Boost-invariant mean field approximation and the nuclear Landau-Zener effect

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We investigate the relation between time-dependent Hartree-Fock (TDHF) states and the adiabatic eigenstates by constructing a boost-invariant single-particle Hamiltonian. The method is numerically realized within a full three-dimensional TDHF which includes all the terms of the Skyrme energy functional and without any symmetry restrictions. The study of free translational motion of a nucleus demonstrates the validity of the concept of boost-invariant and adiabatic TDHF states. The interpretation is further corroborated by the test case of fusion of ^{16}O $+^{16}$ O. As a first application, we present a study of the nuclear Landau-Zener effect on a collision of ^{4}He $+^{16}$ O.

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I. INTRODUCTION

The time-dependent Hartree-Fock (TDHF) approximation, originally proposed by Dirac [1], has found widespread application in nuclear dynamics for more than 30 years [2]. It provides the microscopic foundation for describing various dynamical scenarios in the regime of large amplitude collective motion. Soon after its introduction to nuclear physics, the TDHF approximation was extensively applied to studies of fusion excitation functions, fission, deep-inelastic scattering, collective excitations, and nuclear molecular resonances. These studies shed light on several mechanisms of heavy-ion collisions and resonance dynamics. Reviews on these earlier TDHF applications can be found, e.g., in Refs. [3,4].

At that time, however, limited computer capacity restricted most calculations to axial symmetry and omission of spin-orbit coupling. These limitations turned out to be a hindrance for the development. For example, earlier TDHF calculations underestimated the energy dissipation from the collective kinetic energy into internal excitations so that the energy window of fusion reactions was too small in comparison with experiments. Later work demonstrated that the spin-orbit coupling [5,6] and fully three-dimensional geometry [7–9] enhance dissipation. None of these calculations, however, was able to include all constituents simultaneously. With the steady upgrade of computational power, three-dimensional TDHF calculations employing the full Skyrme force became possible and renewed the interest in nuclear TDHF as seen from recent publications on resonance dynamics [10–14] and heavy-ion collisions [15–18]. One expects that the new generation TDHF calculations may yield more realistic features for heavy-ion collisions at low and medium energies and for resonance dynamics. This revives old questions that have been left unanswered for a while, one of which is the subject of this paper: the analysis of heavy-ion collisions as computed by TDHF in terms of adiabatic states and level-crossing dynamics.

Nucleus-nucleus collisions present different behavior depending on the delicate balance of reaction time and rearrangement time of the mean field. For example, the experimentally observed resonancelike peaks in the inelastic cross sections are explained in terms of the well-known Landau-Zener excitation due to a breakdown of the adiabaticity condition near an avoided level crossing. The Landau-Zener mechanism was first introduced into nuclear physics in Ref. [19]. The Landau-Zener effect and its applications to heavy-ion collisions have been discussed [20–22] in terms of the asymmetric two-center shell model (TCSM) [23], employing the assumption that the nucleons can be described with adiabatic "molecular" states, i.e., the instantaneous eigenstates of the deformed mean field, during the heavy-ion reaction. A review on Landau-Zener dynamics and experimental data in nuclear molecules may be found in Refs. [24,25].

TDHF calculations, however, have never been analyzed in terms of the Landau-Zener effect because their single-particle states and energies have no simple physical interpretation and a construction of corresponding adiabatic states was not readily available. There were early attempts to define a related adiabatic basis by means of density-constrained Hartree-Fock [26,27]. These turned out to be very promising, lacking, however, at that time the exact treatment of the flow contributions. Improved computing power now allows us to revisit the case without technical restrictions. We thus will present here a self-consistent scheme to define and compute two useful analyzing instruments for a given TDHF state: instantaneous single-particle energies and instantaneous adiabatic states. The straightforward expectation values of the single-particle Hamiltonian turn out to be blurred by trivial flow contributions. To take into account the effect of motion on the single-particle wave functions, we define a single-particle Hamiltonian which is invariant under Galilei transformation, in particular under a boost. We call that the boost-invariant Hamiltonian. This dramatically reduces the energy variances of the actual TDHF states, providing better-defined single-particle energies. Moreover, the (instantaneous) eigenstates and energies of the boost-invariant Hamiltonian provide a well-defined adiabatic basis. For example, the single-particle states in free translational motion are exact eigenstates of this boost-invariant Hamiltonian and its expectation values remain the static single-particle energies. While this property is not exact anymore in a situation of two colliding nuclei, we shall demonstrate that this method nevertheless allows us to define meaningful single-particle energies and variances

thereof. Moreover, one can establish an approximate relation of the time-dependent solutions to the adiabatic deformation-dependent spectrum. As a first application we study the Landau-Zener effect in heavy-ion collisions.

