soft-Coulomb and exponential, respectively defined as:

$$v_{\text{int}}^{\text{soft-C}}(x_i, x_j) = \frac{1}{\sqrt{(x_i - x_j)^2 + \alpha^2}}, \tag{1}$$

and

$$v_{\text{int}}^{\text{exp}}(x_i, x_j) = A\ \exp(-\kappa\,|x_i - x_j|), \tag{2}$$

where α, A, and κ are controlled parameters for electrons placed at positions x_i and x_j. In the context of DFT, these

recent instructive manuscripts have considered XC functionals which are valid only for *one* specific choice of α, A, and κ. However, as it has already been mentioned [6], their variation could be used to investigate the transition from weakly to strongly interacting systems. We specifically intend to give a contribution into this sense, that is, constructing XC potentials with an open choice for α, A, and κ. In the sequence, we shall apply our potentials in situations for which strong interactions are known to be relevant.

2 Spin-charge Separation Correction

One-dimensional systems assume non-Fermi-liquid behavior, belonging to a special class of Tomonaga-Luttinger liquids (TLL) [9, 10]. In the context of TLL, the 1D confinement yields strongly interacting electrons which can break their spin and charge into two separated quasiparticles, the first built from uncharged spin$-1/2$ (spinons) and the second from charged spinless electrons (chargons) [11, 12]. This mechanism, entirely predicted by the theoretical TLL approach and usually called spin-charge separation, has recent evidences of experimental observation [4, 5, 13].

Initially proposed in the context of discrete Hubbard chains [14, 15], we here shall apply a spin-charge separation correction (SCSC) in the limit of continuum and to the exchange local-density approximation (xLDA) associated with both, the soft-Coulomb and exponential 1D interaction models. For uniform systems, it can be shown that the (spin-unpolarized) exchange energy per length is given by:

- Soft-Coulomb [7]:

$$e_{\rm x}^{\rm Unif:soft-C.}(n) = -\frac{n^2}{2}\, f\left(\frac{\pi\, n}{2}\right), \tag{3}$$

with

$$f(z) = \int_0^\infty \frac{\sin^2 y}{y^2\sqrt{y^2+\alpha^2\, z^2}}\, dy. \tag{4}$$

- Exponential [8, 16]:

$$e_{\rm x}^{\rm Unif:expon.}(n) = \frac{A\,\kappa}{2\,\pi^2}\left[\ln(1+y^2) - 2\, y\, \arctan\, y\right], \tag{5}$$

with $y = n\,\pi/\kappa$.

In both cases, n labels the uniform electronic density per length. The local-density approximation (LDA) exchange energy is then written as:

$$E_{\rm x}^{\rm LDA} = \int e_{\rm x}^{\rm Unif}(n)\Big|_{n\to n(x)}\, dx. \tag{6}$$

In a noninteracting KS system, charge and spin are intrinsically coupled, leading conventional approaches like LDA to fail when trying to describe strongly interacting systems. Following the original idea of the SCSC approach [14, 15], in order to reproduce the spin-charge separation, we consider that the occupied states of a noninteracting KS system (containing $N = N_\uparrow + N_\downarrow$ electrons) are built by retaining spin and charge together, however, at expense of the presence of holons (the chargon antiparticles), whose densities are given by $\rho^+(x)$, defined as

$$\rho^+(x) = \sum_{i=1}^{N_\uparrow} |\psi_{i,\uparrow}(x)|^2 + \sum_{i=N_\uparrow+1}^{N} |\psi_{i,\downarrow}(x)|^2, \tag{7}$$

with $\psi_{i,\sigma}(x)$ labeling the KS eigenvectors (see Fig. 3 of Ref. [14] and Fig. 1 of Ref. [15]). Then, we shall consider the following KS potential:

$$\begin{aligned} v_{\rm KS}^{\rm SCSC/xLDA}[n](x) &= v_{\rm ext}(x) + v_{\rm H}[n](x) + v_{\rm x}^{\rm LDA}[n](x) \\ &\quad - v_{\rm H}[\rho^+](x) - v_{\rm x}^{\rm LDA}[\rho^+](x) \\ &\equiv v_{\rm ext}(x) + v_{\rm H}[n](x) + v_{\rm xc}^{\rm SCSC/xLDA}[n](x), \end{aligned} \tag{8}$$

