Collective excitations in one-dimensional ultracold Fermi gases: Comparative study

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Time-dependent density-functional theory (TDDFT) is a powerful tool in studying the nonequilibrium dynamics of inhomogeneous interacting many-body systems. Here we show that the simple adiabatic local-spin-density approximation for the time-dependent exchange-correlation potential is surprisingly accurate in describing collective density and spin dynamics in strongly correlated one-dimensional ultracold Fermi gases. Our conclusions are based on extensive comparisons between our TDDFT results and accurate results based on the adaptive time-dependent density-matrix renormalization-group method.

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I. INTRODUCTION

Quantum many-body systems of one-dimensional (1D) interacting particles have attracted an enormous interest for more than fifty years.[1] These systems are nowadays available in a large number of different laboratory realizations ranging from single-wall carbon nanotubes[2] to semiconductor nanowires,[3] conducting molecules,[4] chiral Luttinger liquids at fractional quantum Hall edges,[5] and trapped atomic gases.[6–8]

Regardless of statistics, the effective low-energy description of many of these systems is based on a harmonic theory of long-wavelength fluctuations,[9] i.e., on the "Luttinger-liquid" model.[1] One distinctive feature of the Luttinger liquid is that its low-energy spectrum is completely dominated by collective excitations as opposed to individual quasiparticles that carry both charge and spin. A single-particle excitation in a Luttinger liquid directly decays into collective spin and charge excitations that propagate with different velocities. This phenomenon is called "spin-charge separation."[1]

Tunneling measurements between two parallel quantum wires in GaAs/AlGaAs heterostructures with varying electron density have demonstrated[3] the existence of collective spin and charge excitations with different velocities.

It has also been proposed to study experimentally the dynamics of spin and charge excitations *in real time* using 1D two-component cold Fermi gases,[7] where "spin" and "charge" refer, respectively, to two internal (hyperfine) atomic states and to the atomic mass density.[10–14] In Ref. 15 a different aspect of this collective behavior has been pointed out: namely, spin excitations are intrinsically damped at finite temperature while charge excitations are not.

Important for the experimental observation of the time evolution of excitations in ultracold quantum gases is the creation of a sizable perturbation of the gas (strong enough to be detected). The theoretical description of such strong perturbations, however, needs techniques going beyond the low-energy Luttinger-liquid model.[1] For example, the decay of sizable density perturbations[10] and of a single-particle excitation[11,12] has been recently demonstrated in real time in a numerical time-dependent density-matrix renormalization-group (tDMRG) (Refs. 16 and 17) study of the 1D Fermi-Hubbard model.

The aim of the present work is to provide a conceptually and numerically simple time-dependent microscopic many-body theory that is capable of capturing the main physical features of the time evolution of collective excitations.

A powerful theoretical tool in studying the interplay between interactions and time-dependent inhomogeneous external fields of arbitrary shape is the time-dependent density-functional theory (TDDFT),[18–20] which is based on the Runge-Gross theorem[21] and on the time-dependent Kohn-Sham (KS) equations. Many-body effects enter TDDFT via the time-dependent exchange-correlation (xc) functional, which is often treated by the *adiabatic* local-density approximation (ALDA).[18,22] In this approximation one assumes that the time-dependent xc potential is just the *static* xc potential evaluated at the instantaneous density. The static xc potential is then treated within the static local-density approximation (LDA). The main characteristic of the ALDA is that it is local in time, as well as in space. Memory effects, whereby the xc potential at a time instant might depend on the density at an earlier time, are completely ignored. Very attractive features of the ALDA are its extreme simplicity, the ease of implementation, and the fact that it is *not* restricted to small deviations from the ground-state density, i.e., to the linear-response regime.

Even though several nonadiabatic beyond-ALDA approximate functionals are available nowadays (see, e.g., Refs. 23–27), in this work we focus on a simple adiabatic xc functional and test its performance in describing a particular problem: collective density and spin dynamics in strongly correlated inhomogeneous lattice systems. Building upon earlier ideas described at length in Refs. 28–32, we here employ a lattice TDDFT scheme in which the time-dependent xc potential is determined *exactly* at the adiabatic local-spin-density-approximation level through the Bethe-*Ansatz* (BA) solution of the homogeneous 1D Hubbard model.[33] The numerical results based on this scheme are tested against accurate adaptive tDMRG simulation data for both spin-unpolarized and spin-polarized systems.

The contents of the paper are briefly described as follows. In Sec. II we introduce the model lattice Hamiltonian that we

use to study collective excitations and we briefly summarize its exact solution in the absence of external potentials. In Sec. III we present the self-consistent lattice TDDFT scheme that we use to deal with the time-dependent inhomogeneous system and introduce the Bethe-*Ansatz* adiabatic local-spin-density approximation (LSDA) that we employ for the xc potential. In Sec. IV we report and discuss our main numerical results in comparison with tDMRG simulation data. Finally, in Sec. V we summarize our main conclusions and future perspectives.

II. MODEL

We consider a two-component repulsive Fermi gas with N atoms confined to a 1D tube and subjected to an optical lattice potential applied in the direction of the tube. The optical lattice has unit lattice constant and L lattice sites. For times $t \leq 0$ the system is in the presence of a spin-selective focused laser-induced potential, which creates a strong local disturbance in the ultracold gas. At time $t=0^+$ this local potential is *suddenly* turned off: we are interested in the subsequent time evolution of the spin-resolved densities.

