Boost-invariant TDHF theory and the nuclear Landau-Zener effect

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- New generation 3D code
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Brief review of TDHF theory

- Method originally proposed by Bonche, Koonin, and Negele, Phys. Rev. C13, 1226 (1976)

  fusion and fission, deep-inelastic collisions, nuclear molecules, collective excitation and resonance dynamics

- many groups in the late ‘70s and ‘80s performed more extensive calculations in 2 and 3 dimensions, limited by the computers of the time, e.g.,

  K. T. R. Davies, V. Maruhn-Rezvani, K. R. Sandhya-Devi, S. J. Krieger, J. A. M.

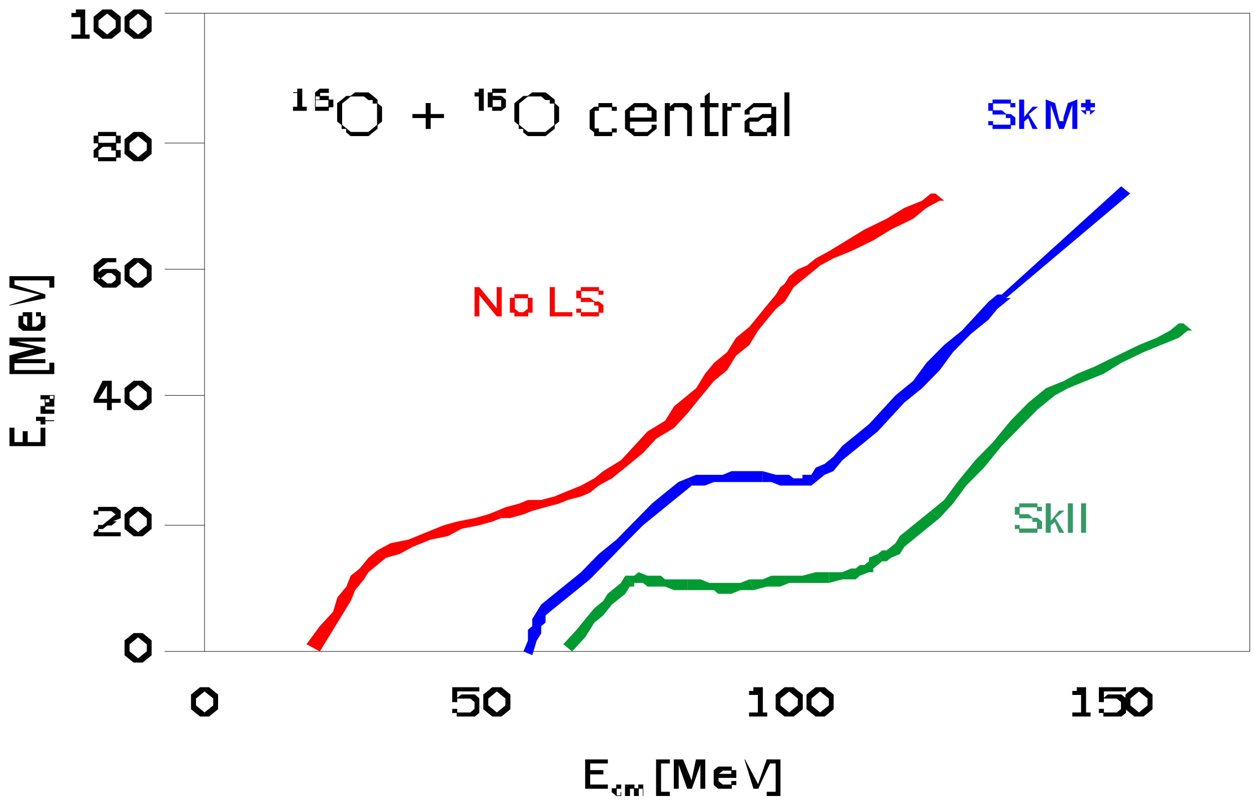
  R. Y. Cusson, H. Stöcker, J. A. M.