where $v_{\rm ext}$, $v_{\rm H}$, and $v_{\rm xc}$ label, respectively, the external, Hartree and XC potentials. Specifically,

$$v_{\rm H}[n](x) = \frac{\delta\, E_{\rm H}[n]}{\delta\, n(x)}, \tag{9}$$

with

$$E_{\rm H}[n] = \frac{1}{2}\int\int v_{\rm int}(x', x'')\, n(x')\, n(x'')\, dx'\, dx'', \tag{10}$$

and

$$v_{\rm x}^{\rm LDA}[n](x) = \left.\frac{\delta\, e_{\rm x}^{\rm Unif}}{\delta\, n}\right|_{n\to n(x)}. \tag{11}$$

Here, $n(x)$ is the ordinary electronic density (of spins + charges together) as a function of position x:

$$n(x) = \sum_{\sigma=\uparrow,\downarrow}\sum_{i=1}^{N_\sigma} |\psi_{i,\sigma}(x)|^2. \tag{12}$$

The SCSC/xLDA XC potential of (8) is not a functional derivative of a known XC energy functional, that is, it is an ad hoc correction to the KS potential. Nevertheless, even though model potentials may suffer from conceptual drawbacks when calculating the associated energy functionals, the use of potentials as seeds are regarded as a promising route to new developments in DFT [17–21]. In addition, note that the SCSC/xLDA XC potential proposed here allows any choices for the soft-Coulomb and exponential parameters α, A, and κ, at almost no increment in computational effort and without the necessity of constructing new correlation density functionals.

3 Application and Results

3.1 Density Oscillations

Friedel oscillations (FO) are oscillations of the electron density which appear in confined systems and around inhomogeneities [22]. They have emerged as a useful laboratory in the study of many-body systems [23, 24], since, particularly in one dimension, FO can be used as a tool to identify the transition from the weakly to the strongly interacting regime: the increase of interaction is accompanied by an increase in the frequency of FO, whose value is known to pass from $2k_F$ (weak) to $4k_F$ (strong interaction). The resulting $4k_F$ Friedel oscillations are usually referred to as Wigner crystal oscillations [25–28], in reference to the Wigner crystallization. Therefore, using the soft-Coulomb and exponential interaction models, we intend to investigate whether the SCSC/xLDA XC potential, by controlling the α, A, and κ parameters, is able to recover the $2k_F \rightarrow 4k_F$ transition. It should be stressed that density functionals are usually not able to yield such a transition. Only few successful examples have been described in recent manuscripts [29–31], which, however, do not employ soft-Coulomb or exponential interaction models, as well as, the spin-charge separation formalism. It is important to mention that the successful results presented by G. Xianlong in 2012 [31] have been obtained by means of considering an infinitesimal spin-symmetry-breaking when $N_\uparrow = N_\downarrow$, leading to a local-spin-density approximation (LSDA). Here, following the original SCSC idea [14], we shall consider an unpolarized formalism, with $N_\uparrow = N_\downarrow$ in all cases, and without any type of spin-symmetry-breaking during the entire self-consistent calculations.

Specifically, we shall consider N interacting electrons in one dimension, with Hamiltonian written as:

$$\hat{H} = \sum_{i=1}^{N}\left[-\frac{1}{2}\frac{d^2}{dx_i^2} + v_{\text{ext}}(x_i)\right] + \frac{1}{2}\sum_{\substack{i,j=1\\(i\neq j)}}^{N} v_{\text{int}}(x_i, x_j), \quad (13)$$

and with a parabolic external potential given by:

$$v_{\text{ext}}(x) = \frac{1}{2}\,\omega^2\,x^2. \quad (14)$$

Two limits are exactly known: (a) noninteracting (NI), with $\alpha \rightarrow \infty$, $A \rightarrow 0$ and trivial analytical solution; (b) strongly interacting (SI), for which $\alpha \rightarrow 0$ and $A \rightarrow \infty$ (with $\kappa \rightarrow 0$). The second case can be also treated analytically by means of the so-called boson-fermion mapping; it is known that strongly interacting electrons behave like noninteracting spinless charges, with orbital occupation equal to one even when $N_\uparrow = N_\downarrow = N/2$ electrons [32–34]. For example, in a case with N noninteracting electrons, the total wave function is given by a $N \times N$ Slater determinant:

$$\Psi(x_1, x_2, ..., x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_\alpha(x_1) & \cdots & \phi_\beta(x_1) \\ \vdots & \ddots & \vdots \\ \phi_\alpha(x_N) & \cdots & \phi_\beta(x_N) \end{vmatrix}, \quad (15)$$

where $\phi_\upsilon(x)$ are the solution of the single-particle Schrödinger equation:

