News from TDHF

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Some Properties of TDHF

- In Time-Dependent Hartree-Fock (since 1972) the time-dependent mean-field equations are solved numerically for nuclear collisions.
- Because of advances in computing, TDHF is being reconsidered by many groups worldwide as a description of low-energy heavy-ion collisions
- It is now possible to use a full Skyrme energy functional and 3D geometry
- TDHF contains only one-body dissipation and no fluctuations: semiclassical behavior
- Results show surprisingly good quantitative description of fusion *without adjusted parameters*
- Many aspects of numerical reliability still need to be investigated more intensively

- Topics
  - Transparency, mass and charge transfer
  - Stability of isomeric states
  - Conservation properties
- Methods
  - Static and time-dependent Hartree-Fock
  - Full Skyrme force
  - Cartesian grid in 3D, no symmetries
  - Differencing using FFT
  - Exact treatment of Coulomb boundary condition

The Skyrme Energy Functional

Red: minimum set of time-odd couplings to assure Galilei invariance

$$E = E_{kin} + \int d^3r \left(\mathcal{E}_{\rm Sk} + \mathcal{E}_{\rm Sk}^{(ls)}\right) + E_C$$

$$E_{kin} = \int d^3r \frac{\hbar^2}{2m}\tau$$

$$\mathcal{E}_{\rm Sk} = \frac{b_0}{2}\rho^2 + b_1(\rho\tau - \vec{j}^{\,2}) - \frac{b_2}{2}\rho\Delta\rho + \frac{b_3}{3}\rho^{\alpha+2}$$

$$- \sum_q \left[\frac{b_0'}{2}\rho_q^2 + b_1'(\rho_q\tau_q - \vec{j}_q^{\,2}) + \frac{b_2'}{2}\rho_q\Delta\rho_q + \frac{b_3'}{3}\rho^\alpha\rho_q^2\right]$$

$$\mathcal{E}_{\rm Sk}^{(ls)} = -b_4\left[\rho\nabla\cdot\vec{J} + \vec{\sigma}\cdot(\nabla\times\vec{j})\right]$$

$$+ b_4'\sum_q[\rho_q(\nabla\cdot\vec{J}_q) + \vec{\sigma}_q\cdot(\nabla\times\vec{j}_q)]$$

$$E_C = \frac{e^2}{2}\int d^3r\, d^3r'\rho_p(\vec{r})\frac{1}{|\vec{r}-\vec{r}'|}\rho_p(\vec{r}') - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\int d^3r[\rho_p(\vec{r})]^{\frac{4}{3}}$$

with

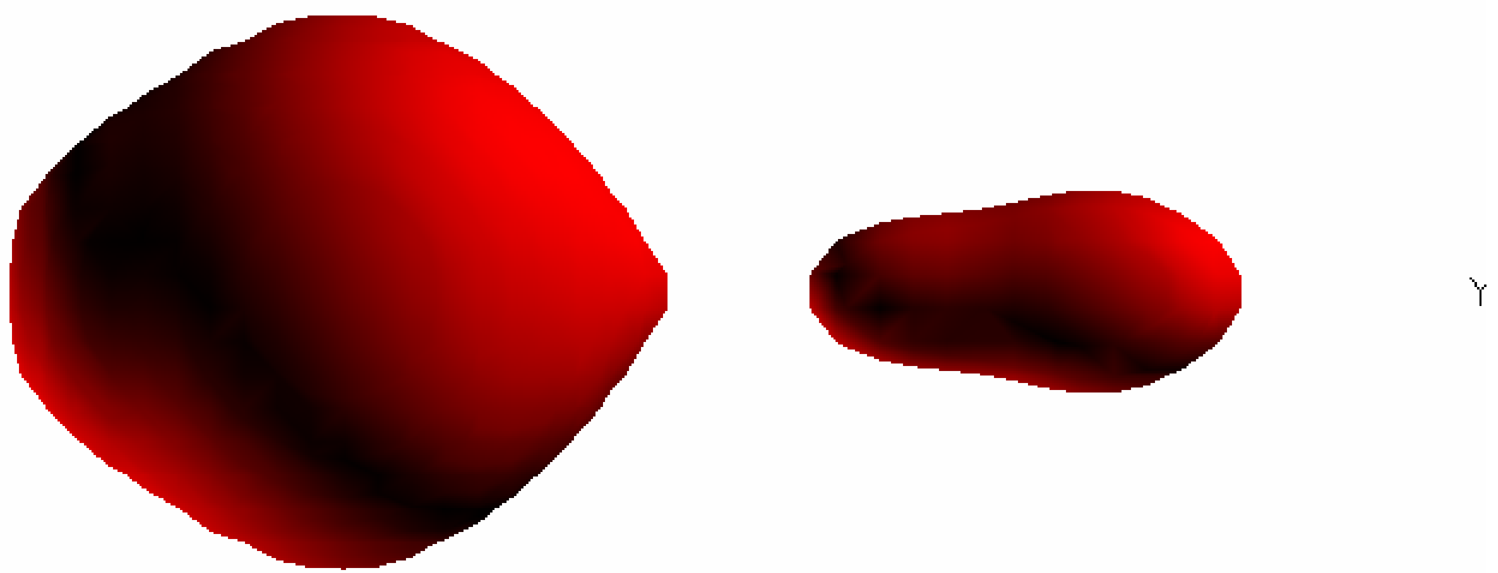
$$\vec{\sigma}_q(\vec{r}) = \sum_q \varphi_\alpha^{+}(\vec{r})\hat{\vec{\sigma}}\varphi_\alpha(\vec{r})$$