The paper is organized as follows: Section II briefly recalls the Skyrme energy functional and TDHF. In Sec. III, we construct a boost-invariant Hamiltonian and test its validity for free translational motion of a nucleus. Section IV applies the newly developed scheme to the analysis of level crossings in heavy-ion collisions. Section V is devoted to the summary and conclusions.

II. COMMENTS ON TDHF WITH SKYRME FORCES

Most nuclear TDHF calculations by far are based on the Skyrme energy functional; for a recent extensive review, see Ref. [28]. It is also used in the present applications. The starting point is the Skyrme energy-density functional $\mathcal{E}_{Sk} = \mathcal{E}(\rho, \tau, \vec{\sigma}, \vec{j}, \vec{J})$, which is expressed in terms of a few local densities and currents: density ρ, kinetic density τ, spin density $\vec{\sigma}$, current $\vec{j}$, and spin-orbit density $\vec{J}$. It includes free kinetic energy, Skyrme interaction, Coulomb energy, and the center-of-mass correction. The pairing energy is ignored here, as we will deal with collisions of closed-shell nuclei. There are various parametrizations of the Skyrme force [28]. Since the present study is concerned with fundamental effects which should not depend on the detailed force used, we thus chose just one parametrization out of many, namely, the force SLy6 [29] which is widely used and provides a reliable description of nuclear structure and dynamics.

Using the principle of least action and varying with respect to the single-particle state φ_α^*, we obtain the TDHF equations (in the following, units with $\hbar = 1$ are used)

$$\mathrm{i}\partial_t \varphi_\alpha = \hat{h}(\rho, \tau, \vec{\sigma}, \vec{j}, \vec{J})\varphi_\alpha, \tag{1}$$

where $\hat{h}$ is the time-dependent mean field Hamiltonian depending on the occupied single-particle wave functions through densities and currents. Given the initial conditions, $\{\varphi_\alpha(\vec{r}, t = 0)\}$, the TDHF equations (1) determine the wave functions for all later times. In the stationary limit, we obtain the static mean field equation

$$\hat{h}\varphi_\alpha = \varepsilon_\alpha \varphi_\alpha, \tag{2}$$

where the single-particle energies ε_α appear naturally as eigenvalues of the mean field Hamiltonian $\hat{h}$. The question is how to generalize the definition of the single-particle energy to TDHF. The naive definition is to use the expectation value of the instantaneous mean field $\hat{h}(t)$. This, however, raises difficulties, as we will see. Possible improvements will be developed in the sequel.

A few words on the numerical solution are in order. The set of nonlinear TDHF equations is solved on a three-dimensional Cartesian coordinate-space grid employing a Fourier representation for the derivatives. All contributions of the full Skyrme force were included and no symmetry restrictions imposed. The coordinate-space grid consists of $24 \times 24 \times 24$ points with a grid spacing of 1 fm. For the dynamical time stepping, we use a Taylor series expansion of the unitary mean field propagator up to sixth order [8] and a time step of 0.2 fm/c. These numerical parameters provide good conservation of particle number and total energy during the dynamic evolution. The static HF equations were solved with the damped gradient iteration method [30,31].

III. SINGLE-PARTICLE ENERGIES IN A MOVING FRAME

A. Adiabatic expansion as a propaedeutic example

Adiabatic single-particle states are eigenstates of a single-particle Hamiltonian for a given set of deformation parameters. For a first introduction, we will discuss that concept in this section on the grounds of a given, properly parametrized, single-particle Hamiltonian, such as, e.g., that of the TCSM [23]. Such a Hamiltonian usually depends on a few collective deformation parameters which characterize the wanted reaction path. For simplicity, let us just deal with internuclear distance R as the sole such parameter and skip trivial complications such as spin and isospin. The proper choice of an R-dependent single-particle potential $V(\vec{r}; R)$ and the subsequent solution of the eigenvalue problem yield a set of adiabatic single-particle states $\phi_k(\vec{r}; R)$ and corresponding eigenenergies $\epsilon_k(R)$. Using the adiabatic single-particle states, we expand the time-dependent (but still independent-particle) solution as

$$\psi_j(\vec{r}, t) = \sum_k c_{jk}(t)\phi_k(\vec{r}; R(t))e^{-\mathrm{i}\int_{t'}^{t} dt' \epsilon_k[R(t')]}. \tag{3}$$

Such an expansion underlies, e.g., the cranking model [32,33]. This expansion has the problem that it relies on a stationary basis in which the current vanishes for all states. Any flow has to be described through the complex expansion coefficients c_{jk}. This limits the ansatz (3) to extremely slow motion.

