Nonadiabatic electron dynamics in one dimension within the time-dependent density functional theory

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We study electron fluid confined in a quasi-one-dimensional potential using the nonadiabatic time-dependent density-functional theory. We analyze the memory effects associated with the nonadiabatic dynamics of the electron fluid and get an insight in exchange-correlation effects by transforming to the Lagrangian frame comoving with electron fluid.

INTRODUCTION

In this work, we analyze the electron dynamics beyond the ALDA approximation within the C-TDDFT and L-TDDFT theories [**?**] based on one-dimensional models of single and double quantum wells.

INTRODUCTION TO C-TDDFT AND L-TDDFT

C-TDDFT time-dependent Kohn-Sham (TDKS) equation

$$i\frac{\partial\varphi_\alpha(\mathbf{r},t)}{\partial t}=\left[\frac{1}{2}\left(-i\nabla+\frac{1}{c}\mathbf{A}_{\rm KS}(\mathbf{r},t)\right)^2+V_{\rm KS}(\mathbf{r},t)\right]\varphi_\alpha(\mathbf{r},t),$$

where $\mathbf{A}_{\rm KS}(\mathbf{r},t)=\mathbf{A}_{\rm ext}(\mathbf{r},t)+\mathbf{A}_{\rm xc}(\mathbf{r},t)$, and $V_{\rm KS}(\mathbf{r},t)=V_{\rm ext}(\mathbf{r},t)+V_{\rm H}(\mathbf{r},t)$. We use atomic units $\hbar=e=m=1$ throughout. Following Refs. [**? ?**], consider a 3D system whose electron density is uniform along y and z directions while the spatial dependence is along x only. Assume the electron liquid is trapped within the interval $-L\le x\le L$ and its density satisfies zero boundary conditions at the edges, $n(-L,t)=n(L,t)=0$. The TDKS reads,

$$i\frac{\partial\varphi_\alpha}{\partial t}=\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V_{\rm ext}(x,t)+V_{\rm H}(x,t)+V_{\rm xc}(x,t)\right]\varphi_\alpha(x,t),\tag{1}$$

where the vector potential has been turned into the scalar exchange-correlation potential $V_{\rm xc}(x,t)$ by the use of gauge transformations. $V_{\rm xc}(\mathbf{r},t)$ takes the form

$$V_{\rm xc}(x,t)=V_{\rm xc}^{\rm ALDA}(x,t)+V_{\rm xc}^{\rm M}(x,t),$$

$$V_{\rm xc}^{\rm M}(x,t)=-\int_0^x\frac{dx'}{n(x',t)}\nabla_{x'}\sigma_{{\rm xc},xx}(x',t)=-\ n(x,t)\tilde\sigma_{{\rm xc},xx}(x,t)|_0^x-\int_0^x\tilde\sigma_{{\rm xc},xx}(x',t)\frac{\partial n(x',t)}{\partial x'}dx',\tag{2}$$

where we have introduced $\tilde\sigma_{{\rm xc},xx}(x,t)\equiv\sigma_{{\rm xc},xx}(x,t)/n(x,t)^2$. From the continuity equation

$$\frac{\partial n}{\partial t}+\frac{\partial(nv)}{\partial x}=0,$$

we have for the velocity field

$$v(x,t)=-\frac{1}{n(x,t)}\frac{\partial}{\partial t}\int_0^x n(x',t)dx'.\tag{3}$$

DOUBLE QUANTUM WELL

We assume the electron density in the double quantum well is given by

$$n(x,t)=A(x)\cos^2\omega t+B(x)\sin^2\omega t\tag{4}$$

where function $A(x)$ and $B(x)$ satisfy

$$\int_{-\infty}^{\infty} A(x)\,dx = \int_{-\infty}^{\infty} B(x)\,dx \equiv N,$$

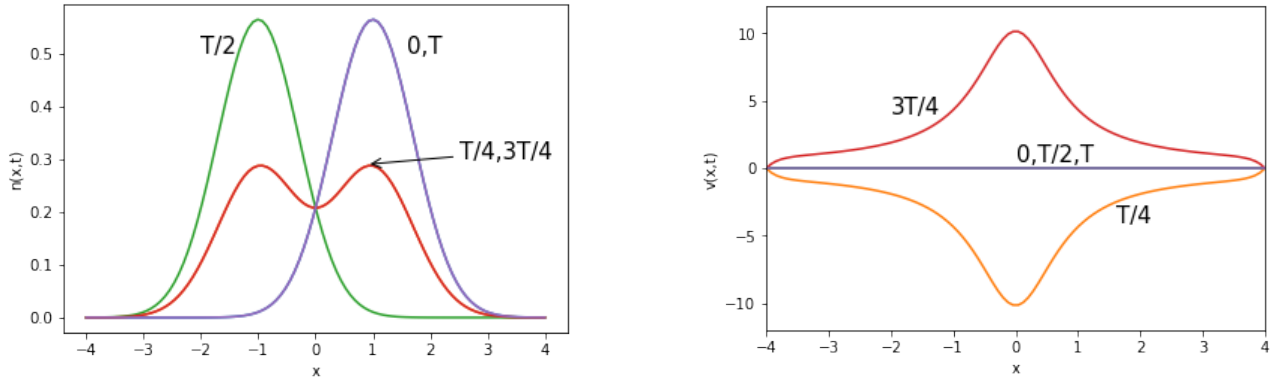
so that the number of particles is conserved at all times and is given by $\int_{-\infty}^{\infty} n(x,t)dx = N$. We shall measure frequencies in units of the average plasmon frequency of the system, given by