$$\vec{J}_q(\vec{r}) = -i\sum_q \varphi_\alpha^{+}(\vec{r})\nabla\times\hat{\vec{\sigma}}\varphi_\alpha(\vec{r})$$

Mg + Pb : Motivation

- Experimental data at GSI seem to hint at „transparency“.
  S. Heinz et al., Eur. Phys. J. A DOI 10.1140/epja/i2008-10671-9
- 25Mg+206Pb near E_{cm}=193 MeV
- Ejected fragment in the forward direction with mass ≈12
- A tentative explanation could be
  - TDHF „feedthrough“ for central collisions
  - Peripheral mass exchange with forward focussing
- *This led to new insights on nucleon exchange in TDHF…*

Transparency does occur at higher energies, here at 550 MeV



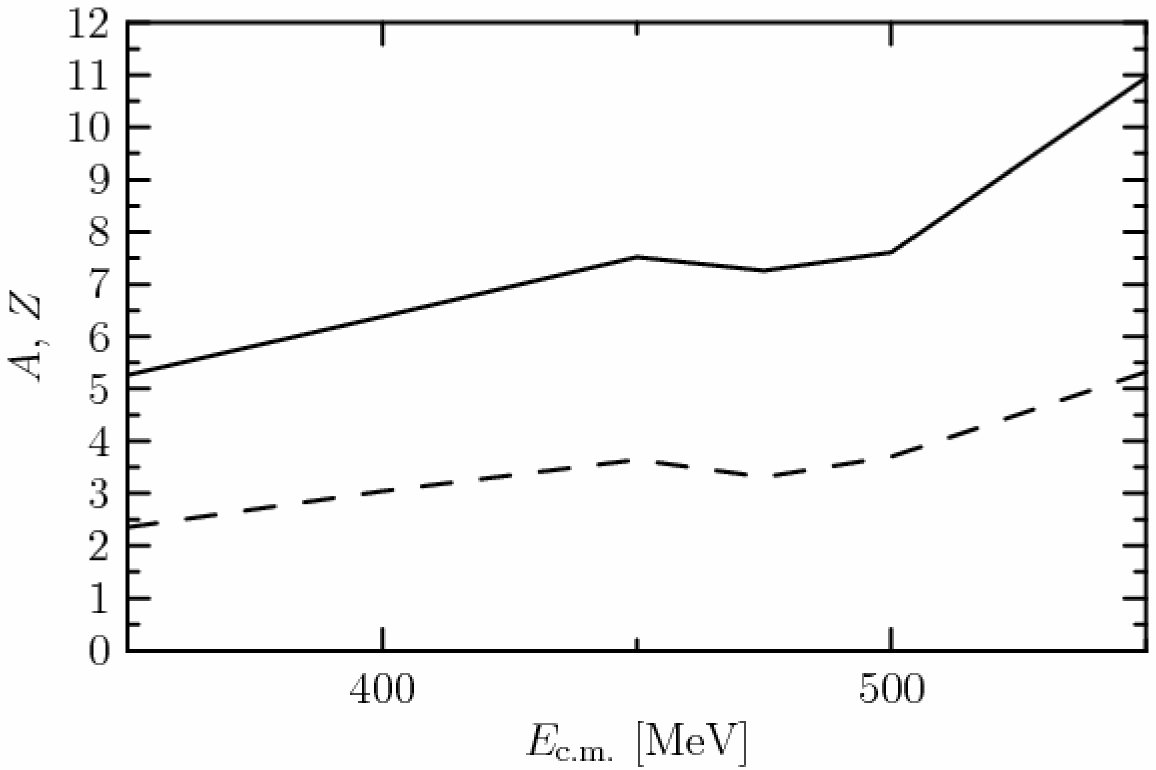
Central collisions

There is increasing transparency at higher energies.