This system is modeled by the following Fermi-Hubbard Hamiltonian,[34]

$$\hat{\mathcal{H}}(t) = -\gamma \sum_{i,\sigma} (\hat{c}_{i\sigma}^{\dagger}\hat{c}_{i+1\sigma} + \text{H.c.}) + U\sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \sum_{i,\sigma} V_{i\sigma}(t)\hat{n}_{i\sigma}$$
$$\equiv \hat{\mathcal{H}}_{\text{ref}} + \hat{\mathcal{H}}_{\text{ext}}(t). \quad (1)$$

In Eq. (1), γ is the hopping parameter, $\hat{c}_{i\sigma}^{\dagger}$ ($\hat{c}_{i\sigma}$) creates (destroys) a fermion on the ith site ($i \in [1,L]$), $\sigma = \uparrow, \downarrow$ is a pseudospin-1/2 degree of freedom (hyperfine-state label), $U > 0$ is the strength of the on-site Hubbard repulsion, and $\hat{n}_{i\sigma} = \hat{c}_{i\sigma}^{\dagger}\hat{c}_{i\sigma}$. We also introduce for future purposes the local number operator $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$ and the local-spin operator $\hat{s}_i = \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$.

The "time-dependent" Hamiltonian $\hat{\mathcal{H}}_{\text{ext}}(t)$ models the aforementioned spin-selective focused laser-induced potential. The external potential $V_{i\sigma}(t)$ is taken to be of the following simple Gaussian form

$$V_{i\sigma}(t) = W_{\sigma} \exp\left\{ -\frac{\left[i - (L+1)/2 \right]^2}{2w^2} \right\} \Theta(-t)$$
$$\equiv V_{i\sigma}^{\text{ext}} \Theta(-t), \quad (2)$$

where $\Theta(x)$ is the Heaviside step function. This guarantees that the local potential $V_{i\sigma}^{\text{ext}}$, which is active for all times $t \leq 0$ is suddenly switched off at time $t=0^+$. Note that the time t enters the problem through the step function only. We are not really studying a time-dependent problem but only the dynamics of a system after a sudden local quench: an initial state $|\Psi_0\rangle$, which is an eigenstate of $\hat{\mathcal{H}}_{\text{ref}} + \Sigma_{i,\sigma} V_{i\sigma}^{\text{ext}} \hat{n}_{i\sigma}$, is propagated forward in time with a different Hamiltonian ($\hat{\mathcal{H}}_{\text{ref}}$). $|\Psi(t)\rangle = \exp(-i\hat{\mathcal{H}}_{\text{ref}} t)|\Psi_0\rangle$ is the state of the system at time t. Present-day technology in cold-atom-gas laboratories allows changing of the external potentials on short time scales. By this it is possible to explore the regime where the many-body system is still governed by a unitary evolution but with nonequilibrium initial conditions.

The number of atoms with spin up, $N_{\uparrow} = \Sigma_i \langle \Psi(t)|\hat{n}_{i\uparrow}|\Psi(t)\rangle$, can be different from the number of atoms with spin down, $N_{\downarrow} = \Sigma_i \langle \Psi(t)|\hat{n}_{i\downarrow}|\Psi(t)\rangle$. The particle number $N_{\uparrow}$ and $N_{\downarrow}$ are separately conserved quantities because no spin-flip mechanism is included in the Hamiltonian (1). The model (1) must be accompanied by some boundary conditions: in this work we choose for simplicity open (hard wall) boundary conditions (OBCs). OBCs do not model well the most common experimental setups[6–8] in which a parabolic trapping acts on the Fermi gas to keep it into the optical lattice. However, we have deliberately decided to limit our present investigations to simple OBCs to disentangle spurious effects (mainly spatial coexistence of different quantum phases) that can be induced by the parabolic trapping from fundamental effects related to the dynamics after the quench.

In the absence of $\hat{\mathcal{H}}_{\text{ext}}(t)$ [i.e., for $V_{i\sigma}(t)=0$], the Hamiltonian in Eq. (1) reduces to a 1D homogeneous Hubbard model that has been solved exactly by Lieb and Wu.[33] At zero temperature the properties of $\hat{\mathcal{H}}_{\text{ref}}$ in the thermodynamic limit ($N_{\sigma}, L \to \infty$) are determined by the spin-resolved filling factors $n_{\sigma} = N_{\sigma}/L$ and by the dimensionless coupling constant $u \equiv U/\gamma$. For simplicity, we limit the analysis below to $n = n_{\uparrow} + n_{\downarrow} < 1$ and, for definiteness, we take $n_{\uparrow} \geq n_{\downarrow}$.

According to Lieb and Wu,[33] the ground state of $\hat{\mathcal{H}}_{\text{ref}}$ in the presence of repulsive interactions and in the thermodynamic limit is described by two continuous distribution functions $\rho(x)$ and $\sigma(y)$ which satisfy the BA coupled integral equations,

$$\rho(x) = \frac{1}{2\pi} + \frac{\cos x}{\pi} \int_{-B}^{+B} \frac{u/4}{(u/4)^2 + (y - \sin x)^2} \sigma(y) dy, \quad (3)$$

and

$$\sigma(y) = \frac{1}{\pi} \int_{-Q}^{+Q} \frac{u/4}{(u/4)^2 + (y - \sin x)^2} \rho(x) dx$$
$$- \frac{1}{\pi} \int_{-B}^{+B} \frac{u/2}{(u/2)^2 + (y - y')^2} \sigma(y') dy'. \quad (4)$$

The parameters Q and B are determined by the normalization conditions

$$\begin{cases} \int_{-Q}^{+Q} \rho(x) dx = n \\ \int_{-B}^{+B} \sigma(y) dy = n_{\downarrow} \end{cases}. \quad (5)$$

The ground-state energy of the system (per site) is given by

$$\varepsilon_{\text{GS}}(n_{\uparrow}, n_{\downarrow}, u) = -2\gamma \int_{-Q}^{+Q} \rho(x) \cos x \; dx. \quad (6)$$

III. TIME-EVOLUTION WITHIN TIME-DEPENDENT DENSITY-FUNCTIONAL THEORY

In this section we describe the two-step procedure that we have followed to calculate the time-evolution of the spin-

resolved site-occupation profiles $n_{i\sigma}(t)$. We first calculate the spin-resolved site-occupation profiles corresponding to $|\Psi_0\rangle$ for times $t \leq 0$ by means of a static DFT calculation and then find the subsequent time evolution for $t > 0$ by means of TDDFT.