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + v_{\text{ext}}(x)\right]\phi_\upsilon(x) = \varepsilon_\upsilon\,\phi_\upsilon(x), \quad (16)$$

with

$$\phi_\upsilon(x)\frac{1}{\sqrt{2^\upsilon \upsilon!}}\left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} e^{\frac{-\omega x^2}{2}} H_\upsilon\left(\sqrt{\omega}\,x\right), \quad (17)$$

and H_υ are the Hermite polynomials. Considering the ground-state, the density distributions of each limit (with $N_\uparrow = N_\downarrow$) are then given by:

$$n^{\text{NI}}(x) = 2\sum_{\upsilon=0}^{N/2-1}|\phi_\upsilon(x)|^2, \quad (18)$$

$$n^{\text{SI}}(x) = \sum_{\upsilon=0}^{N-1}|\phi_\upsilon(x)|^2. \quad (19)$$

In this context, two examples of curves are shown in Fig. 1, for which we have chosen a system with $N_\uparrow = N_\downarrow = 2$ and $\omega^2 = 0.02$. In this case, we have:

$$n^{\text{NI}}(x) = 2\left(\frac{\omega}{\pi}\right)^{\frac{1}{2}} e^{-\omega x^2}\left[1 + 2\omega x^2\right], \quad (20)$$

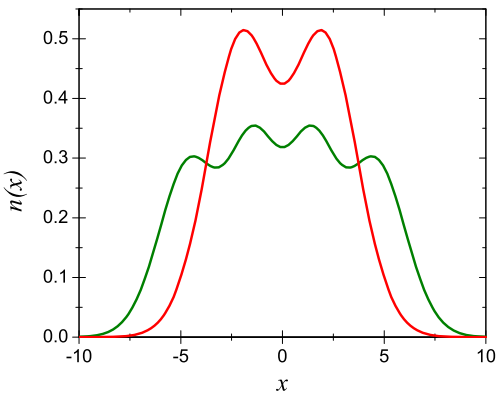

Fig. 1 (*Color online*) 1D systems. Exact density profiles for $N = 4$ electrons (with $N_\uparrow = N_\downarrow$) confined in a harmonic potential given by (14) and with $\omega^2 = 0.02$. The *curve with two peaks* corresponds to the noninteracting limit expressed in (20), for which the soft-Coulomb and exponential parameters of (1) and (2) are given by $\alpha \rightarrow \infty$ and $A \rightarrow 0$. The *curve with four peaks*, given by (21), refers to the strongly interacting limit, with $\alpha \rightarrow 0$ and $A \rightarrow \infty$ (with $\kappa \rightarrow 0$)