An instructive example is the uniform center-of-mass translation of an unexcited nucleus with velocity $\vec{v} = \vec{p}/m$. It is described by coherently moving single-particle states $\psi_k(\vec{r}, t) = \phi_k(\vec{r} - \vec{v}t)\exp(\mathrm{i}(\vec{k} \cdot \vec{r} - \epsilon_k t))$. Clearly, the trivial plane-wave factor which produces the correct flow is missing from the basis states in Eq. (3). It has to be reconstructed laboriously by the expansion coefficients. A much more efficient description could be obtained by properly extending the scheme to a dynamic basis $\phi_k(\vec{r}; R, \dot{R})$ which already accounts for collective flow. This step was found to be crucial for the derivation of microscopic theories for collective motion in the framework of adiabatic TDHF [34]. We will now use the extension for the definition of adiabatic reference states in TDHF. The example of center-of-mass motion will be used as guidance.

B. Flow-induced variances

We will now discuss the case of self-consistent mean fields. To simplify the formal considerations, we restrict the discussion to one spatial dimension and think in terms of the simplest energy functional $\mathcal{E} = \mathcal{E}(\rho)$ depending only on the

local density and producing a purely local mean field, i.e.,

$$\hat{h}[\rho] = \frac{\hat{p}^2}{2m} + U(x,t), \quad U(x,t) = \frac{\delta \mathcal{E}}{\delta \rho(x,t)}, \tag{4}$$

where U is obtained from $\mathcal{E}$ by functional derivation. The ground-state wave functions $\{\varphi_{0,\alpha}\}$ fulfill the equations

$$(\hat{h}_0 - \varepsilon_\alpha)\varphi_{0,\alpha}(x) = 0, \tag{5}$$

with ε_α being the static single-particle energies.

As a test case, consider center-of-mass motion of the HF ground state. The motion is initialized by a boost with total momentum $P = MV$ where V is the velocity of the center of mass and $M = Nm$ the total mass. The same boost is applied to all single-particle wave functions

$$\varphi_{0,\alpha} \to \varphi_\alpha(x,t) = e^{\mathrm{i}P\hat{x}/N}\varphi_{0,\alpha}(x - Vt)e^{-\mathrm{i}\tilde{\varepsilon}_\alpha t}, \tag{6a}$$

$$\tilde{\varepsilon}_\alpha = \varepsilon_\alpha + \frac{P^2}{2M}. \tag{6b}$$

The local density is then propagated with velocity V as $\rho(x,t) = \rho_0(x - Vt)$, and this, in turn, carries through to the mean field motion as $U(x,t) = U_0(x - Vt)$. The boosted wave functions together with the similarly moving mean field are the solution of the TDHF equations (1). The action of the mean field on the boosted wave function can be expressed in terms of the static solution as

$$\hat{h}\varphi_\alpha = e^{\mathrm{i}P\hat{x}/N}e^{-\mathrm{i}\tilde{\varepsilon}_\alpha t}\left(\tilde{\varepsilon}_\alpha + \frac{P}{M}\hat{p}\right)\varphi_{0,\alpha}. \tag{7}$$

The expectation value is simply $\langle\varphi_\alpha|\hat{h}|\varphi_\alpha\rangle = \tilde{\varepsilon}_\alpha$. Both together allow evaluation of the variance of the single-particle Hamiltonian explicitly as

$$\langle\varphi_\alpha|\Delta\hat{h}^2|\varphi_\alpha\rangle = \frac{P^2}{M^2}\langle\varphi_{0,\alpha}|\hat{p}^2|\varphi_{0,\alpha}\rangle. \tag{8}$$

It is obvious that the moving wave function φ_α is not an eigenstate of the instantaneous mean field Hamiltonian $\hat{h}$. The variance grows quadratically with the boost momentum P, i.e., proportionally to the center-of-mass energy. The expectation value $\tilde{\varepsilon}_\alpha$ also becomes misleading. The kinetic contribution makes the binding properties invisible. This problem was already noticed by Thouless and Valatin [35] while they were studying Galilean invariance of the TDHF equation.

