ACCURACY OF FISSION DYNAMICS WITHIN THE TIME-DEPENDENT SUPERFLUID LOCAL DENSITY APPROXIMATION*

J. Grineviciute[a], P. Magierski[a,b], A. Bulgac[b], S. Jin[b], I. Stetcu[c]

[a]Faculty of Physics, Warsaw University of Technology
Koszykowa 75, 00-662 Warszawa, Poland
[b]Department of Physics, University of Washington
Seattle, WA 98195–1560, USA
[c]Theoretical Division, Los Alamos National Laboratory
Los Alamos NM 87545, USA

(Received December 5, 2017)

We investigate properties of the method based on time dependent superfluid local density approximation (TDSLDA) within an application to induced fission of ^{240}Pu and surrounding nuclei. Various issues related to accuracy of time evolution and the determination of the fission fragment properties are discussed.

DOI:10.5506/APhysPolB.49.591

1. Introduction

The time-dependent superfluid local density approximation (TDSLDA) is an extension of time-dependent Density Functional Theory (TDDFT) to superfluid systems using local pairing field. It is designed to describe real-time dynamics of inhomogeneous fermionic systems subjected to perturbations of arbitrary strength. The method is flexible and allows for applications in various quantum systems which are defined through a suitable energy density functional. It is also microscopic in a sense that fermionic degrees of freedom are treated and evolved explicitly without any additional phenomenological input. Various successful applications of TDSLDA include physics of ultracold atomic gases [1], low-energy nuclear physics [2, 3], and physics of the neutron star crust [4]. The main advantage of TDSLDA consists of treating paired fermions as a dynamic field which has its own modes

* Presented at the XXXV Mazurian Lakes Conference on Physics, Piaski, Poland, September 3–9, 2017.

of excitations. Indeed, the correct treatment of pairing is crucial when describing nuclear reactions, such as fission, that are strongly influenced by pairing correlations [3, 5].

In the context of nuclear reactions, the typical scenario in which TDDFT is used consists of a system being initially in a ground state or a state characterized by a certain deformation achieved using a constraint solution (obtained within the standard DFT). Subsequently, the nucleus is acted upon by a perturbation that drives it out of equilibrium. The external perturbation in the nuclear system can be of various origins: it can be caused by photon absorption, by neutron capture, or the perturbation can arise as an interaction between the projectile and the target nucleus. It has to be emphasized that the perturbation may be of arbitrary strength since TDDFT can be applied both in the linear-response regime as well as in the nonlinear regime. In particular, the external perturbations can be strong enough to compete with, or even override the internal interactions that provide the structure and stability of atomic nucleus, as in the case of induced fission process.

The typical procedure used in the context of nuclear reactions is the following:

— Prepare the initial state by solving static Kohn–Sham equations for a nucleus (or nuclei if more than one system is involved in the reaction process), to get a set of ground-state Kohn–Sham orbitals and orbital energies.

— The time evolution can be obtained by applying certain external field simulating *e.g.*, the photon absorption, or through generating nonzero velocities of nuclei towards each other. Then one solves the time-dependent Kohn–Sham equation from the initial time to the desired final time. The time propagation of the orbitals determines the time-dependent densities.

— During time evolution, one may calculate the desired observable(s) as functionals of densities used as building blocks of the energy density functional. It implies that TDDFT is particularly well-suited to calculate one-body observables.

Hence, it is clear that in particular for calculations of induced fission the stability of the evolution of nuclear system is crucial as it influences the nascent fragment properties. In this paper, we discuss issues pertaining to accuracy of induced fission of selected Pu isotopes within TDSLDA employing Skyrme SLy4 nuclear energy density functional (NEDF).