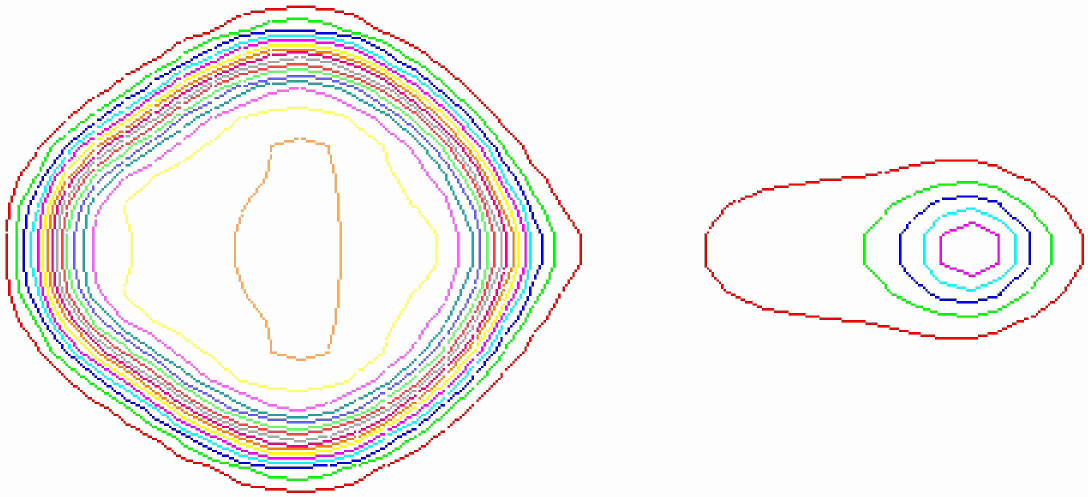
Analysis shows that 90% of the ejected fragment wave functions are from the initial projectile.

The properties of the ejected material are quite unusual, however.

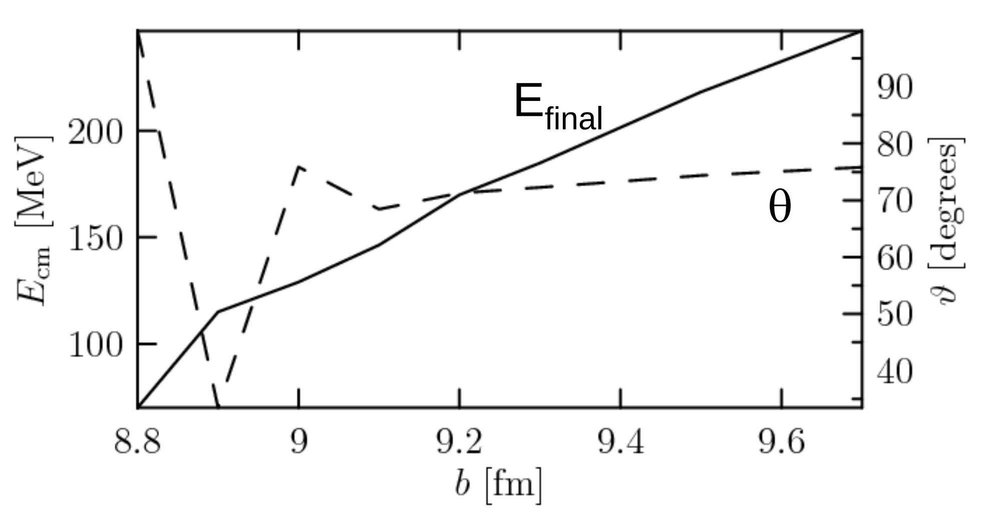
Properties of fragment in forward direction