C. Construction of a boost-invariant mean field

The above example of center-of-mass motion is instructive. The variance of the mean field Hamiltonian grows, although we know that the system remains intrinsically unaltered. All that happens is a trivial kinematical effect. Thus there should be ways to undo it equally trivially. In the center-of-mass case, we could simply transform the single-particle momentum into the intrinsic frame as $\hat{p} \to \hat{p} - P/N$ and use that in the kinetic energy operator. That indeed provides a reasonable boost-invariant Hamiltonian for that particular case. A generalization can be obtained with the concept of the local momentum distribution $\bar{p}(x)$ as given by the local current $j(x)$. This suggests the definition of a locally boost-invariant momentum

$$\hat{p} \to \hat{p}_{\mathrm{inv}} = \hat{p} - \bar{p}(x), \quad \bar{p}(x) = \frac{j(x)}{\rho(x)}, \tag{9}$$

which can be extended to a boost-invariant kinetic-energy density $\tau_{\mathrm{inv}} = \sum_\alpha |\hat{p}_{\mathrm{inv}}\varphi_\alpha|^2 = \tau - j^2/\rho$. It is interesting to note that this is practically the Galilean-invariant combination $\tau\rho - j^2$ of kinetic contributions in the interaction part of the Skyrme energy functional [28,36]. This gives confidence in the above generalization.

The idea thus is to define an "intrinsic" energy functional by replacing the kinetic energy $\propto \int d^3r\,\tau$ by the boost-invariant kinetic energy

$$E_{\mathrm{kin,inv}} = \frac{1}{2m}\int dx \left(\tau - \frac{j^2}{\rho}\right). \tag{10}$$

The potential energy was already boost-invariant, and thus the total functional becomes so. This functional is to be used for the purpose of analysis only, and it plays no role for the computation of the time evolution as such. Variation leads to the corresponding boost-invariant mean field Hamiltonian

$$\hat{h}_{\mathrm{inv}} = \frac{\hat{p}^2}{2m} + U(x,t) - \frac{1}{2m}\left\{\frac{j(x)}{\rho(x)}, \hat{p}\right\} + \frac{j^2(x)}{2m\rho^2(x)}, \tag{11}$$

where $\{\ldots,\ldots\}$ is the anticommutator and $U(x,t)$ the usual time-dependent mean field potential. The first two terms are exactly the same as in the usual TDHF Hamiltonian, and the last two stem from the boost-invariant kinetic energy. The corrected Hamiltonian then defines a boost-invariant single-particle energy

$$\varepsilon_\alpha^{(\mathrm{inv})} = \langle\varphi_\alpha|\hat{h}_{\mathrm{inv}}|\varphi_\alpha\rangle. \tag{12}$$

Next we will show that the boost-invariant Hamiltonian has the boosted TDHF wave functions as eigenstates in the case of free translation.

D. Test case: Free translational motion

The construction of the boost-invariant Hamiltonian (11) was guided by the example of free center-of-mass translation, so that the natural test case is the global center-of-mass boost (6a). In that case, the local momentum distribution is given by

$$\bar{p}(x) = \frac{j(x)}{\rho(x)} = \frac{P}{N} = \text{const.}, \tag{13}$$

while the boost-invariant Hamiltonian reduces to

$$\hat{h}_{\mathrm{inv}} = \frac{\hat{p}^2}{2m} + U(x,t) - \frac{P}{M}\hat{p} + \frac{P^2}{2M}, \tag{14}$$

and finally the expectation value of the boost-invariant Hamiltonian and its variance become

$$\langle\varphi_\alpha|\hat{h}_{\mathrm{inv}}|\varphi_\alpha\rangle = \epsilon_\alpha, \tag{15a}$$

$$\langle\varphi_\alpha|\Delta\hat{h}_{\mathrm{inv}}^2|\varphi_\alpha\rangle = 0, \tag{15b}$$

where ε_α are the static single-particle energies.

The zero variance means that the boosted TDHF wave function φ_α according to Eq. (6a) is an eigenstate of the boost-invariant Hamiltonian $\hat{h}_{\rm inv}$, and its eigenvalue remains static solution ε_α as defined in Eq. (5).

These results for free translation suggest the boost-invariant Hamiltonian $\hat{h}_{\rm inv}$ as an appropriate instrument for analyzing the single-particle states of TDHF. The single-particle energies computed as expectation values of the boost-invariant Hamiltonian (11) can be considered as "intrinsic" single-particle energies representing the actual binding independent from trivial kinematical contributions. It is to be noted that these equations are also applicable for a nonlocal mean field Hamiltonian such as the Skyrme force.