2. Time step and pairing coupling constant

The set of equations originated from TDSLDA has the following form:

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} U_\mu(\boldsymbol{r},t) \\ V_\mu(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} h(\boldsymbol{r},t) & \Delta(\boldsymbol{r},t) \\ \Delta^*(\boldsymbol{r},t) & -h^*(\boldsymbol{r},t) \end{pmatrix}\begin{pmatrix} U_\mu(\boldsymbol{r},t) \\ V_\mu(\boldsymbol{r},t) \end{pmatrix}, \qquad (1)$$

where h and Δ are determined by the energy density functional through the densities which are constructed from amplitudes U and V (for clarity we omit here spin and nucleon indices). Therefore, TDSLDA represents a system of coupled, nonlinear time-depended partial differential equations. In nuclear applications, the number of equations is of the order of hundreds of thousands (depending on the lattice size). The time interval of the evolution of the system depends on the physical problem studied, and in the case of induced fission, it is set by the time needed for a nucleus to move from saddle point to separated fragments, which requires around half a million time steps.

In the case of induced fission, the time-depended equations of TDSLDA are solved on a spatial lattice discretized by a lattice constant a. The lattice spacing $a = 1.25$ fm sets the cubic momentum cutoff $p_c = \hbar k_c \approx 860$ MeV$/c$, where $k_c = \sqrt{3}\pi/a$ [7]. For fission of ^{240}Pu, ^{238}Pu and ^{242}Pu, the $(25\text{ fm})^2 \times 50$ fm box is used, which is large enough to determine properties of two separated fission fragments.

The time evolution is performed using the fifth-order Adams–Bashforth–Milne predictor–modifier–corrector method [8]. The number of evolved amplitudes U_μ, V_μ is equal to $4N_{xyz}$, where N_{xyz} is the number of lattice points (factor 4 originates from two spin and two isospin values). This is due to the fact that Bogoliubov transformation, which is defined at each time step, has to fulfill completeness relations and, thus, requires to include all states within the space defined by the lattice. Note that this is in contrast to the static SLDA calculations, where the energy cutoff can be set at much lower energies. In TDSLDA, one can prove that the energy of the system is conserved only when all states are evolved (see Ref. [6] for discussion related to the energy cutoff in TDDFT). In practice, however, if only a short time evolution is required, imposing a lower energy cutoff is enough as the discrepancies occur only after a certain time interval. It is illustrated in Fig. 1, where ^{240}Pu is evolved at $E^* = 8.08$ MeV on a $(22.5\text{ fm})^2 \times 50$ fm lattice for 3 different cutoff energies: 75 MeV (black/dashed line), 100 MeV (green/dotted line), 120 MeV (blue/solid line). The relation between pairing coupling constants for three energy cutoffs is set according to Ref. [10]. Clearly, the discrepancy between these three solutions is cutoff-dependent. However, for short time scales, even a relatively low-energy cutoff is sufficient to obtain accurate solutions.