A. Preparation of the initial state

As we have already noted, for times $t \leq 0$ the Hamiltonian (1) with OBCs describes an equilibrium ground-state problem. We can calculate accurately the ground-state spin-resolved site-occupation profiles of the inhomogeneous system described by $\hat{\mathcal{H}}(t \leq 0) = \hat{\mathcal{H}}_{\text{ref}} + \Sigma_{i,\sigma} V_{i\sigma}^{\text{ext}} \hat{n}_{i\sigma}$ by means of a DFT scheme based on Eqs. (3)–(6). We have in fact generalized the site-occupation-functional theory (SOFT) scheme proposed in Ref. 30 and based on the BA local-density approximation to the case in which the external potential is spin dependent (spin SOFT). We here summarize the main steps that we have followed to calculate the ground-state spin-resolved site-occupation profiles $n_{i\sigma}(t \leq 0)$.

Within spin SOFT $n_{i\sigma} \equiv n_{i\sigma}(t \leq 0)$ can be obtained by solving self-consistently the static lattice KS equations,

$$\sum_j [-\gamma_{ij} + V_{i\sigma}^{\text{KS}} \delta_{ij}] \varphi_{j\sigma}^{(\alpha)} = \varepsilon_\sigma^{(\alpha)} \varphi_{i\sigma}^{(\alpha)}, \tag{7}$$

together with the closure

$$n_{i\sigma} = \sum_{\alpha,\text{occ.}} |\varphi_{i\sigma}^{(\alpha)}|^2, \tag{8}$$

where the sum runs over the occupied orbitals. Here $\gamma_{ij} = \gamma > 0$ if i and j are nearest-neighbor sites and zero otherwise, and $V_{i\sigma}^{\text{KS}} = U n_{i\bar{\sigma}} + V_{i\sigma}^{\text{xc}} + V_{i\sigma}^{\text{ext}}$ where $\bar{\sigma} = -\sigma$. The first term in the effective Kohn-Sham potential $V_{i\sigma}^{\text{KS}}$ is the Hartree mean-field contribution while $V_{i\sigma}^{\text{xc}}$ is the (not exactly known) xc potential. As already stressed in Ref. 30, exchange interactions between parallel-pseudospin atoms have been effectively eliminated in the Hubbard model (1) by restricting the model to one orbital per site. Hence parallel-pseudospin interactions are not treated dynamically in solving the Hamiltonian but are accounted for implicitly via a restriction of the Hilbert space. To stress the analogy of the present work with *ab initio* applications of standard DFT, we nevertheless continue to call $V_{i\sigma}^{\text{xc}}$ the exchange-correlation potential but it is understood that the exchange contribution to this quantity is exactly zero.

The LSDA has been shown to provide an excellent account of the ground-state properties of a large variety of inhomogeneous systems.[18,35,36] In this work we have employed the following BA-based LSDA (BA-LSDA) functional

$$V_{i\sigma}^{\text{xc}} \simeq V_{i\sigma}^{\text{xc}}|_{\text{BA–LSDA}} \equiv v_{\text{xc},\sigma}^{\text{hom}}(n_\uparrow, n_\downarrow, u)|_{n_\sigma \to n_{i\sigma}}, \tag{9}$$

where, in analogy with *ab initio* spin DFT, the xc potential $v_{\text{xc},\sigma}^{\text{hom}}(n_\uparrow, n_\downarrow, u)$ of the reference system described by $\hat{\mathcal{H}}_{\text{ref}}$ is defined by

$$v_{\text{xc},\sigma}^{\text{hom}}(n_\uparrow, n_\downarrow, u) = \frac{\partial}{\partial n_\sigma} [\varepsilon_{\text{GS}}(n_\uparrow, n_\downarrow, u) - \varepsilon_{\text{GS}}(n_\uparrow, n_\downarrow, 0) - U n_\sigma n_{\bar{\sigma}}]. \tag{10}$$

Thus, within the LSDA scheme proposed in Eqs. (9) and (10), the only necessary input is the xc potential $v_{\text{xc},\sigma}^{\text{hom}}(n_\uparrow, n_\downarrow, u)$ of the homogeneous reference system, which can be calculated exactly following a very similar procedure to that outlined in Ref. 30.

The self-consistent scheme represented by Eqs. (7)–(10) can be solved numerically for each set of parameters $\{L, N_\uparrow, N_\downarrow, u, W_\sigma/\gamma, w\}$. The outcome of these calculations is $n_{i\sigma}$, which is used in the next section as the initial condition for the time evolution.

B. Time-evolution within time-dependent density-functional theory

The spin-resolved site-occupation profiles of the many-body system described by the Hamiltonian (1) at time t can be obtained by solving single-particle-like time-dependent lattice KS equations,

$$i\hbar \partial_t \psi_{i\sigma}^{(\alpha)}(t) = \sum_j [-\gamma_{i,j} + V_{i\sigma}^{\text{KS}}(t) \delta_{ij}] \psi_{j\sigma}^{(\alpha)}(t), \tag{11}$$

with initial conditions $n_{i\sigma}(0) = n_{i\sigma}$. As in the static case, the spin-resolved time-dependent site occupations $n_{i\sigma}(t)$ are calculated by adding up the contributions of the orbitals that are occupied at the initial time,

$$n_{i\sigma}(t) = \sum_{\alpha,\text{occ.}} |\psi_{i\sigma}^{(\alpha)}(t)|^2. \tag{12}$$

In Eq. (11) $V_{i\sigma}^{\text{KS}}(t) = U n_{i\bar{\sigma}}(t) + V_{i\sigma}^{\text{xc}}(t)$ is the spin-resolved KS. The first term in the effective KS potential is the instantaneous Hartree mean-field contribution while $V_{i\sigma}^{\text{xc}}(t)$ is the (not exactly known) xc potential. The time-dependent spin-resolved KS potential must be determined self-consistently with the site-occupation profiles $n_{i\sigma}(t)$. This means that, in practice, the initial ground-state densities $n_{i\sigma}$ determine the initial KS potential, which is then used to recalculate the site-occupation profiles at an infinitesimally later time, and so on.