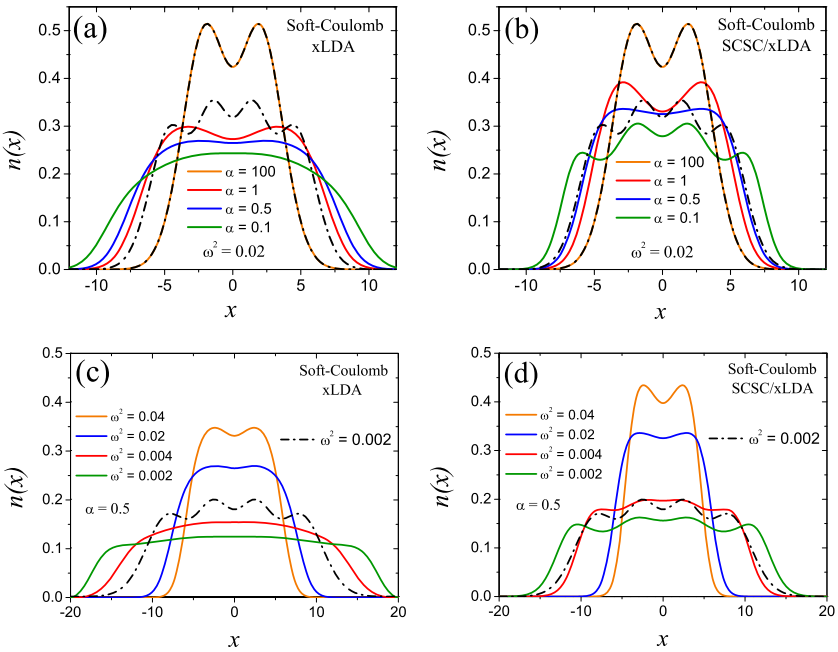

Fig. 2 (*Color online*) 1D systems. Density profiles obtained by means of the xLDA and SCSC/xLDA approaches, as defined in (8), considering $N = 4$ electrons (with $N_\uparrow = N_\downarrow$) confined in harmonic potentials. **a**, **b** Different values of the soft-Coulomb parameter α, with $\omega^2 = 0.02$. **c**, **d** Different values of ω, with $\alpha = 0.5$. The sof-Coulomb interaction is defined in (1), with ω given in accordance with (14)

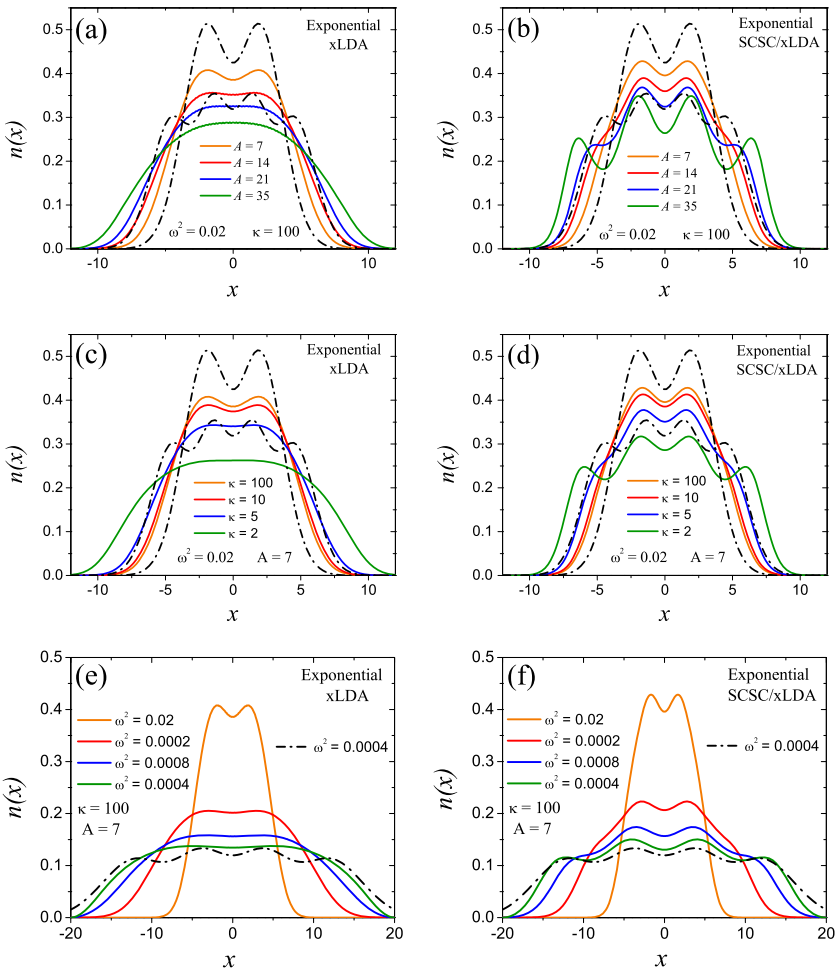

Fig. 3 (*Color online*) The same as Fig. 2, but for the exponential interaction potential. For each panel, two of the three parameters (A, κ, and ω) are maintained fixed. The exponential interaction is defined in (2)

and

$$n^{\mathrm{SI}}(x)=\frac{3}{2}\left(\frac{\omega}{\pi}\right)^{\frac{1}{2}} e^{-\omega x^2}\left[1+2\omega x^2-\frac{4}{3}\omega^2x^4+\frac{8}{9}\omega^3x^6\right]. \tag{21}$$

Note a change in the frequency of Friedel oscillations, with two peaks ($2k_F$) in the noninteracting limit and four peaks ($4k_F$) in the strongly interacting situation. The last case is a signature of strong interaction, with four peaks identifying electrons as far apart as possible.