The density, however, …

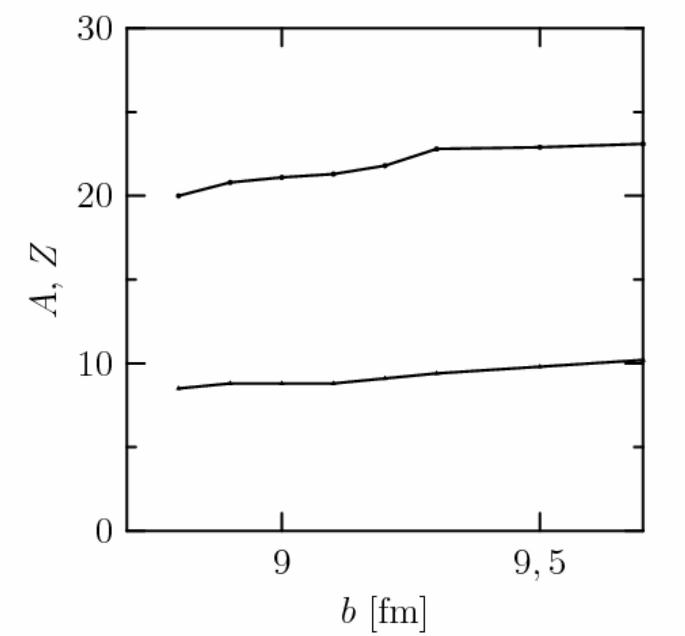


Peripheral Collisions at 350 MeV

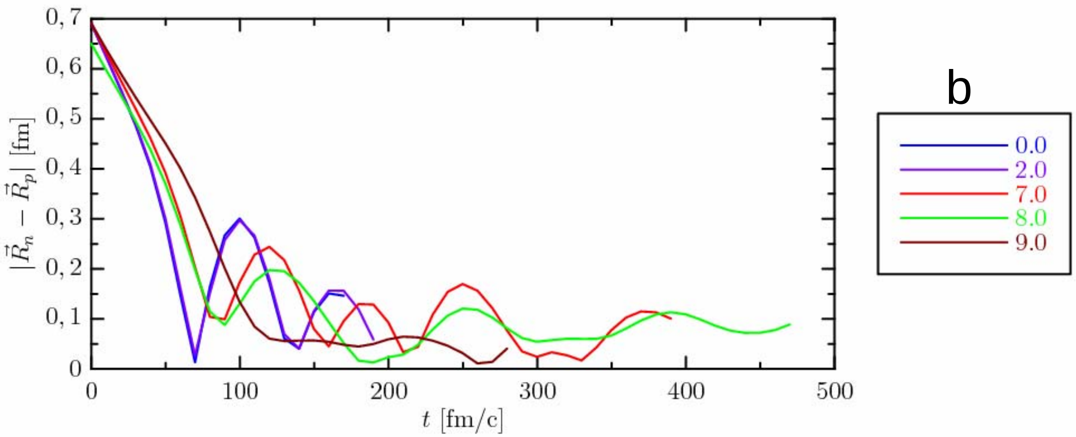


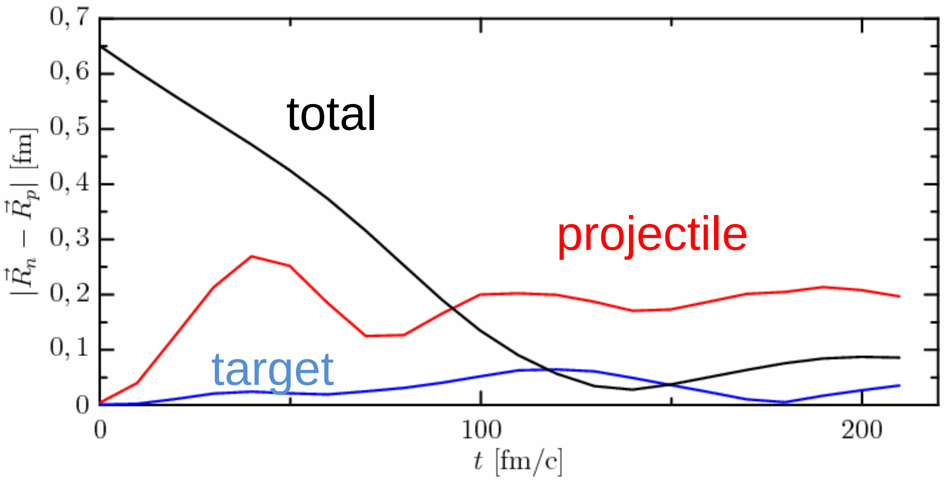
- There is a systematic increase in transfer with decreasing *b*