  H. Flocard, M. S. Weiss

mostly calculation in 2D axial geometry,
no l*s-force (essential for correct shell structure) ⇒ **hindrance**

Spin-orbit coupling solved puzzle of small fusion window

Omission of l*s-coupling underestimated the energy dissipation so that the energy window of fusion reactions was too small in comparison with experiments



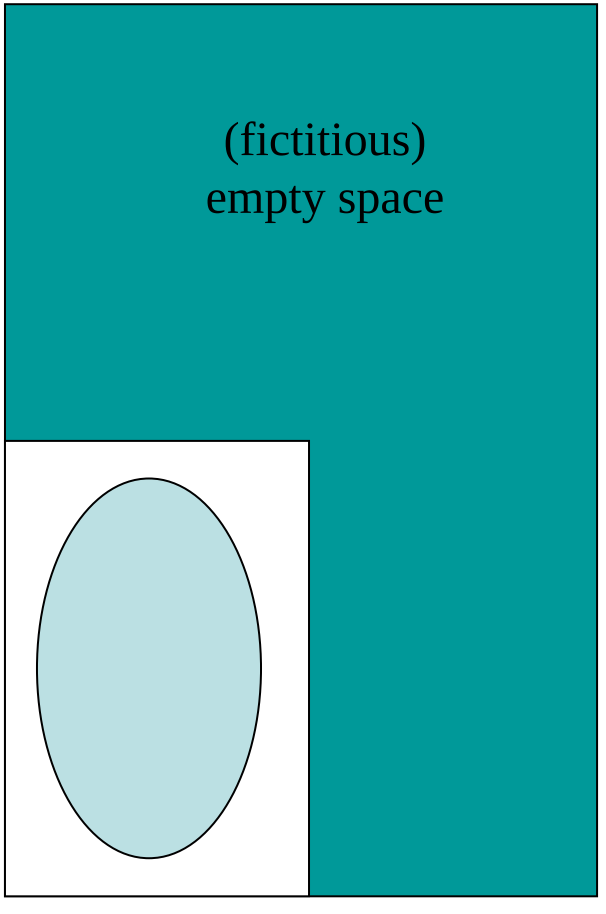
The dissipation is generally increased when symmetries are relaxed and new degrees of freedom enter.

New 3D TDHF code **being revived with many restrictions removed**

- All variations of *full Skyrme forces* can be treated
- 3-D Cartesian geometry *without any symmetry restrictions* both static and *time-dependent*
- Differencing based on *Fast-Fourier-Transform*
- Fourier treatment of Coulomb allows *correct solution*
- *for isolated charge distribution*
- Parameter-free calculations! Nothing is fitted to reactions!
- Coded in Fortran-95
- TDHF version can run on message-passing *parallel machines*

Fourier calculation of potential for isolated charge distributions

The wave functions have periodic boundary conditions, but for the Coulomb filed interaction with images must be avoided