In this work we have chosen to approximate the time-dependent xc potential $V_{i\sigma}^{\text{xc}}(t)$ with a BA-based adiabatic local-spin-density approximation (BA-ALSDA):

$$V_{i\sigma}^{\text{xc}}(t) \simeq V_{i\sigma}^{\text{xc}}(t)|_{\text{BA–ALSDA}} \equiv v_{\text{xc},\sigma}^{\text{hom}}(n_\uparrow, n_\downarrow, u)|_{n_\sigma \to n_{i\sigma}(t)}. \tag{13}$$

IV. NUMERICAL RESULTS AND DISCUSSION

In this section we report some illustrative numerical results that we have obtained applying the TDDFT/BA-ALSDA method described above.

All the numerical results presented below correspond to a system with $N = 28$ atoms on $L = 72$ sites, the OBCs being imposed at the sites $i = 0$ and $i = 73$. We compare the results obtained with the TDDFT/BA-ALSDA with results of the

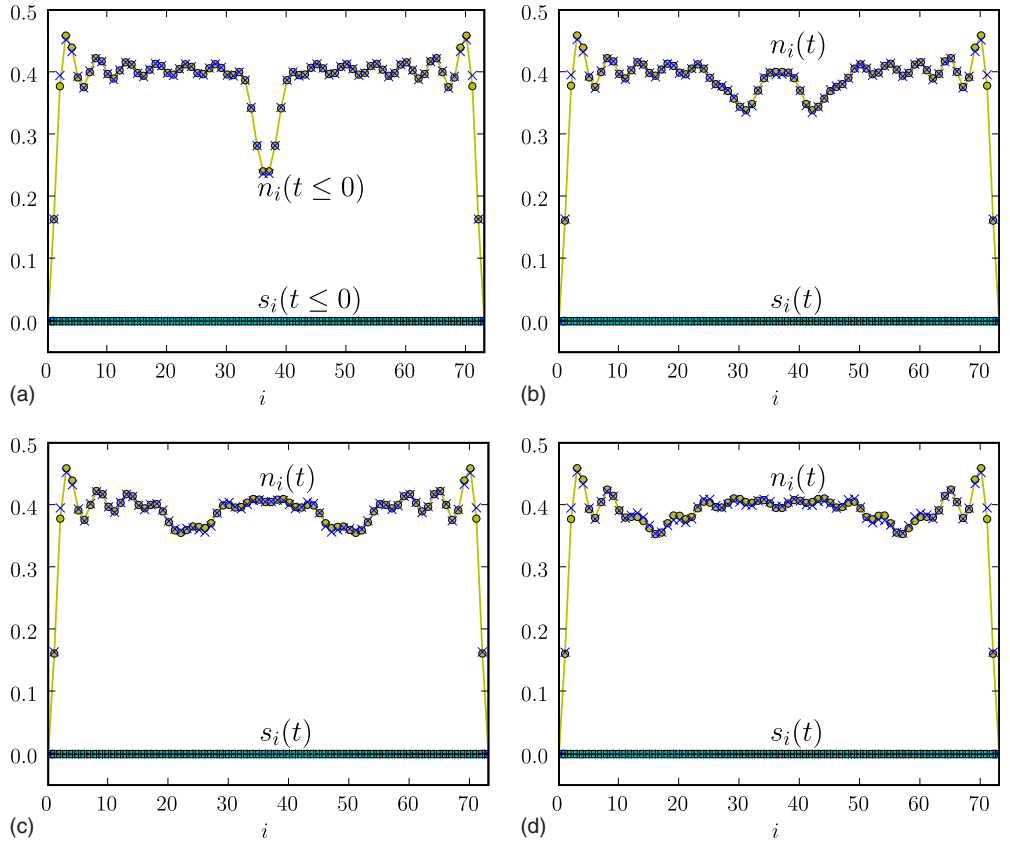

FIG. 1. (Color online) Charge $n_i(t)$ and spin $s_i(t)$ occupations as functions of lattice site i and time t for $L=72$ (the hard-wall boundary conditions are imposed at the sites 0 and 73), $N_\uparrow=N_\downarrow=14$, $u=+2$, $W_\uparrow/\gamma=W_\downarrow/\gamma=-7/18$, and $w=2$. TDDFT data (filled circles and squares) are compared with tDMRG data ($\times$ and $+$). Top left panel: ground-state charge and spin occupations for times $t\le 0$. Top right panel: same as in the top left panel but at time $t=5\hbar/\gamma$. Bottom left panel: same as in the top panels but at time $t=10\hbar/\gamma$. Bottom right panel: same as in the bottom left panel but at time $t=15\hbar/\gamma$.

adaptive tDMRG. The adaptive tDMRG relies on the use of an effective Hilbert space of dimension M adapted at each time step. In the current work the time evolution is performed using a Suzuki-Trotter decomposition. Several hundred density-matrix renormalization-group (DMRG) states are kept (up to $M=800$) and time steps of the order of $\mathcal{O}(0.1\hbar/\gamma)$ are used to achieve accurate results up to long times. For a discussion of the sources of uncertainties, we refer the reader to the work by Gobert *et al.*[37]

In Fig. 1 we show results for a spin-unpolarized system ($N_\uparrow=N_\downarrow=14$) with $U=+2\gamma$. In this special simulation the external potential is chosen to be spin independent: $W_\uparrow=W_\downarrow=-7/18$ [see Eq. (2)]. The initial charge $n_i=n_{i\uparrow}+n_{i\downarrow}$ and spin local occupations $s_i=n_{i\uparrow}-n_{i\downarrow}$ are shown in the top left panel. The spin occupation is identically zero in this spin-unpolarized situation simply due to the symmetry between the $\uparrow$- and $\downarrow$-spin atoms. The effect of the external potential results in a local perturbation of the charge-density distribution, i.e., the dip in Fig. 1. Additional deviations from a homogeneous distribution are due to OBCs which cause Friedel oscillations.