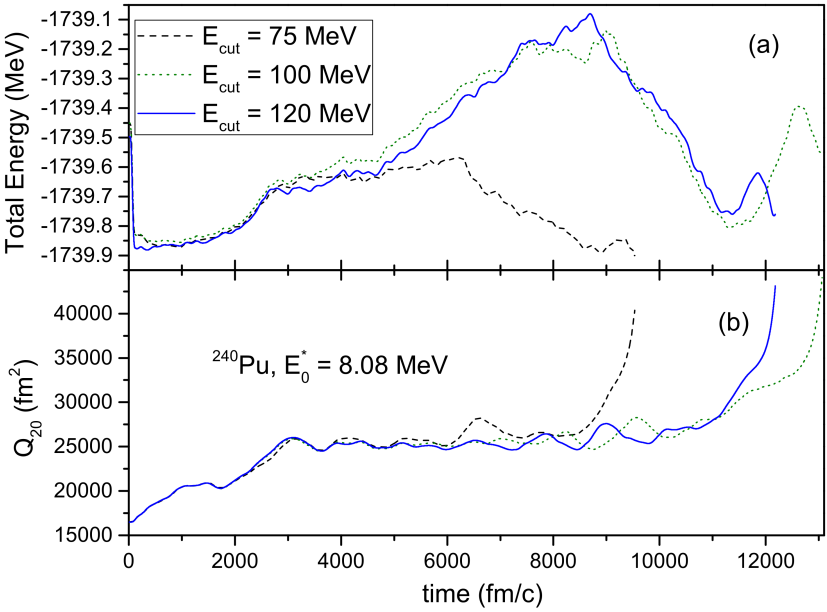

Fig. 1. (Color online) Time evolution of induced fission of ^{240}Pu compound nucleus with pure volume pairing on a $18^2 \times 40$ lattice with a lattice constant of 1.25 fm at $E^* = 8.08$ MeV using a spherical cutoff for 3 different cutoff energies: 75 MeV (black dashed line), 100 MeV (green dotted line), 120 MeV (blue solid line). Subfigure (a) shows total energy as a function of time, and subfigure (b) shows quadrupole Q_{20} moment as a function of time.

In the induced fission studies, however, a long-time evolution is required and, therefore, one needs to include all the states. The pairing coupling constant needs to be renormalized through the relation [9]

$$\begin{aligned} \Delta(\boldsymbol{r}) &= -g_{\text{eff}}\chi(\boldsymbol{r}), \\ \frac{1}{g_{\text{eff}}} &= \frac{1}{g} - \frac{m_{\text{eff}}K}{4\pi\hbar^2 b}, \end{aligned} \tag{2}$$

where χ is the anomalous density, b is the lattice constant and $K = 2.4427496$ is a numerical factor, resulting from the expression:

$$K = \frac{12}{\pi}\int_0^{\pi/4} \mathrm{d}\theta \ln\left(1 + 1/\cos^2\theta\right) \tag{3}$$

as in Ref. [9].

Using the cubic cutoff renormalization and evolving all the states, the energy cutoff $E_{\max} \approx 400$ MeV is three times larger as compared to calculations with spherical cutoff [3] and, therefore, a time step $\Delta t \sim 1/E_{\max}$ for the dynamic calculation needs to be reduced. Consequently, the time step $\Delta t = 0.03$ fm/c ($\approx 10^{-25}$s) turns out to be sufficient to get a stable solutions within the required time interval. The relative error for evolutions with two different time steps is shown in Fig. 2. Namely, the time evolution of ^{242}Pu nucleus at $E^* = 4.90$ MeV for $T < 4000$ fm/c with $\Delta t_0 = 0.03$ fm/c and $\Delta t_0 = 0.024$ fm/c has been plotted. Note that for this case, the total energy difference between the two trajectories with two different time steps is within 1 eV!

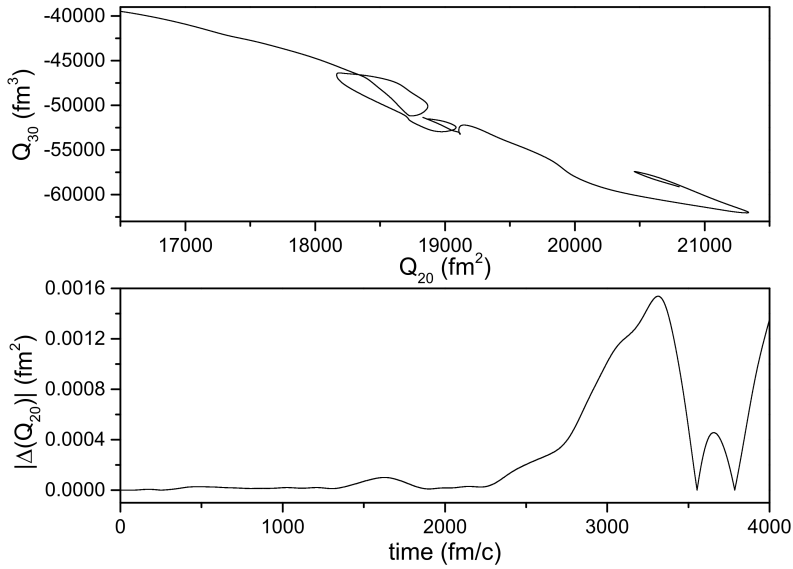

Fig. 2. Time evolution of fissioning ^{242}Pu up to 4000 fm/c. Top: octupole Q_{30} moment as a function of quadrupole Q_{20} moment (time step: $\Delta t = 0.030$ fm/c). Bottom: the differences in the quadrupole moment for two evolutions obtained with time steps: $\Delta t = 0.030$ fm/c and $\Delta t = 0.024$ fm/c.