The solution constructed via

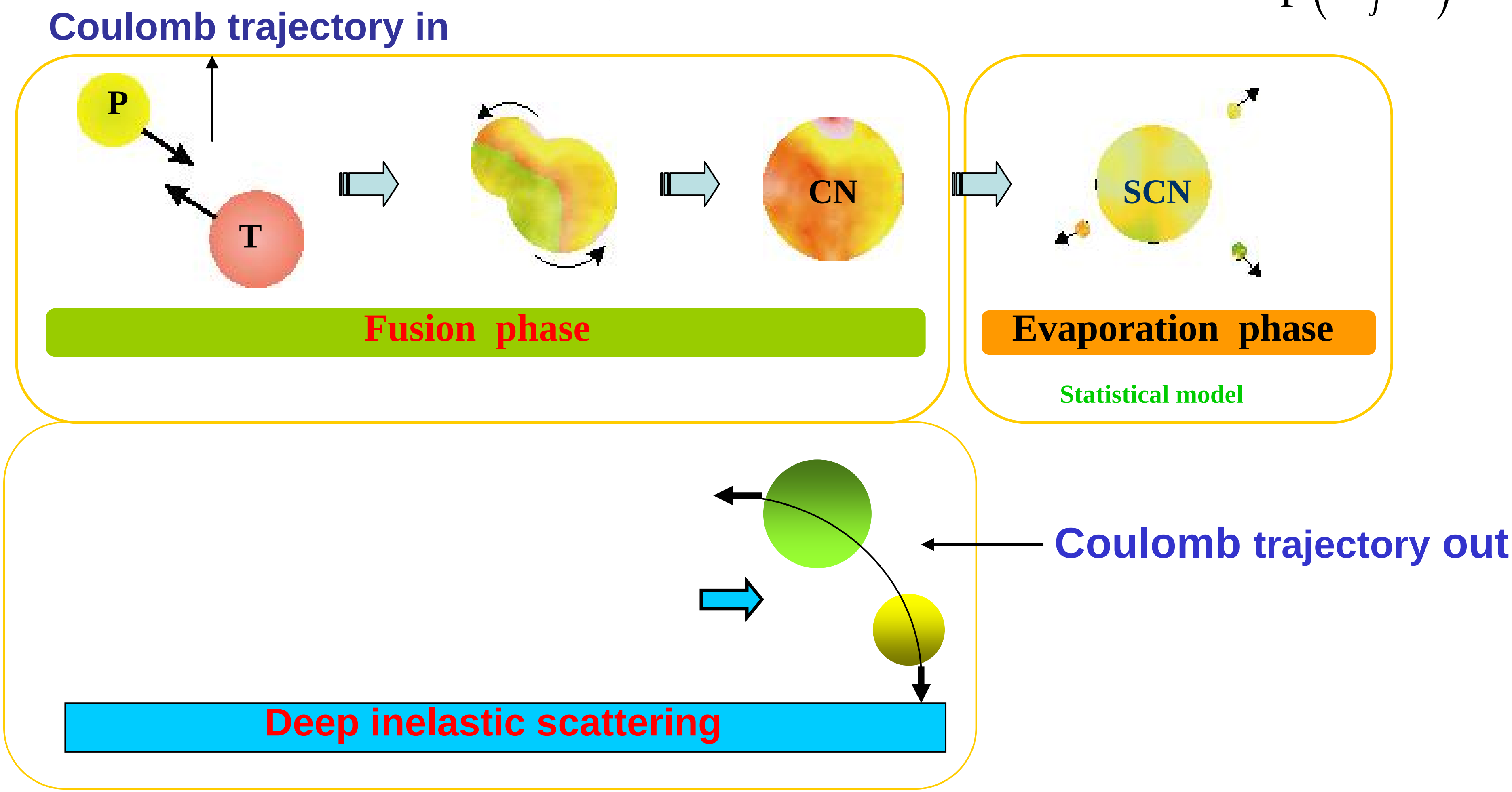
$$V(\vec{k}) = \frac{4\pi}{k^2}\rho(\vec{k})$$

with two FFT operations in the enlarged region with *periodic* boundary conditions fulfills the boundary condition for an isolated charge distribution in the physical region

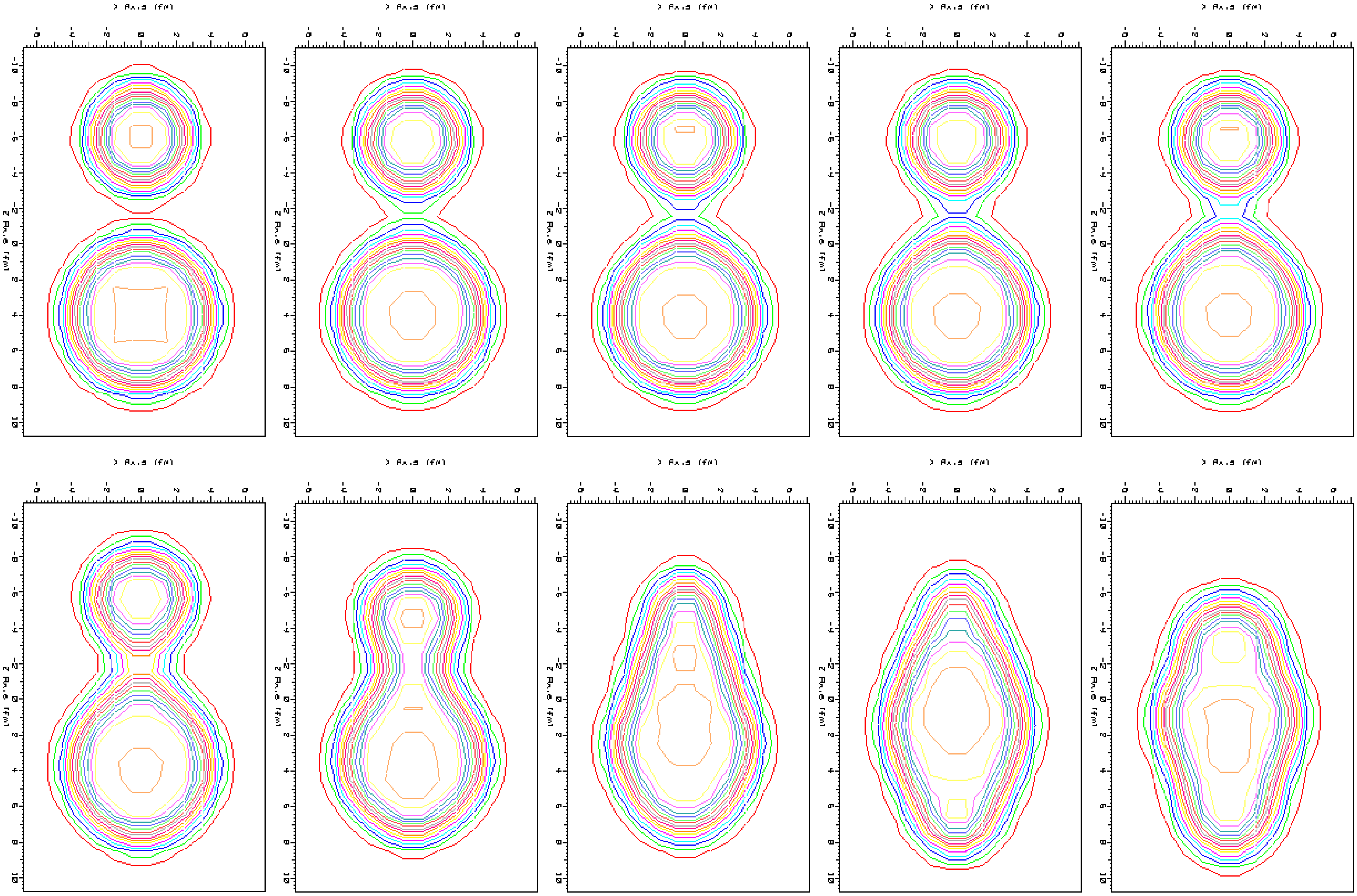
R.W. Hockney, Meth. Comp. Phys. 9, 135 (1970).