The practical computation of the boost-invariant Hamiltonian is a bit demanding because of the density in the denominator. Nevertheless, for free translation of the nucleus ^{16}O we achieve variances of about 0.02–0.05 MeV and expectation values stay within $10^{-4} \sim 10^{-5}$ MeV of the static ones with the full three-dimensional TDHF which includes all the terms of the Skyrme energy functional and without any symmetry restrictions.

E. Adiabatic states

True intrinsic excitations in more general dynamical situations add some energy variance to the TDHF states. The eigenstates of the instantaneous boost-invariant Hamiltonian,

$$\hat{h}_{\rm inv}\phi_i = \varepsilon_i^{\rm (adia)}\phi_i, \tag{16}$$

then become something different. They correspond to some extent to the adiabatic states, and we will therefore use the expressions "adiabatic states" and "adiabatic energies" in the following. A given TDHF state φ_α imbued with some intrinsic excitation is distributed over the adiabatic basis $\{\phi_i\}$. This can be quantified through the adiabatic occupation probability

$$P_i^{\rm (occ)} = \sum_{\alpha\in{\rm occ}} |\langle\varphi_\alpha|\phi_i\rangle|^2, \tag{17}$$

where the sum runs over the occupied TDHF states φ_α. That quantity is the probability to find the state ϕ_i occupied when expanding the actual TDHF Slater state into the adiabatic basis. Complementarily we have the hole probability $P_i^{\rm (unocc)} = 1 - P_i^{\rm (occ)}$. The occupation probability quantifies in its way the amount of intrinsic excitation carried in the TDHF states. The value of unity means no excitation at all for states of the adiabatic basis below the Fermi level, and lowering below unity is closely related to excitation.

IV. ANALYSIS OF HEAVY-ION COLLISIONS

A. Level schemes

For the investigation of heavy-ion collisions, the wave functions of the two fragments are placed symmetrically on the grid 5 fm off the center of box and then boosted to the desired relative center-of-mass energies. This is the initial state for TDHF dynamical propagation. Besides the calculation of the usual TDHF states $\{\varphi_\alpha\}$ of the colliding system, diagonalization of the boost-invariant Hamiltonian gives the adiabatic single-particle energies and wave functions $\{\phi_i\}$. It should be noted that in a collision situation, the boost-invariant Hamiltonian cannot be expected to eliminate the kinetic effects completely, because it depends on the *local* conditions. It is hoped, however, that for the initial stages of the interaction the behavior of the levels can still be extracted. For the symmetric system, parity projection has been done for the boost-invariant wave functions.

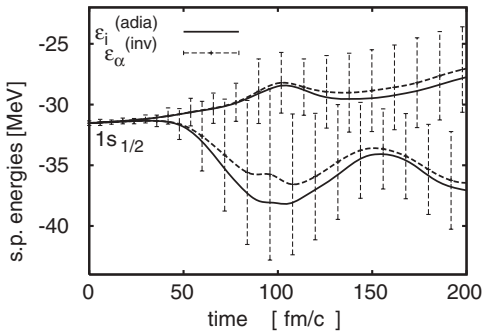

FIG. 1. Time evolution of boost-invariant and adiabatic observables for a central ^{16}O+^{16}O collision at 25 MeV. The dashed lines with error bars show the boost-invariant single-particle energies $\varepsilon_\alpha^{\rm (inv)}$ and their variances $\Delta\varepsilon_\alpha^{\rm (inv)}$ for the lowest ($1s_{1/2}$) proton states, and solid lines the adiabatic energies $\varepsilon_i^{\rm (adia)}$ for comparison.

To illustrate the performance of boost-invariant and adiabatic states, Fig. 1 shows a typical result for the splitting of an initially highly degenerate state during a heavy-ion reaction. The test case is a central ^{16}O+^{16}O collision with center-of-mass energy of 25 MeV. Shown are the two lowest levels (the proton $1s_{1/2}$ levels in the right and left collision partner). The first few fm/c show the initial phase with nearly free c.m. motion of the two nuclei toward each other. Boost-invariant and adiabatic states remain identical, and the energy variance is zero within the limit of numerical precision. The nuclei start to interact around 30 fm/c. At this time, the initially degenerate $1s_{1/2}$ states split into two levels, as expected. The way the levels split into the various substates is very similar to what is expected from a two-center approach as in Ref. [23]. At the same time, the energy variance of the boost-invariant states grows, because the collision mixes forward with backward flow such that we have an increasing spread of flow around its decreasing average. It is to be noted that the variances of the boost-invariant Hamiltonian are much smaller than those of the usual TDHF Hamiltonian. The latter comes up to several tens of MeV, clearly showing that the single-particle energies from the TDHF states have no meaning at all. Furthermore, the boost-invariant energies become slightly larger than the adiabatic ones, which expresses the amount of true intrinsic excitation piling up in the boost-invariant states. It is very satisfying to see that the energy difference is proportional to the variance of the boost-invariant states. The signals confirm each other as measure for intrinsic excitation, and they give credibility to both forms of energy expectation values. Altogether, Fig. 1 clearly demonstrates the usefulness of the