- Proton transfer sets in much more rapidly



Dipole Development

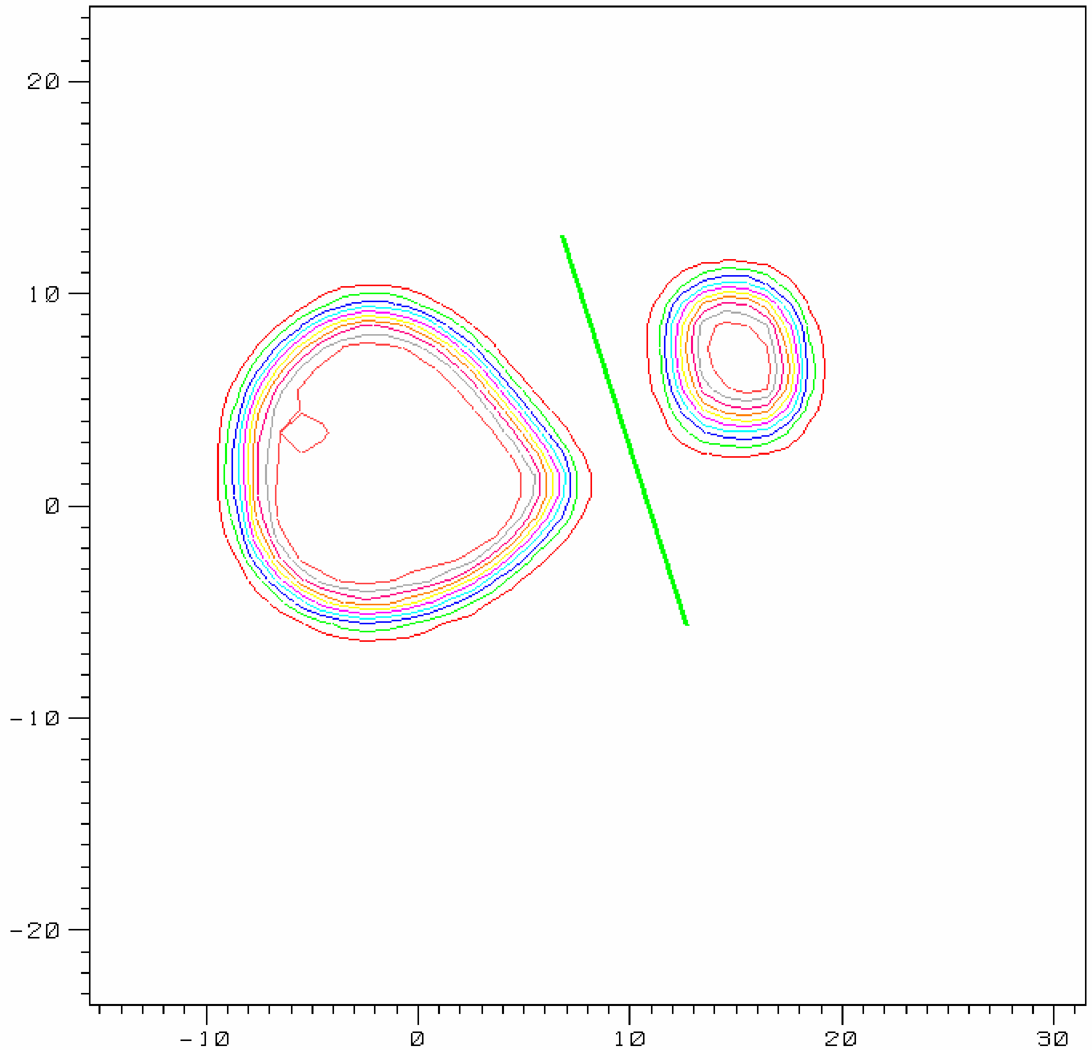