Next, we shall proceed KS-DFT calculations employing the KS potential of (8). In Fig. 2a and b, we display curves of density for the xLDA and SCSC/xLDA approaches, with different values of the soft-Coulomb parameter α and $\omega^2 = 0.02$. The dashed-doted lines correspond to the curves presented in Fig. 1. Note that only for the SCSC the reduction of α is accompanied by a change in the frequency of the Friedel oscillations, from two to four peaks, indicating a correct weakly-strongly interacting transition. In Fig. 2c and d, we consider different values of ω for a single $\alpha = 0.5$, where the dashed-doted lines indicate the strongly interacting limit for $\omega^2 = 0.002$. It is known that a reduction of average density in a confined region is accompanied by an increment of correlation. Particularly, from Fig. 2d, we observe that only SCSC/xLDA is able to recover such an increment, with the transition $2k_F \rightarrow 4k_F$ clearly present. It is interesting to mention a known drawback of LDA: Electrons tend to be excessively delocalized, what is usually called *delocalization error* [3, 35, 36].

As second group in our analysis, we shall consider the exponential interaction and its two open parameters, A and κ. In each panel of Fig. 3, two of the three parameters (A, κ, and ω) are maintained fixed. The same as the previous figure, only the SCSC/xLDA XC potential is able to recover the $2k_F \rightarrow 4k_F$ transition as A is increased, as well as, κ and ω are decreased, in accordance with the expected results. As additional observation, different from Fig. 2a and b, in Fig. 3a–d the accurate reproductions of the analytical weakly interacting curves are not present. Actually, we could obtain such a reproduction by changing the parameters A and κ. However, this is not our aim here, but verify the $2k_F \rightarrow 4k_F$ transition.

3.2 Highest Occupied Kohn-Sham Eigenvalues

An alternative to infer the accuracy of the approximations adopted here is to analyze the constancy of the highest occupied (HO) KS eigenvalues ($\varepsilon_{\mathrm{HO}}$) upon fractional electron numbers. Even though they do not exist, systems with fractionary electrons are widely employed as a tool to examine exact constraints density functionals must satisfy. In a