concept and the relation between the boost-invariant states containing local flow and the quasistationary adiabatic states.

Figure 2 shows the time evolution of the other occupied proton states in our example of a $^{16}O + ^{16}O$ collision. As for the $1s_{1/2}$ levels above, we again see the splitting of the asymptotically degenerate states $1p_{3/2}$ and $1p_{1/2}$ with increasing interaction. The difference between adiabatic and boost-invariant energies indicates the degree of internal excitation. It can be very different for the different states. It is, e.g., somewhat surprising that the lower state (left panels) acquires excitation rather early, while some higher states wait for much longer. The lower panels of Fig. 2 show the occupation probabilities (17). They start at unity as they should for a yet unexcited state where adiabatic and boost-invariant states are still identical. Their subsequent decrease reflects the degree of intrinsic excitation. The two indicators for intrinsic excitation, occupation probability and difference $\varepsilon^{(\mathrm{inv})} - \varepsilon^{(\mathrm{adia})}$, agree nicely for all states shown. The adiabatic energies in the upper panels of Fig. 2 show the interesting phenomenon of level crossings, quite similar to that observed in former studies using deformed shell models [20–23]. The arrows connect these points with the lower panels where the occupation probabilities seem to jump. But that is merely a labeling effect when sorting the states always according to adiabatic energy. Following the states diabatically through the crossings would produce smooth evolution of energies and occupation probabilities. Such a diabatic tracking, however, is only possible if we ignore pairing, as we do here. Inclusion of pairing would smoothen the crossings and enforce adiabatic tracking with subsequent "smooth jumps" in the observables.

B. Landau-Zener effect

As mentioned in the Introduction, reactions of complex many-body systems like nuclei or molecules often produce the Landau-Zener effect. It happens at level crossings with only small coupling between the two energetically close levels. There is a competition between the speed with which the levels evolve and the time necessary for the rearrangement of the occupations. Very slow motion leaves sufficient time such that always the energetically lower level is fully occupied. That is the adiabatic limit. Increased velocity causes transitions (= diabaticity) where the occupation partially crosses over into the then higher level, thus turning collective energy to internal excitation. That is the much celebrated Landau-Zener effect. In this section, we will employ the boost-invariant and adiabatic states as analyzing tools to a study of the Landau-Zener effect in a self-consistent mean field description of heavy-ion collisions. For this purpose an asymmetric reaction is more appropriate, and we select a head-on collision of $^{4}He + ^{16}O$.

Figure 3(a) shows the rms radius of the colliding system as a function of time. It is clear that both the collisions with 75 and 125 MeV are deep-inelastic scattering. The adiabatic occupation probability as defined in Eq. (17) for the last occupied neutron state labeled at initial stage as $1p_{1/2}$ is presented in Fig. 3(b). The assignment "occ." and "unocc." in Fig. 3 refers to the situation in the initial stage, while in the colliding region the adiabatic occupation probability gives information on the actual occupation.

The occupation probability is, of course, nearly unity during the initial stage of nearly free translation and starts decreasing as the two colliding nuclei approach each other.