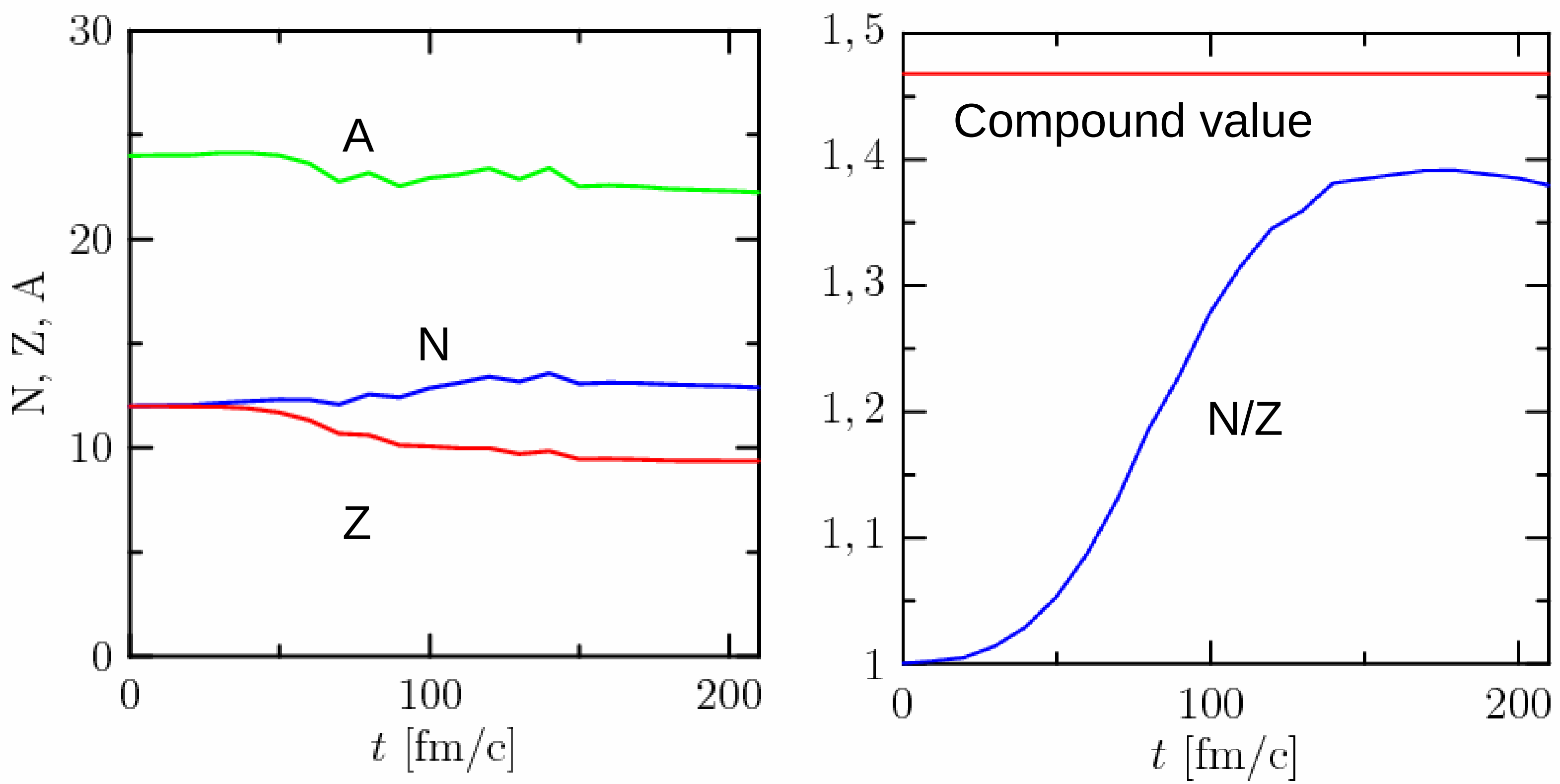
The dipole seems to indicate rapid relaxation with oscillations superimposed.