We find an excellent agreement between the ground-state DFT/BA-LSDA results (see Sec. III A) and the DMRG results. Small differences between the two are visible only when close to the boundaries and in the local perturbation. OBCs are very severe boundary conditions for BA-LSDA: the performance of this approximation increases in the presence of soft boundaries, such as those created by a parabolic trapping potential—see Ref. 30. Our finding is in agreement with earlier studies[38] in which the inability of the BA local-density approximation to reproduce the correct Friedel oscillations in the presence of a single impurity (or close to a sharp boundary) has been noted. In general, no local-density approximation for the xc potential is expected to produce Friedel oscillations with an amplitude that scales as a power law as a function of the distance from the impurity/boundary, with an exponent that is controlled by the interaction strength. Of course, this inadequacy of BA-LSDA is more severe at strong coupling: see, for example, the top left panel in Fig. 6.

The time evolution of charge and spin occupations subsequent to the sudden switching off of the external local potential is illustrated in the other three panels of Fig. 1 for times $t=5\hbar/\gamma$, $10\hbar/\gamma$, and $15\hbar/\gamma$. For small times $t<5\hbar/\gamma$ the initial dip in the charge density starts splitting into two counterpropagating perturbations. After the splitting the perturbations move with a certain velocity toward the boundaries. During the evolution a deformation of the shape of the density perturbations can be seen. Scattering of the perturbation from the Friedel oscillations and the boundaries occurs.

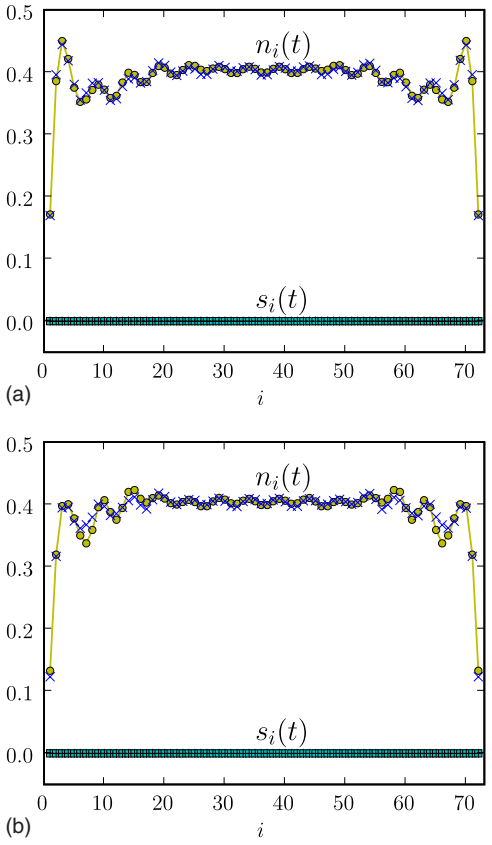

FIG. 2. (Color online) Same as in Fig. 1 but for $t=20\hbar/\gamma$ (top panel) and $t=30\hbar/\gamma$ (bottom panel).

We see how TDDFT/BA-ALSDA results are in full quantitative agreement with the tDMRG data. The agreement remains quite decent even at times later than $t=15\hbar/\gamma$, when reflections from the boundaries and interference with the microscopic Friedel oscillations are expected to spoil the performance of TDDFT/BA-ALSDA. For example, in Fig. 2 we have reported the comparison between TDDFT/BA-ALSDA and tDMRG data at $t=20\hbar/\gamma$ and $30\hbar/\gamma$.

In the results shown in Figs. 1 and 2 the spin dynamics is trivial: $s_i(t)\equiv 0$ at all times. In order to check the predicting power of TDDFT/BA-ALSDA in regard to spin dynamics, in Fig. 3 we show results for a spin-polarized system ($N_\uparrow=20$ and $N_\downarrow=8$). Note that the local external potential in this case is again spin independent (as it was in the case of Fig. 1) and couples only to the total-charge sector. Nonetheless, due to the imbalance between the number of atoms with different spin, this local disturbance generates a nontrivial spin dynamics. This is a consequence of the fact that the spin and charge sectors of the spin-polarized 1D Hubbard model away from half filling are coupled.[12,39–42] The coupling affects the dynamics considerably. In contrast to the spin-balanced case, the perturbation does not decay into noninteracting charge and spin perturbations. As before the charge-density perturbation evolves into two counterpropagating perturbations. However, the creation of a pronounced dip at the center of the system, which is due to the interaction with the slower spin perturbation, can be observed. We clearly see from Fig. 3 how the agreement between TDDFT/BA-ALSDA and tDMRG is also very satisfactory in this spin-polarized case. Deviations are mainly observed close to the boundaries.

All numerical results shown in Figs. 1–3 have been obtained for $U=+2\gamma$. We have also checked how the relative strength U/γ of interactions influences the reliability of TDDFT/BA-ALSDA. In Figs. 4–6 we show results for spin-unpolarized and spin-polarized systems at $U=+4\gamma$ and $U=+6\gamma$. With increasing coupling strength, the deviations between the two methods increase both for the initial state and the time evolution. For the initial state the Friedel oscillations are not captured correctly (mainly the $4k_F$ component[38]) and large deviations at the boundaries arise. In particular, the results for the spin-density profiles at $U=+6\gamma$ show considerable differences between the two methods. In the time evolution, in contrast to smaller couplings, the form of the charge perturbation shows deviations between the results of the two methods even in the unpolarized case (see the top right panel in Fig. 6). However, the main features of the tDMRG data are qualitatively reproduced by TDDFT/BA-ALSDA (e.g., the splitting into two counterpropagating perturbations with approximately the correct velocity). From these plots we can see how the predicting power of TDDFT/BA-ALSDA is quite acceptable also at strong coupling.