TDHF collision process

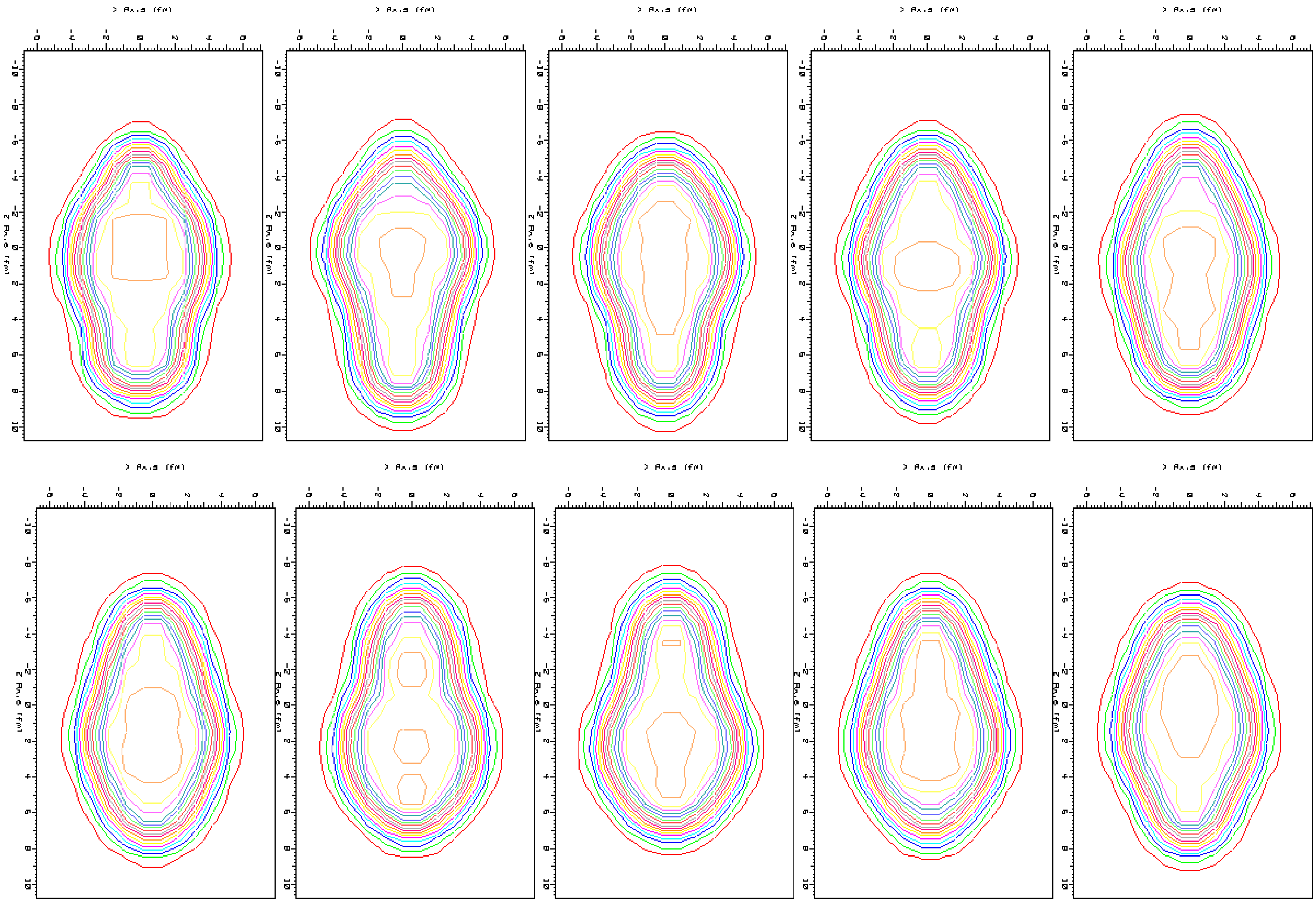
1. **Get wave functions for each nucleus from static Hartree-Fock solution**
2. **Set up the fragments at a finite distance**
3. **Boost wave functions in fragment *j* by phase factors** ⟹ $\exp\left(ik_j \cdot r\right)$