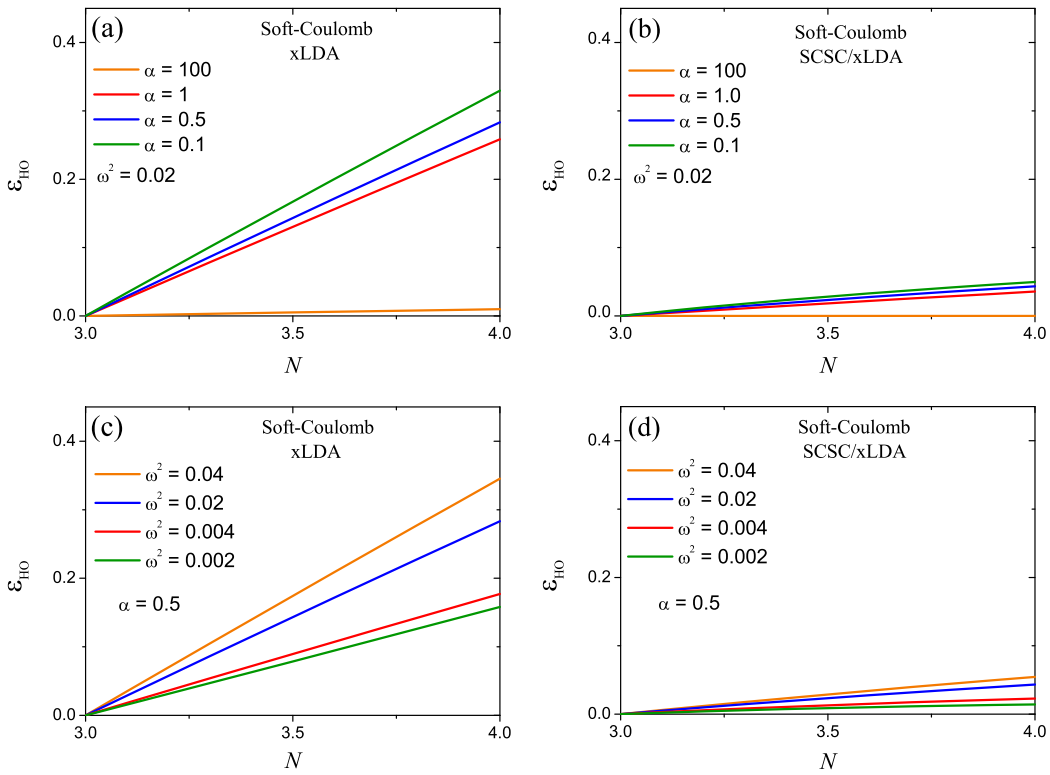

Fig. 4 (*Color online*) Highest occupied KS eigenvalues ($\varepsilon_{\mathrm{HO}}$) upon a fractionary number of electrons N (with $N_\uparrow = N_\downarrow$), considering the soft-Coulomb interaction potential. All presented values have been subtracted by a constant factor, such that $\varepsilon_{\mathrm{HO}} = 0$ for $N = 3$

system with $M = N + w$ $(0 \leq w \leq 1)$ electrons, the total ground-state energy is given by [15, 37]:

$$E(N + w) = (1 - w)E(N) + wE(N + 1), \tag{22}$$

with density written as:

$$n(x) = \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^{N_\sigma} f_{i,\sigma} \left|\psi_{i,\sigma}(x)\right|^2, \tag{23}$$

and $0 \leq f_{i,\sigma} \leq 1$. Assuming that only the HO KS orbital can be fractionally occupied, Janak [38] has proved that:

$$\frac{\delta E}{\delta M} = \varepsilon_{\rm HO} = \text{constant}. \tag{24}$$

In order to test the exact constraint of (24), we shall considere systems containing $3 \leq N \leq 4$ electrons (with $N_\uparrow = N_\downarrow$ in all cases). Thus, (7) can be rewritten as:

$$\rho^+(x) = \sum_{i=1}^{2} |\psi_{i,\uparrow}(x)|^2 + \sum_{i=3}^{4} f_{\rm HO} \, |\psi_{i,\uparrow}(x)|^2, \tag{25}$$

since $\psi_{i,\uparrow}(x) \equiv \psi_{i,\downarrow}(x)$ in our cases, with $0.5 \leq f_{\rm HO} \leq 1$ (see Fig. 1 of Ref. [15]). In addition, we shall consider the same harmonic external potential given by (14). In Fig. 4, we present the comparison for the approximations xLDA and SCSC/xLDA, obtained by means of the soft-Coulomb interaction. Observe a clearer constancy provided by the SCSC in comparison with the xLDA, upon the variation of either parameters, α or ω. In Fig. 5, considering the exponential interaction, the conclusions are equivalent, that is, the SCSC/xLDA approaches tested here yield much more accurate KS potentials.

Upon variation of parameters α, A, and κ, from Figs. 4 and 5, we observe the expected behavior, that is, the increment of interaction induces $\varepsilon_{\rm HO}$ to be less and less constant. This is also commonly associated with the previously mentioned delocalization error of density-functionals. Upon variation of ω, the more opened the harmonic external potential is, the more constant $\varepsilon_{\rm HO}$ appears to be. A possible explanation is the way LDA is designed, using homogeneous systems to describe inhomogeneous ones. Thus, the decrease of ω induces a more homogenous situation.