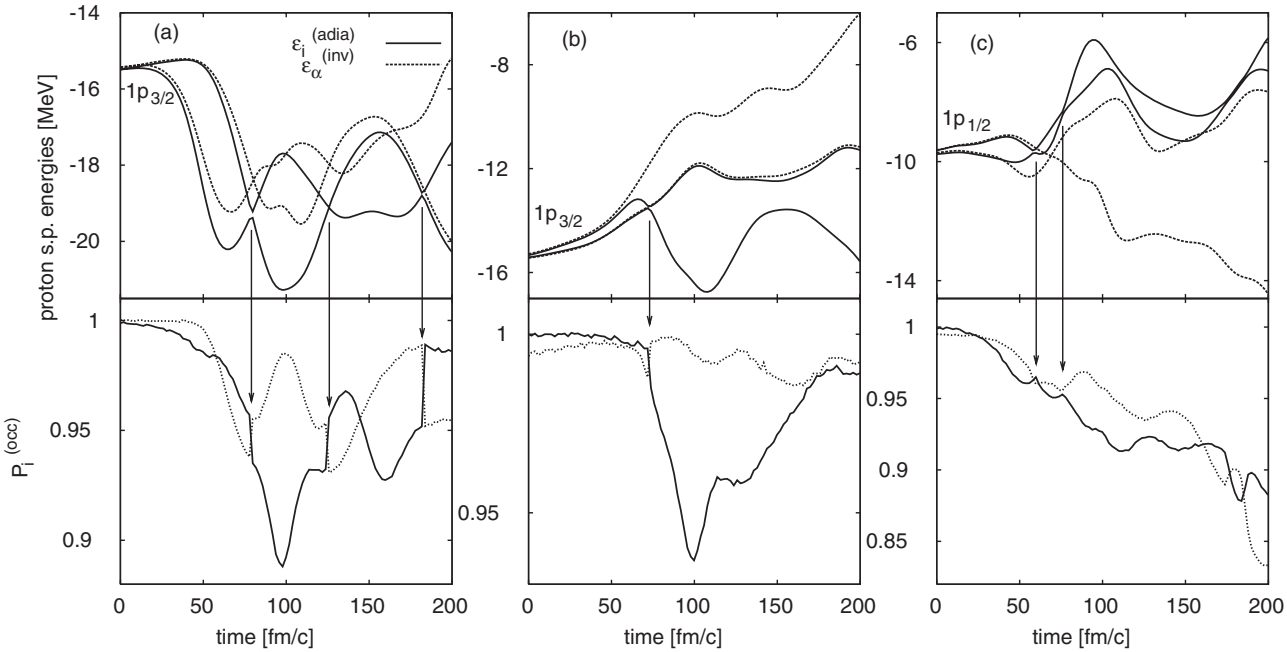

FIG. 2. Time evolution of higher lying proton states for a central collision of $^{16}O + ^{16}O$ with a center-of-mass energy of 25 MeV. The upper panels show the boost invariant single-particle energies $\varepsilon_\alpha^{(\mathrm{inv})}$ (dashed) and the adiabatic energies $\varepsilon_i^{(\mathrm{adia})}$ (full lines). The lower panels show the corresponding adiabatic occupation probabilities. The arrows pointing from the upper panels to the lower ones indicate the level crossings where occupation changes rapidly. The labels of the single-particle states at $t = 0$ are indicated near the left axis.