3. Energy conservation

The initial state for the simulation of the fission process has been prepared by solving the static DFT equations with the constraint, which produced reflection asymmetric shape with a quadrupole moment $q_0 \approx 16\,500$ fm^2. It corresponds to an excited configuration slightly beyond the outer barrier ($q_0 \approx 14\,000$ fm^2). The initial state of ^{240}Pu nucleus is 8.08 MeV

above the ground state and corresponds to the neutron incident energy $E_n = 1.54$ MeV. Analogously, the constrained static solution for ^{238}Pu nucleus is 4.64 MeV above the ground state. The constraint has been released adiabatically, and the number of steps in the saddle-to-scission time evolution is about 300–500 thousand. The average particle number in time-evolution is conserved. The precision of the total energy conservation of the system during the time evolution varies from 0.5 MeV to 3.5 MeV, which is 0.03% to 0.2% of the total energy, respectively (see Fig. 3).

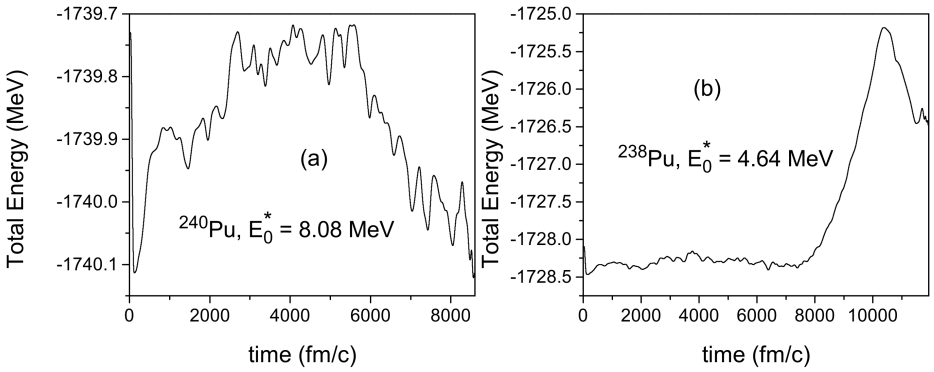

Fig. 3. Total energy as a function of time during saddle-to-scission induced fission. Subfigure (a) shows fission of ^{240}Pu compound nucleus, and subfigure (b) shows ^{238}Pu compound nucleus. Initial states of compound nuclei with a quadrupole constraint $q_0 = 16500$ fm^2 correspond to $E_x = 8.08$ MeV and $E_x = 4.64$ MeV, respectively.

Note that as shown in Fig. 2, top, the fission path for Pu isotopes is not smooth. At various times during evolution, the nucleus rearranges its structure and various internal degrees of freedom are excited along the fission path. When the nucleus keeps rearranging, but cannot find a fission path, the error in total energy keeps increasing and the nucleus does not fission.

4. TKE and excitation energies of the fragments

Within the framework of TDSLDA, one can easily extract the total kinetic energy (TKE) and, hence, the total excitation energy (TXE) of the fragments, as well as the excitation and kinetic energies of each fragment separately. It is one of the main advantages of TDSLDA over those based on adiabatic assumptions or treating internal degrees of freedom within semi-classical approaximation (*e.g.*, based on the Langevin-type equation). TKE of the fragments can be extracted when fragments are well-separated, *i.e.*, at distances larger than 10 fm. The typical accuracy of TKE determination is about 0.5 MeV, that is 0.3 %.

The agreement of TKE with experimental data for ^{239}Pu(n,f) at $E_n < 6\,\mathrm{MeV}$ [11] is within 3.5 MeV, which corresponds to 2% error. For example: TKE ($E_n = 1.54\,\mathrm{MeV}$) = 173.8 MeV (exp. 177.3 MeV), TKE ($E_n = 5.63\,\mathrm{MeV}$) = 176.1 MeV (exp. 175.8 MeV).