$^{16}O + {}^{48}Ca$, Boost 0.3 MeV / nucleon, t=0-450 fm/c



^{16}O + ^{48}Ca, Boost 0.3 MeV / nucleon, t=500-950 fm/c



Construction of boost-invariant TDHF theory: **why?**

A. Flow-induced dynamic variances

The ground state wavefunctions fulfill the equations

$$\left(\hat{h}_0 - \varepsilon_\alpha\right)\varphi_{0,\alpha}(x) = 0\ ,\quad \hat{h}_0 = \frac{\hat{p}^2}{2m} + U(x)$$

We apply a boost with total momentum *P*

$$\varphi_{0,\alpha}(x) \rightarrow \varphi_\alpha(x,t) = \exp(ip\hat{x})\varphi_{0,\alpha}(x - Vt)\exp\left(-i\tilde{\varepsilon}_\alpha t\right)$$

Boosted WF and mean field are the solution of TDHF equation

The expectation value of s.p. hamiltonian and its variance

misleading

$$\langle\varphi_\alpha|\hat{h}|\varphi_\alpha\rangle = \tilde{\varepsilon}_\alpha = \varepsilon_\alpha + \frac{P^2}{2M}$$

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

⇒ Moving WF is not an eigenstate of hamitonian h

quadratically proportional to the center-of-mass energy

Construction of boost-invariant TDHF theory: how?

B. Construction of boost-invariant mean field

$$E_{\mathrm{kin}} = \frac{\hbar^2}{2m}\int dx\ \tau \Rightarrow$$

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

where, τ is the kinetic energy density, j is the local current, and ρ is the density.

Construction of boost-invariant TDHF theory: how?

Variation leads to the corresponding boost-invariant mean-field Hamiltonian

Potential with Skyrme functional is boost-invariant

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

where, {, } denotes anti-commutator and U(x,t) is the usual time-dependent mean field potential. The above Hamiltonian defines a "boost invariant" single-particle energy

$$\varepsilon_\alpha^{(\text{inv})} = \langle \varphi_\alpha | \hat{h}_{\text{inv}} | \varphi_\alpha \rangle$$

Construction of boost-invariant TDHF theory: what?

C. Free translational motion of a nucleus

For the case of the global center-of-mass motion, the boost Invariant Hamiltonian reduces to

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

and finally

static s.p. energies

$$\hat{h}_{\text{inv}}\varphi_\alpha = \varepsilon_\alpha \varphi_\alpha$$

Numerically 10^{-4} ~10^{-5} MeV

eigenstate

$$\langle \varphi_\alpha | \Delta \hat{h}^2_{\text{inv}} | \varphi_\alpha \rangle = 0$$

→ **Numerically 0.02~0.05 MeV**

Free translational motion of nucleus O16 with 3D TDHF code

Construction of boost-invariant TDHF theory: what?