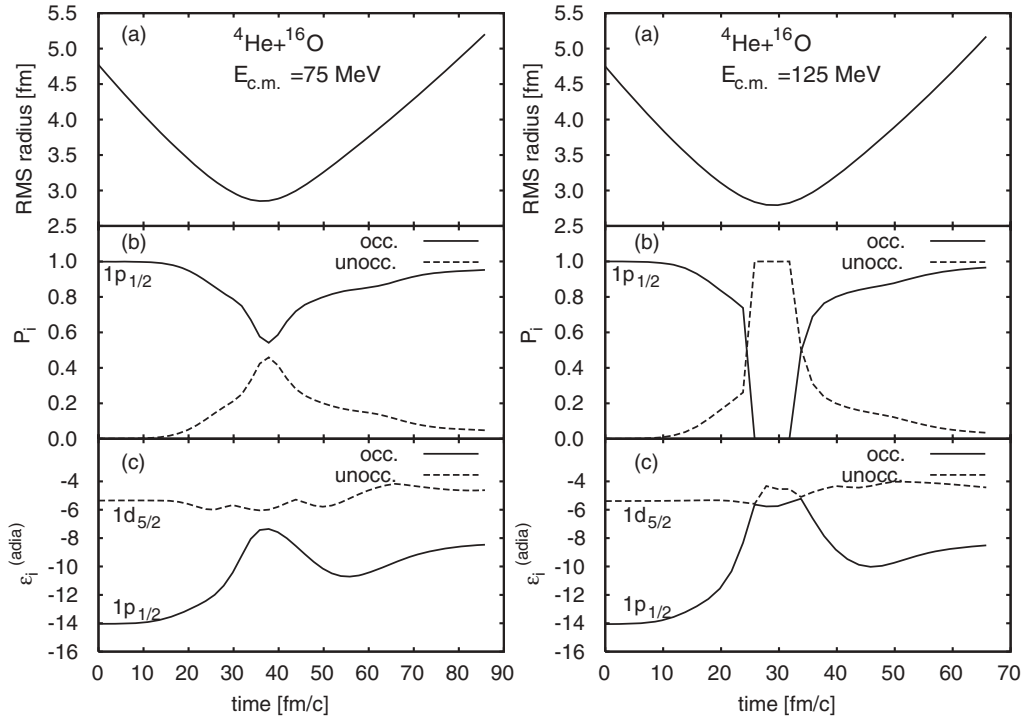

FIG. 3. Time evolution of the central collision of ^{4}He $+^{16}$O with c.m. energies of 75 and 125 MeV. (a) rms radius for the colliding system as a function of time; (b) adiabatic occupation probability P_i of the last occupied neutron state; and (c) interacting single-particle adiabatic states. The labels of the single-particle states at $t = 0$ are near the left axis.

It then increases again and finally returns to nearly unity, not quite attaining it owing to the small transfer and evaporation probabilities after the separation. The corresponding adiabatic single-particle energies of the highest-lying occupied and the lowest-lying unoccupied neutron states, labeled at the initial stage as $1p_{1/2}$ and $1d_{5/2}$, respectively, are shown in Fig. 3(c). In the initial stage of dynamic propagation, the adiabatic single-particle energies are almost the same as those of the static ground states (realized exactly at $t = 0$).

This behavior is easy to understand since the boost-invariant and adiabatic states only reflect the excitation and interaction of colliding nuclei. The two adiabatic states display the feature of avoided crossing around the smallest distance of two colliding nuclei. The same feature also appears in the adiabatic occupation probability. The right panel with larger bombarding energy of 125 MeV shows that the mixing of occupied and unoccupied components in the colliding stage becomes much stronger such that the occupied and unoccupied states are exchanged completely. Since the two interacting single-particle states belong to the nucleus ^{16}O, we find that two neutrons are excited from the uppermost occupied state to the lowest unoccupied state. This excitation is activated gradually with increasing incident energy. This is a clear signal of a nuclear Landau-Zener transition in the TDHF description of a deep inelastic collision.

V. SUMMARY

In this work, we have constructed a boost-invariant single-particle Hamiltonian to eliminate the dynamically induced variances coming from the local velocity field in TDHF. For the case of free translational motion of a nucleus, the boost-invariant Hamiltonian produces eigenstates which have zero dynamical variances and reproduce the stationary single-particle energies. In the case of a reaction, true intrinsic excitations take place, and the TDHF states do not remain eigenstates of the boost-invariant Hamiltonian anymore. Their variances then become a measure of intrinsic excitation, and the expectation values still remain useful measures of single-particle energies. Moreover, the eigenstates of the boost-invariant Hamiltonian can be considered as the (instantaneous) adiabatic states which contain no flow. The relation between boost-invariant and adiabatic single-particle energies is also related to the intrinsic excitation energy, similar to the energy variances. As a further measure of excitation, we introduce occupation probabilities, i.e., the probabilities to find a given adiabatic state within the space of occupied TDHF states. Adiabatic states and occupation probabilities serve as analyzing tools, e.g., to investigate the nuclear Landau-Zener effect within self-consistent mean field models. The scheme has been implemented numerically in fully three-dimensional TDHF without any symmetry restrictions and with all the terms of the Skyrme energy functional included.

Two test cases of head-on collisions were considered, fusion of the ^{16}O+^{16}O system at low scattering energy and deep inelastic scattering of ^{4}He+^{16}O. The newly defined boost-invariant and adiabatic single-particle energies show the expected behaviors. For the symmetric ^{16}O+^{16}O system, the splitting of the asymptotically degenerate levels in the interaction regime is clearly seen. In both cases, one finds the

mutually complementing signals for intrinsic excitation and, in particular, several nicely developed level crossings with, in the case of ^{4}He+^{16}O, all signatures of a nuclear Landau-Zener effect. The trend from more adiabatic evolution at low energies to clean diabatic transitions at high collisional energy, e.g., is clearly apparent.

These first results are very encouraging. The boost-invariant Hamiltonian with its single-particle energies and the corresponding adiabatic basis are promising tools for analyzing TDHF simulations of heavy-ion reactions and understanding their relation to the other widely used time-dependent method based on single-particle orbitals, the expansion in the adiabatic basis.

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