The surprising accuracy and success of the simple adiabatic approximation (13) in the present strongly correlated system call for an explanation, which we try to offer in what follows.

To begin with, we would like to note that, in the charge channel, the excitation spectrum of 1D interacting systems at finite momentum q and frequency ω resembles in many ways that of a 1D noninteracting Fermi system.[18] In particular, its support [defined by the region of the (q,ω) plane in which the density of excitations is largest] is qualitatively similar in the two cases. The main differences are (i) the Fermi velocity of the interacting system is corrected by particle-particle interactions, and (ii) the spectral density of excitations of the interacting system at the absolute zero of temperature [the density-density dynamic structure factor $S_{nn}(q,\omega)$] can have pronounced substructures as power-law singularities at the kinematic boundaries of the spectrum.[43–47] Quantitative calculations of the excitation spectrum in the spin channel and of the spin-spin dynamic structure factor $S_{ss}(q,\omega)$ have been carried out in Refs. 45 and 47. Also in this channel power-law singularities (at the low-energy onset of the two-spinon continuum) have been found.[45]

In our TDDFT approach, electron-hole excitations at finite q and ω are naturally contained in the auxiliary noninteracting system that is used in the Kohn-Sham mapping [Eqs. (11) and (12)]. It is the task of the exchange-correlation potential to take into account the effects (if any) of (i) and (ii) on the propagation of a density (spin) packet. The effect of (i) is very important (since it controls the velocity of propagation of the packet) and is obviously taken into account by the static part of our exchange-correlation potential, $v_{\mathrm{xc},\sigma}^{\mathrm{hom}}(n_\uparrow,n_\downarrow,u)$ in Eq. (13). Our functional simply "knows" the exact thermodynamic compressibility and spin susceptibility (and thus the exact charge and spin velocities) from the Bethe-*Ansatz* solution of the 1D Hubbard model described by $\hat{\mathcal{H}}_{\mathrm{ref}}$ in Eq. (1). The effect of (ii) is not so clear. However,

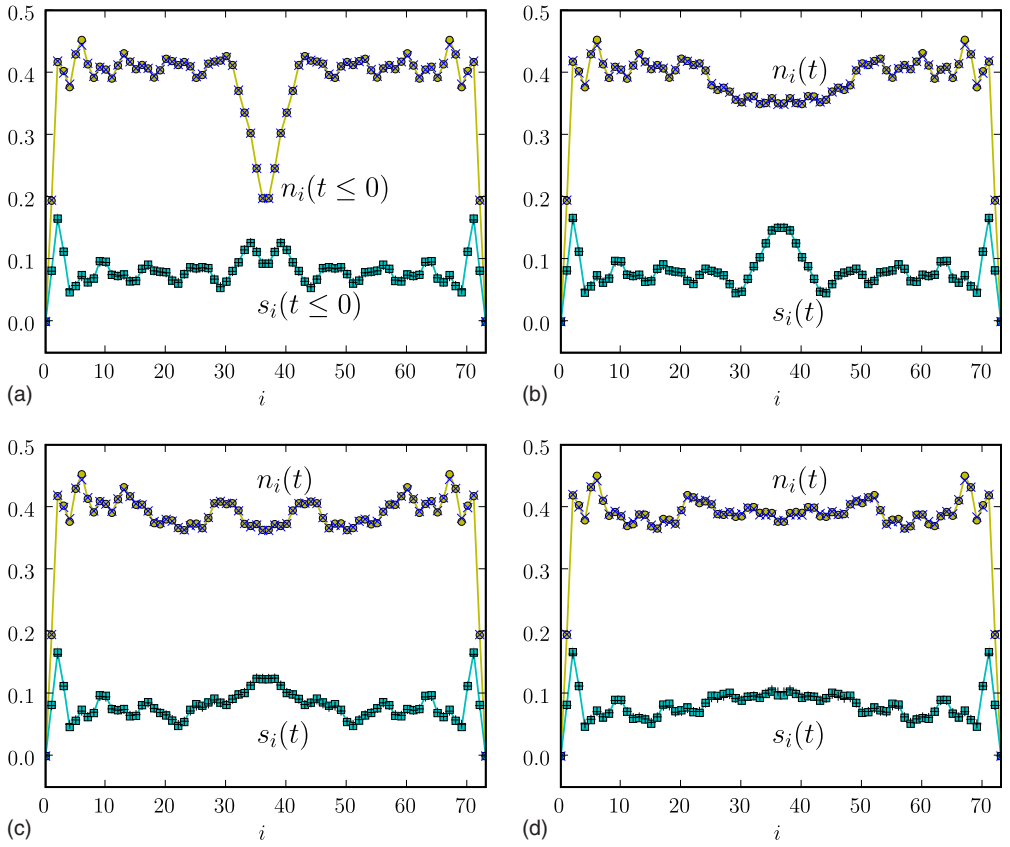

FIG. 3. (Color online) Same as in Fig. 1 but for $N_\uparrow=20$, $N_\downarrow=8$, $u=+2$, $W_\uparrow/\gamma=W_\downarrow/\gamma=-5/9$, and $w=2$.