D. Adiabatic eigenstate

For collision situation → not eigenstate

$$\hat{h}_{\rm inv}\varphi_\alpha \neq \varepsilon_\alpha \varphi_\alpha, \quad \langle \varphi_\alpha | \Delta \hat{h}_{\rm inv}^2 | \varphi_\alpha \rangle \neq 0$$

Intrinsic excitation and collision dynamics

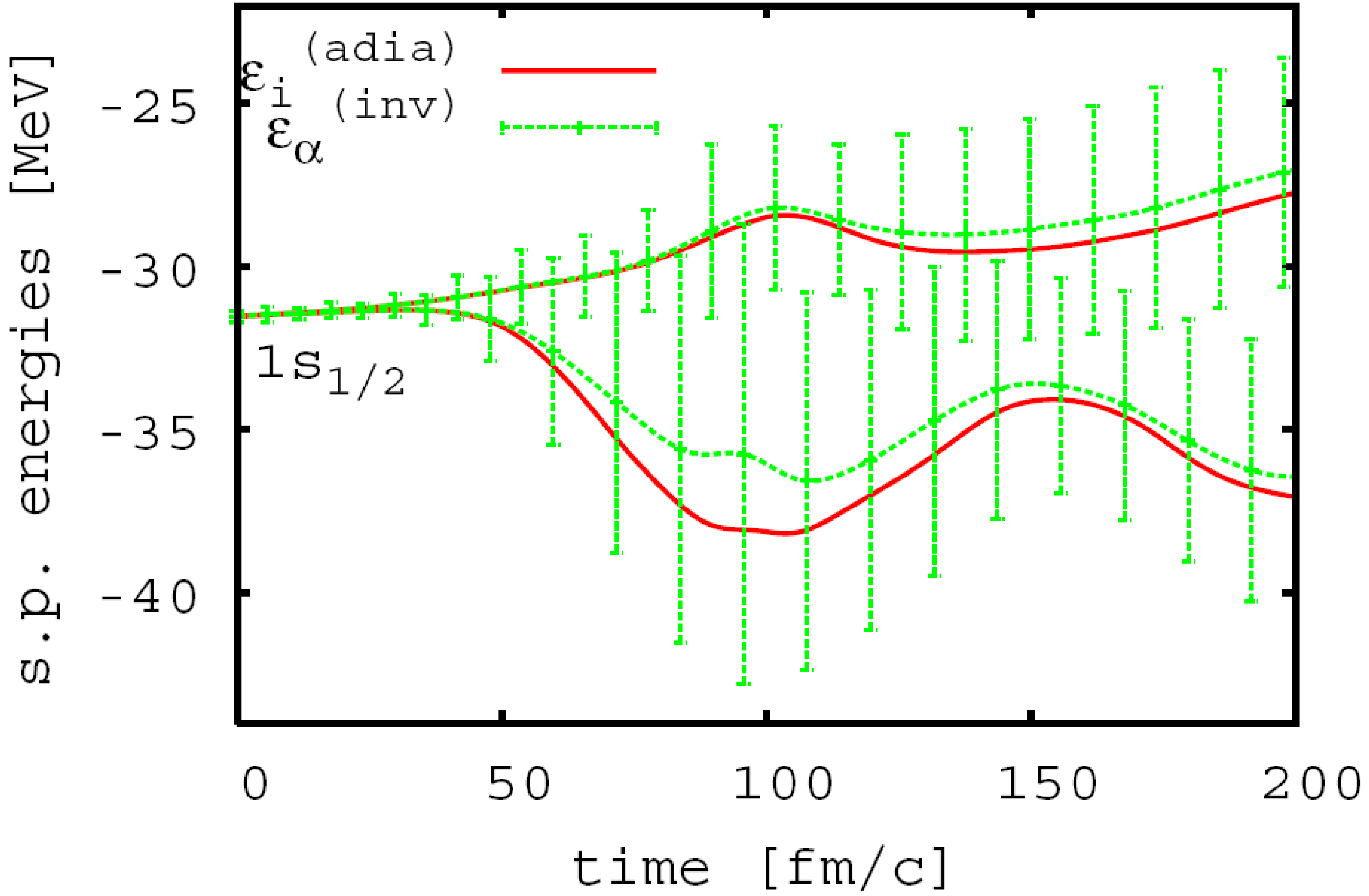
Eigenstate of boost-invariant hamiltonian is defined as