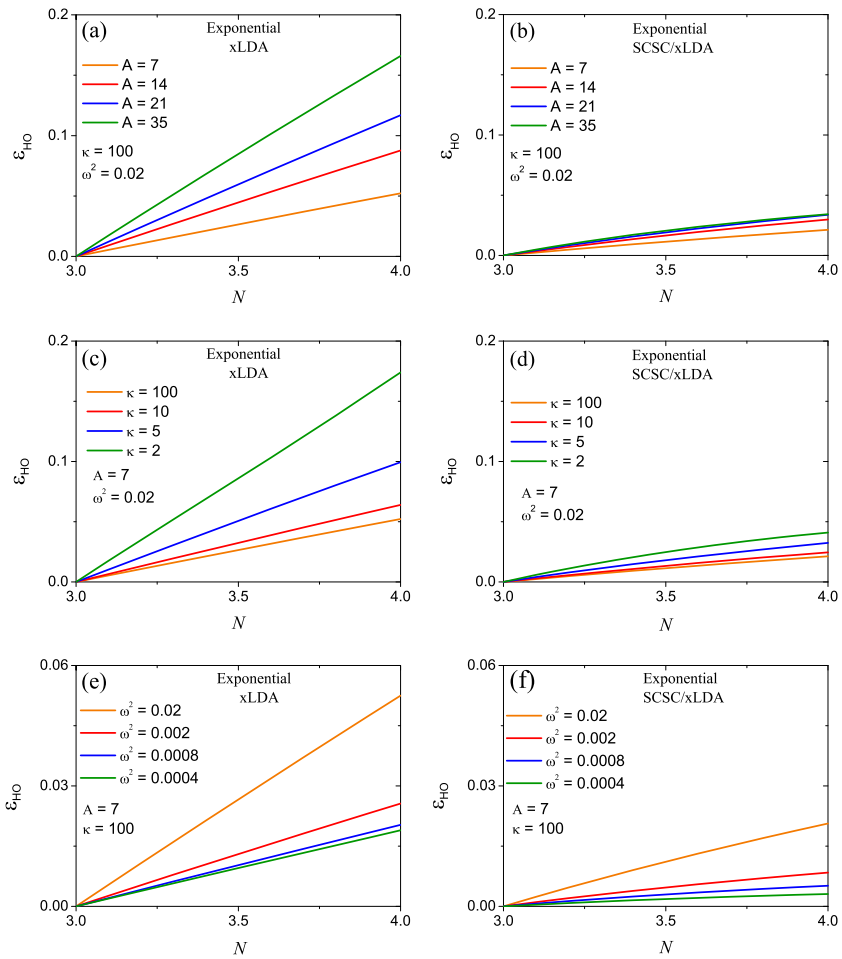

Fig. 5 (*Color online*) The same as Fig. 4, but for the exponential interaction potential

4 Summary

We have dealt with two interaction models—soft-Coulomb and exponential—in one-dimensional systems. The XC local-density approximations available in the literature for both cases are limited to specific choices of parameters (α, A, and κ), preventing the possibility of investigating the crossover between the weak and strong correlation regimes. We here have proposed a generalization, by means of a spin-charge separation formalism applied to DFT (the SCSC correction). This new XC potentials, for both soft-Coulomb and exponential, are able to recover the $2k_F \rightarrow 4k_F$ transition in the Friedel oscillations, as signatures of the transition from weak to strong interactions. It should be mentioned density functionals are usually not able to yield such a transition, with few exceptions presented in recent manuscripts [29–31]. SCSC also yields good results in reproducing the constancy of the highest occupied Kohn-Sham eigenvalues upon fractional electron charges, which is one of the exact constraints to be satisfied by density functionals—at any interaction magnitudes.

The SCSC has been initially proposed in the context of discrete Hubbard chains. We here have extended the idea to the continuum, with a totally different Hamiltonian, and the conclusion about its capacity of recovering the weak-strong interaction transition remained unchanged. For this reason, we believe the SCSC formalism, which is a very simple approach—at almost no increment in computational effort—may be successfully applied to other classes of systems and density functionals, such as the generalized-gradient approximations (GGAs).

In spite of recovering the correct $2k_F \rightarrow 4k_F$ transition, the SCSC/xLDA potentials presented here do not necessarily reproduce the exact curves in the strongly interacting limit. As improvement, beyond xLDA, the SCSC formalism can be applied to LDA functionals which also incorporate correlation explicitly as a function of parameters α, A, and κ.

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