Unfortunately it contains a strong distance dependence and local internal GDRs of the fragments

Details at b = 9.3 fm, Ecm=170 MeV

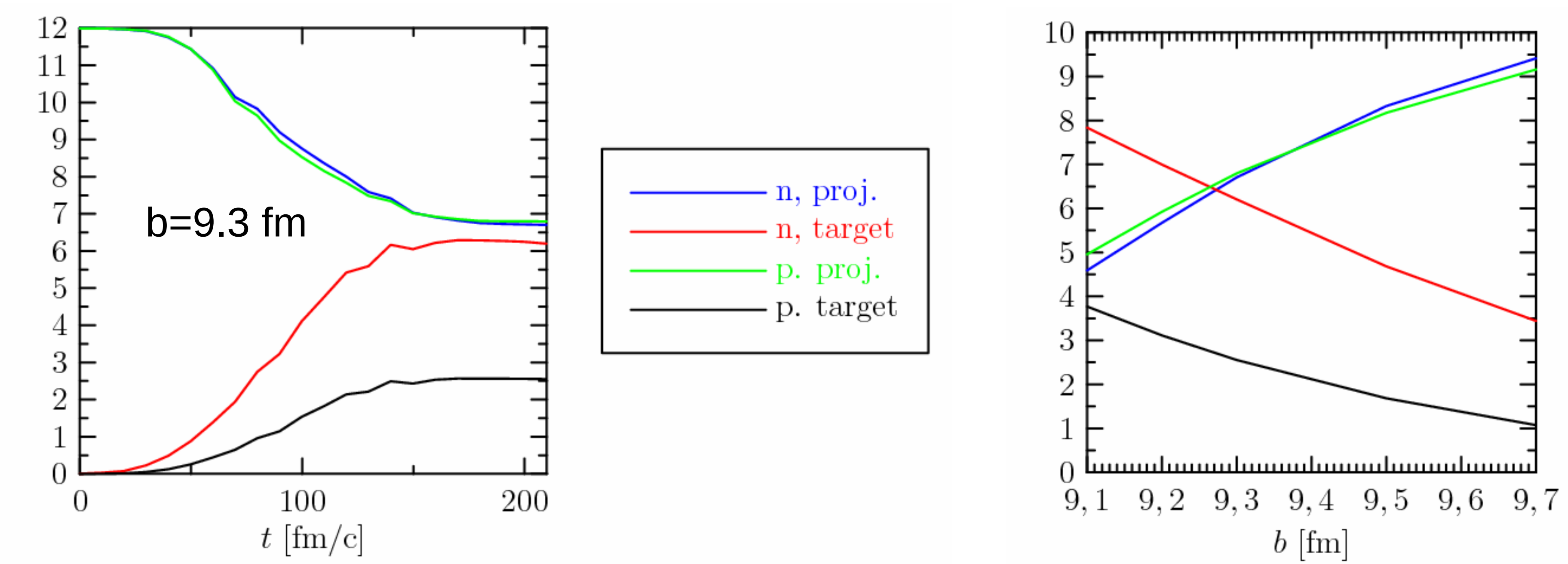


Time-dependence of Transfer



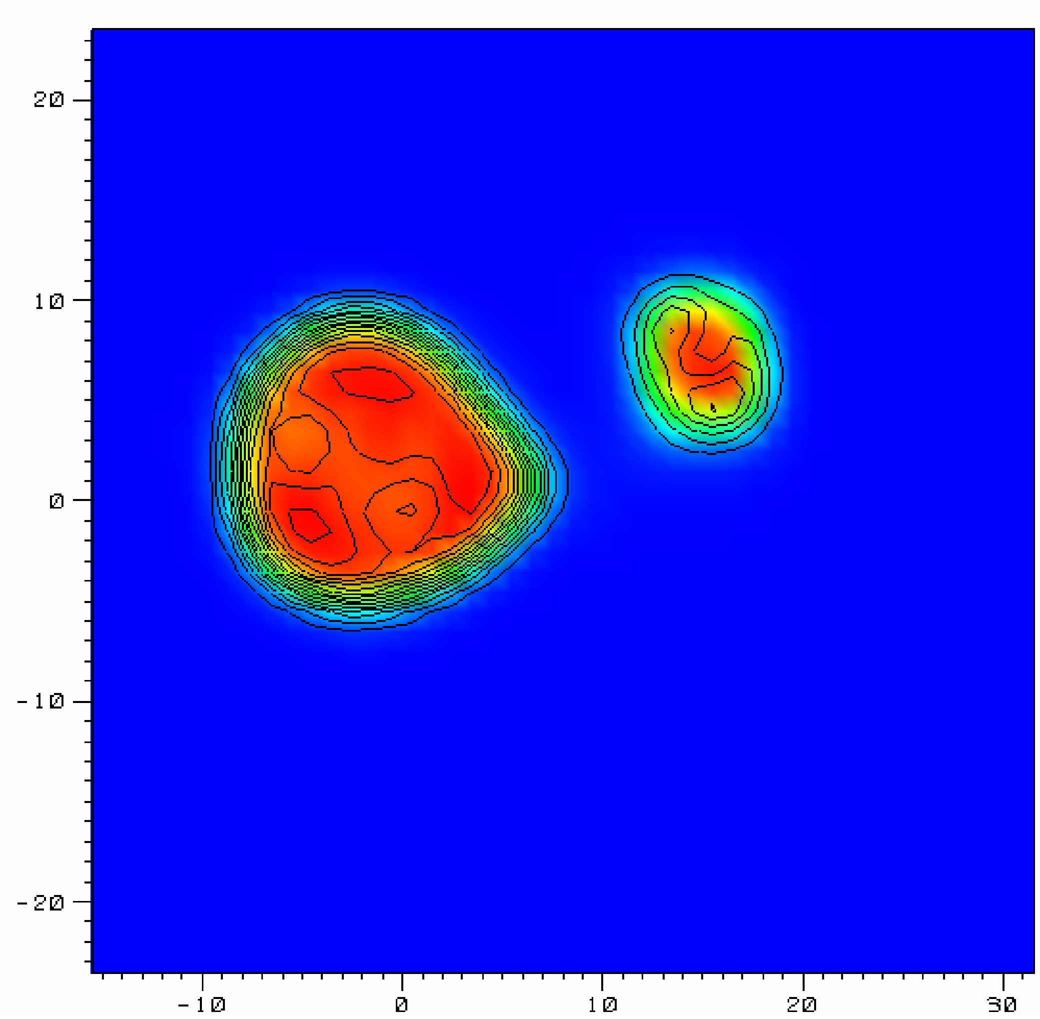
The proton and neutron numbers in the smaller fragment seem to rapidly stabilize and approach the compound value.
E = 350 MeV, b = 9.3 fm