$$\hat{h}_{\rm inv}\phi_i = \varepsilon_i^{(adia)}\phi_i$$ → Adiabatic basis

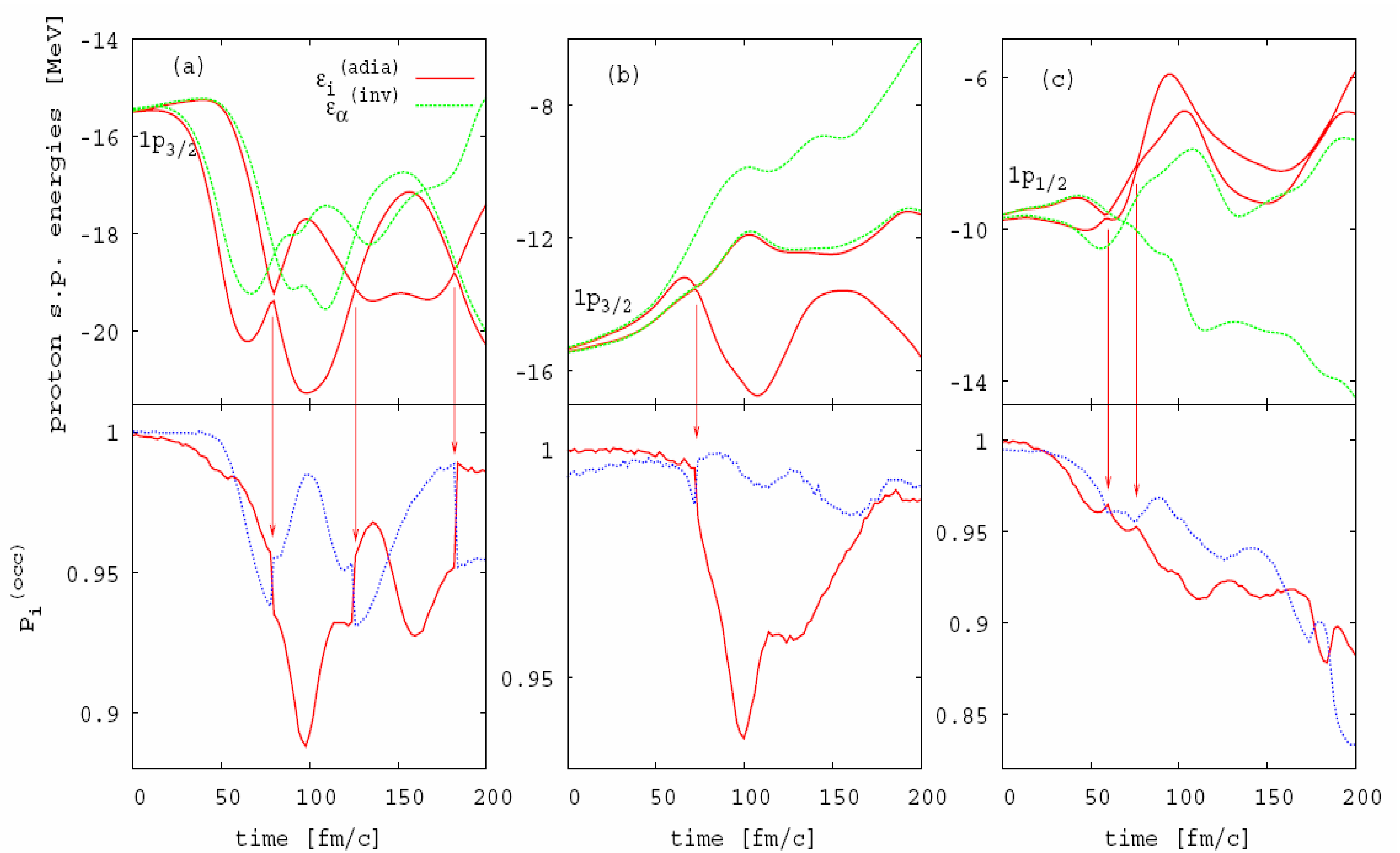
We define adiabatic occupation probability as