$$\bar{\omega}_p = \frac{1}{L}\int dx\omega_p(n_0(x)) = \frac{1}{L}\int dx\sqrt{4\pi e^{-(x+1)^2}}, \tag{5}$$

that equals $\bar{\omega}_p = 0,555$ for $L = 8$. We take functions in the Gaussian form

$$A(x) = \frac{1}{\sqrt{\pi}}e^{-(x+1)^2}, \quad B(x) = \frac{1}{\sqrt{\pi}}e^{-(x-1)^2}, \tag{6}$$

which satisfy the conditions above. Using (3), one can find the velocity $v(x,t)$. Corresponding evolution of these quantities over time is represented by FIG 1. Here we define $T = \frac{\pi}{\omega}$.



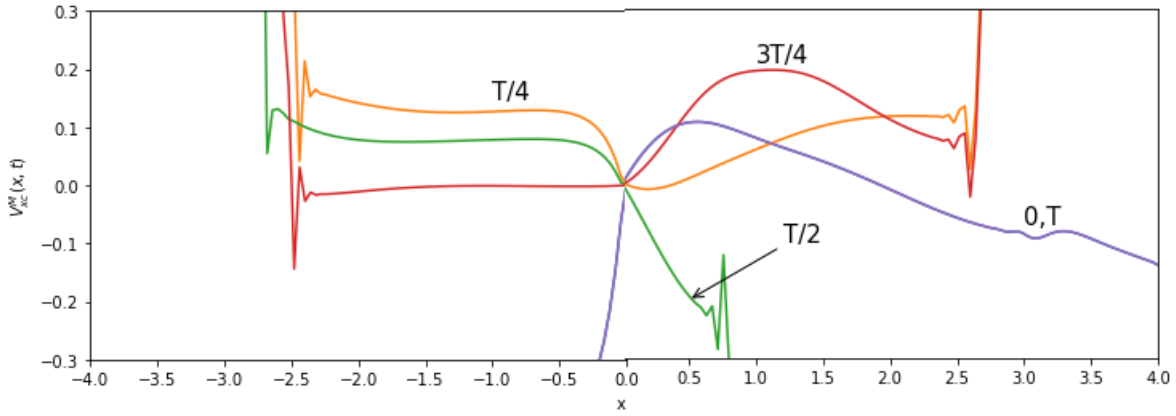
a) b)

FIG. 1. Distribution of electron density $n(x,t)$ (a) and velocity $v(x,t)$ (b), taken at times $t = 0, T/4, T/2, 3T/4$.

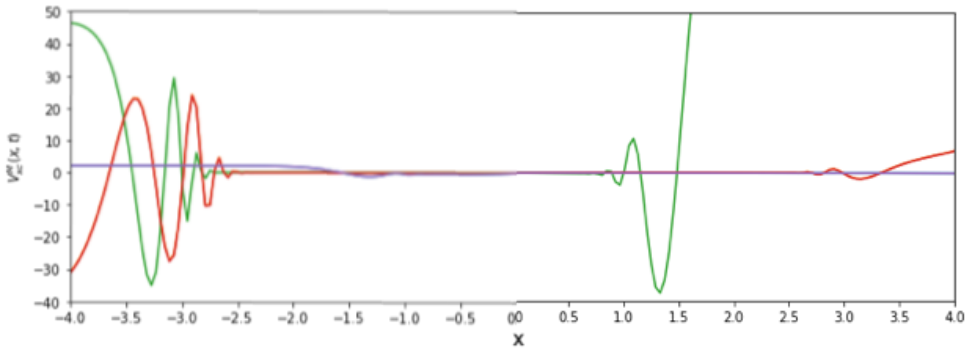
Then memory part of scalar potential was calculated by (2), the result is on FIG 2

CONCLUSIONS

We have analyzed the memory effects associated with the nonadiabatic dynamics of the electron fluid in one-dimensional systems. An insight in the role of exchange-correlation effects has been obtained and transforming to the Lagrangian frame comoving with the electron fluid.



a)



b)

FIG. 2. a) Evolution of V_{xc}^{M}, taken at times $t = 0, T/4, T/2, 3T/4$ for frequency $\omega = 2.22\bar{\omega}$. In b) the same, but potential scale is greater.