5. Conclusions

The superfluid TDDFT in the framework of TDSLDA is a perfect candidate to provide a fully microscopic description of nuclear fission and low-energy nuclear reactions, among other approaches that have been suggested over the years, with various degrees of theoretical assumptions about the character of the fission dynamics (see [12] and references therein). As we discussed above, the method, when applied on a leadership-class supercomputers, is capable to provide results concerning fission like TKE, TXE and provide energy sharing between fragments, *i.e.*, data which can be compared directly to experiment. As discussed above, the accuracy of the description of the fission process within TDSLDA is within 0.1 % of the total energy and the calculated TKE allow for the 0.2% precision. These values can be gradually decreased by employing higher order integration methods and smaller lattice constants.

Authors acknowledge support of the National Science Centre, Poland (NCN) grants: decision No. DEC-2013/08/A/ST3/00708 and UMO-2016/23/B/ ST2/01789. We acknowledge PRACE for awarding us access to resource Piz Daint based in Switzerland at the Swiss National Supercomputing Centre (CSCS), decision No. 2016153479. We also acknowledge Interdisciplinary Centre for Mathematical and Computational Modelling (ICM) of the University of Warsaw for computing resources at Okeanos (grant No. GA67-14).

REFERENCES

[1] A. Bulgac, S. Yoon, *Phys. Rev. Lett.* **102**, 085302 (2009); A. Bulgac *et al.*, *Science* **332**, 1288 (2011); A. Bulgac, M.M. Forbes, G. Wlazłowski, *J. Phys. B* **50**, 014001 (2017).

[2] I. Stetcu, A. Bulgac, P. Magierski, K.J. Roche, *Phys. Rev. C* **84**, 051309 (2011); I. Stetcu *et al.*, *Phys. Rev. Lett.* **114**, 012701 (2015); P. Magierski, K. Sekizawa, G. Wlazłowski, *Phys. Rev. Lett.* **119**, 042501 (2017).

[3] A. Bulgac, P. Magierski, K.J. Roche, I. Stetcu, *Phys. Rev. Lett.* **116**, 122504 (2016).

[4] G. Wlazłowski *et al.*, *Phys. Rev. Lett.* **117**, 232701 (2016).

[5] D.M. Brink, R.A. Broglia, *Nuclear Superfluidity: Pairing in Finite Systems*, Cambridge University Press, 2005; J. Sadhukhan *et al.*, *Phys. Rev. C* **90**, 061304 (2014).

[6] P. Magierski, in "Progress of Time-dependent Nuclear Reaction Theory", ed. Yoritaka Iwata in the ebook series: "Frontiers in Nuclear and Particle Physics", Bentham Science Publishers [arXiv:1606.02225 [nucl-th]; P. Magierski, J. Grineviciute, K. Sekizawa *Acta Phys. Pol. B* **49**, 281 (2018), this issue.

[7] A. Bulgac, M.M. Forbes, *Phys. Rev. C* **87**, 051301 (2013).

[8] R. Hamming, *Numerical Methods for Scientists and Engineers*, New York: Dover Publications, 2012, p. 408.

[9] W. Zwerger, ed., *The BCS-BEC Crossover and the Unitary Fermi Gas*, Springer, Berlin 2012, Vol. **836**.

[10] A. Bulgac, Y. Yu, *Phys. Rev. Lett.* **88**, 042504 (2002); A. Bulgac, *Phys. Rev. C* **65**, 051305 (2002).

[11] N.I. Akimov *et al.*, *Sov. J. Nucl. Phys.* **13**, 272 (1971).

[12] J. Sadhukhan, W. Nazarewicz, N. Schunck, *Phys. Rev. C* **93**, 011304(R) (2016); P. Goddard, P. Stevenson, A. Rios, *Phys. Rev. C* **92**, 054610 (2015); **93**, 014620 (2016); D. Regnier, N. Dubray, N. Schunck, M. Verriere, *Phys. Rev.C* **93**, 054611 (2016); Y. Tanimura, D. Lacroix, S. Ayik, *Phys. Rev. Lett.* **118**, 152501 (2017).