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

Application of boost-invariant TDHF theory: heavy-ion collision

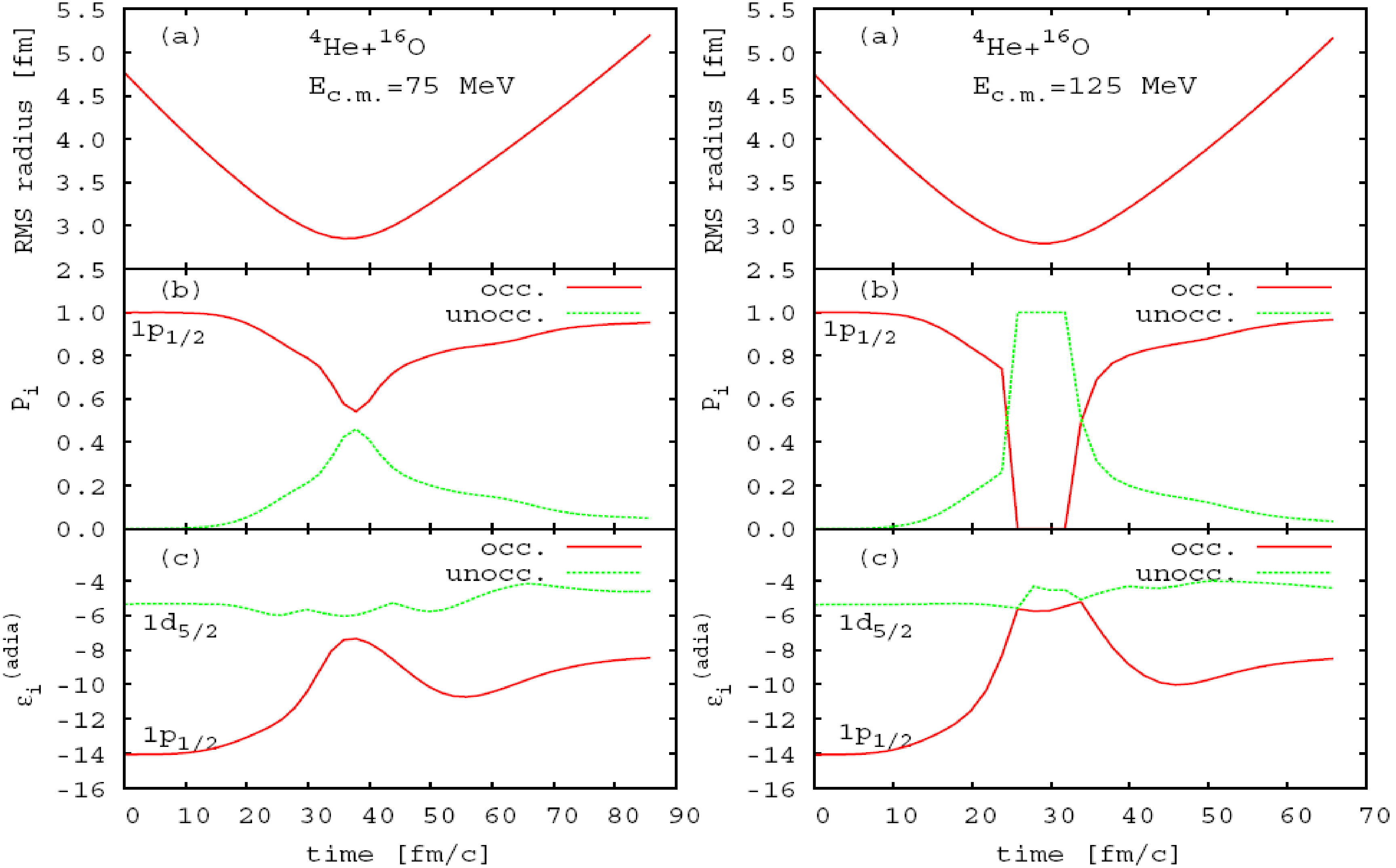


Application of boost-invariant TDHF theory: heavy-ion collision



Application of boost-invariant TDHF theory: Landau-Zener effect

reaction time ⟷ rearrangement time near level crossing



Summary

1. **We constructed boost-invariant TDHF theory**

2. **Free translational motion of a nucleus**

3. **Fusion of the O16+O16: level crossing**

4. **Deep inelastic scattering of He4+O16: Landau-zener effect**

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