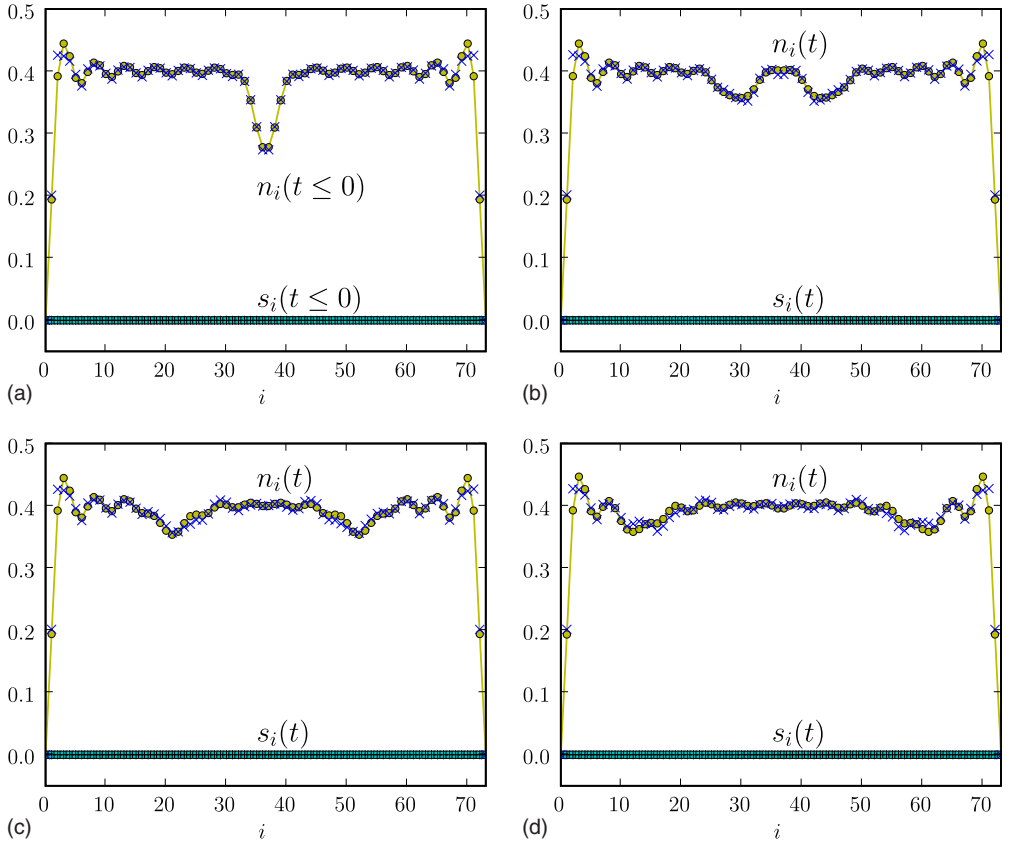

FIG. 4. (Color online) Same as in Fig. 1 but for $u=+4$.

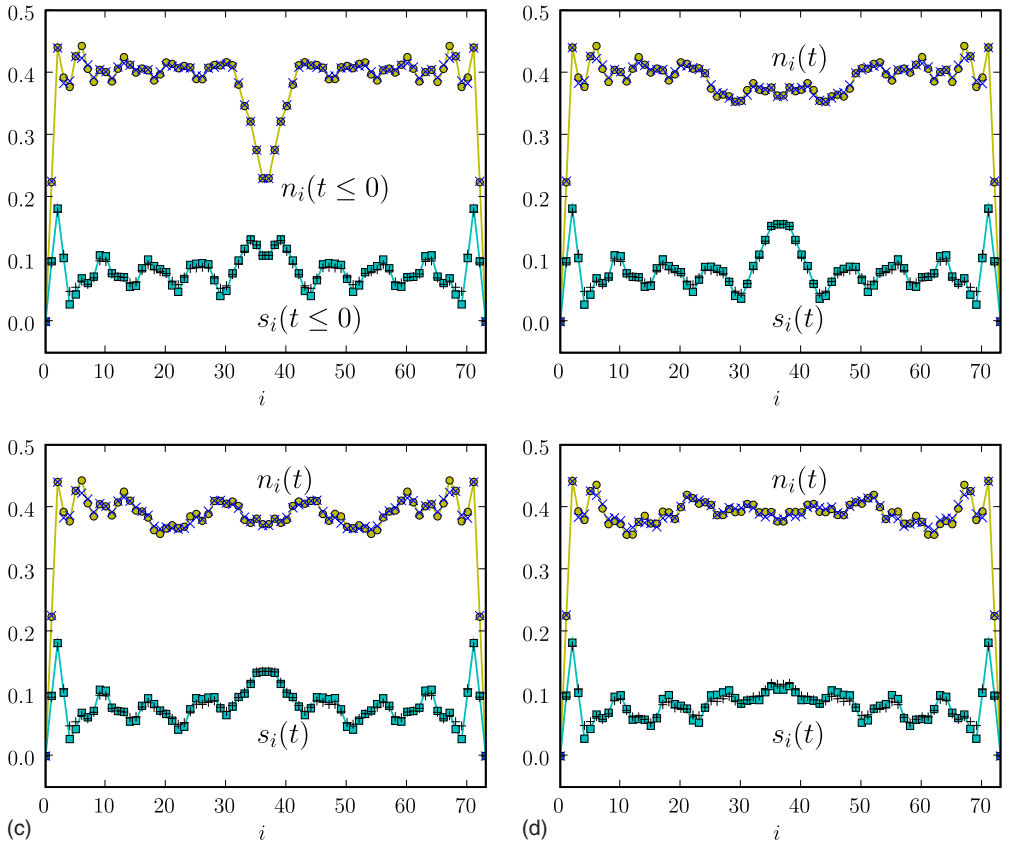

FIG. 5. (Color online) Same as in Fig. 3 but for $u=+4$.

it seems unlikely that the details of the spectral distribution would show up in the considered evolution of collective excitations in the particle and/or spin density. This expectation is fully confirmed by the tDMRG results, in which the excitations only show a slight broadening and a decay on the time scales considered in this work.

Second, we would like to mention that the adiabatic approximation is very well known to perform extraordinarily well in reproducing the frequency of collective excitations such as plasmons[48,49] in a large variety of systems. However, the linewidth of these collective resonances is strictly *zero* within the adiabatic approximation and one has to go beyond it to capture, e.g., intrinsic damping (due to many-body effects) of the collective modes (see for example Ref. 48 for a theoretical calculation of the linewidth of the intersubband plasmon in two-dimensional (2D) quantum wells and Ref. 50 for a calculation of the same quantity in tunnel-coupled double-layer electron gases).

V. CONCLUSIONS AND FUTURE PERSPECTIVES

In summary, we have carried out an extensive numerical study of the collective spin and charge dynamics in strongly correlated ultracold Fermi gases confined in one-dimensional tight tube. We have compared the results obtained from time-dependent density-functional theory within a suitable (Bethe-*Ansatz*-based) adiabatic local-spin-density approximation with accurate results based on the adaptive time-dependent density-matrix renormalization-group method. We have found the simple adiabatic local-spin-density approximation for the time-dependent exchange-correlation potential to be reliable and surprisingly accurate in describing the collective evolution of density and spin-wave packets in a wide range of coupling strengths and spin polarizations.

The adiabatic scheme proposed in this work can also be used and tested in many other interesting problems. For example, one can study spin-charge dynamics after a local quench in Luther-Emery liquids [which can be modeled by Eq. (1) with $U<0$], Andreev reflection[51] in ultracold two-component Fermi gases, and, of course, quantum dynamics in the presence of truly time-dependent external potentials.

In this last respect, we can anticipate that more sophisticated functionals in which the main ALDA assumptions, i.e., (i) locality in space *and* time and (ii) the complete neglect of memory effects, are relaxed may be needed to handle truly time-dependent problems. The importance of spatial versus temporal nonlocality has already been commented at length in earlier literature.[52] More recent numerical results[32] of a TDDFT study of small (i.e., $L=4-12$) Hubbard chains seem to indicate that *both* (i) and (ii) have to be transcended to describe the time dynamics of strongly correlated systems.

Finally, we would like to mention that adiabatic and beyond-adiabatic exchange-correlation functionals based on time-dependent current-spin-density-functional theory have also been recently applied[53] to study collective spin and charge dynamics at finite temperature in one-dimensional continuum models.

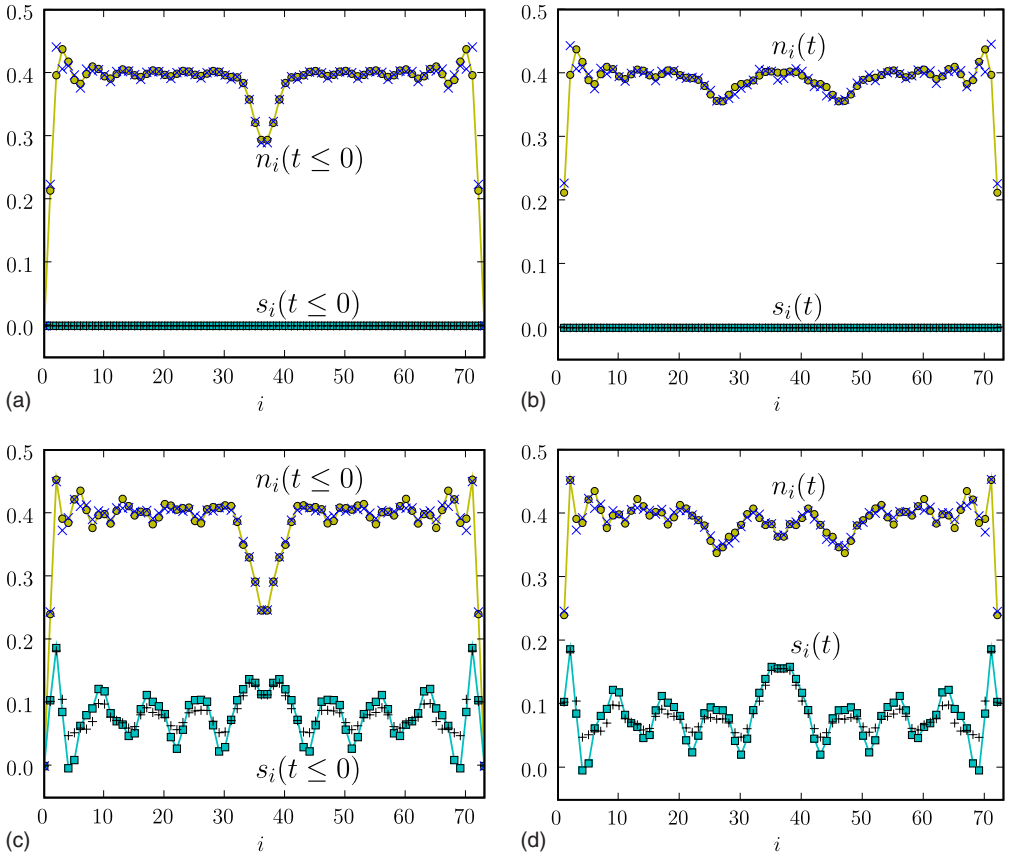

FIG. 6. (Color online) Top panels: Charge $n_i(t)$ and spin $s_i(t)$ occupations as functions of lattice site i and time t for $L=72$, $N_\uparrow=N_\downarrow=14$, $u=+6$, $W_\uparrow/\gamma=W_\downarrow/\gamma=-7/18$, and $w=2$. TDDFT data (filled circles and squares) are compared with tDMRG data ($\times$ and +). Left: ground-state charge and spin occupations for times $t\le 0$. Right: same as in the left panel but at time $t=6\hbar/\gamma$. Bottom panels: same in the top panels but for $N_\uparrow=20$ and $N_\downarrow=8$.

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