Detailed Exchange

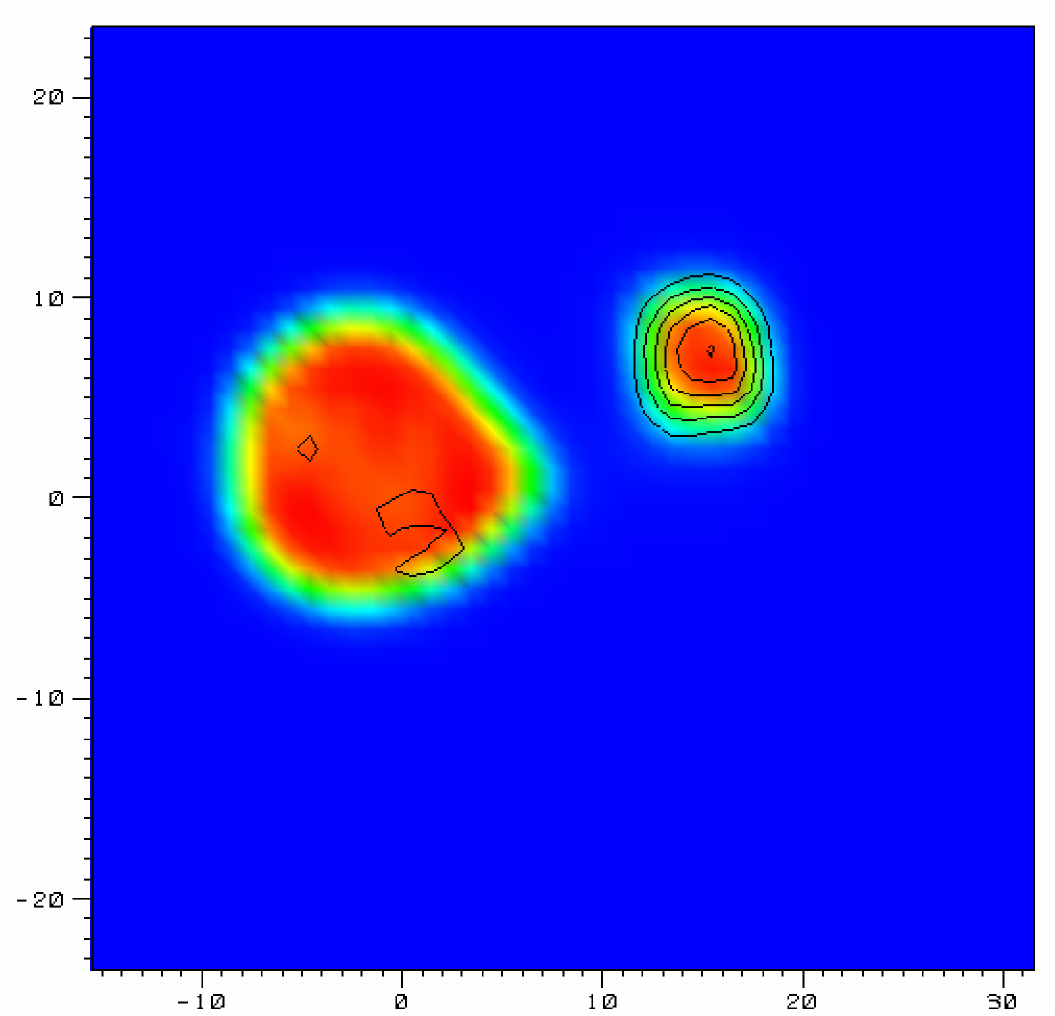


- Transfer set in very rapidly even for peripheral collisions
- No evidence for oscillations in this regime
- Statistical mixing seems to be the mechanism
- Projectile neutron/proton transfer ratio close to 1, but for target larger than N/Z . Reason?
- Mixing of projectile & target matter is very strong
- To be checked: is the neck size or the interaction time the limiting factor?

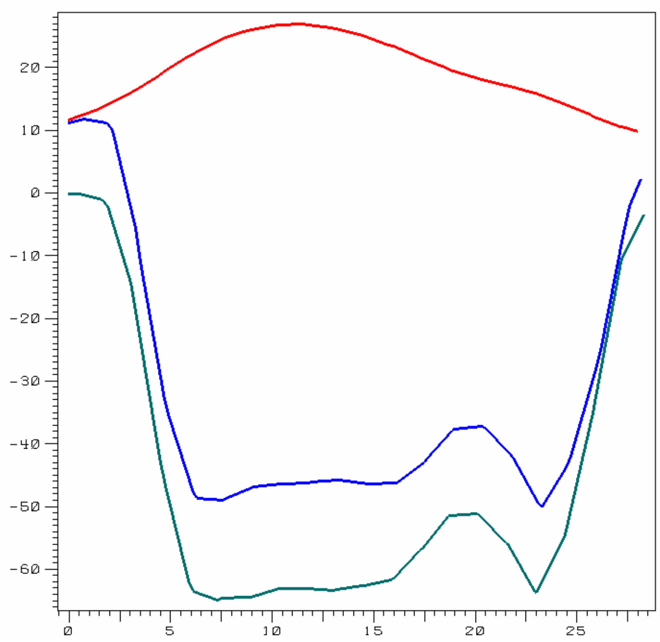
Target Material Development

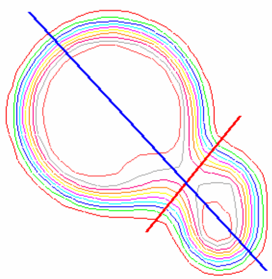


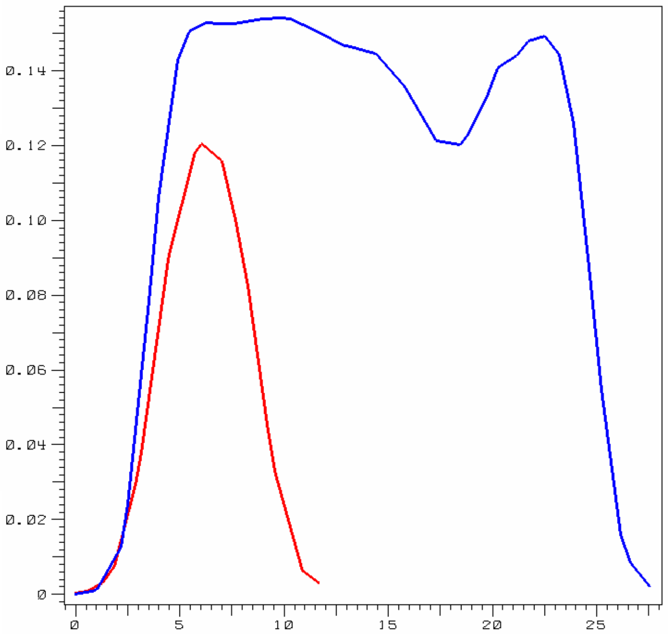
Projectile Material Development



Density and Potential

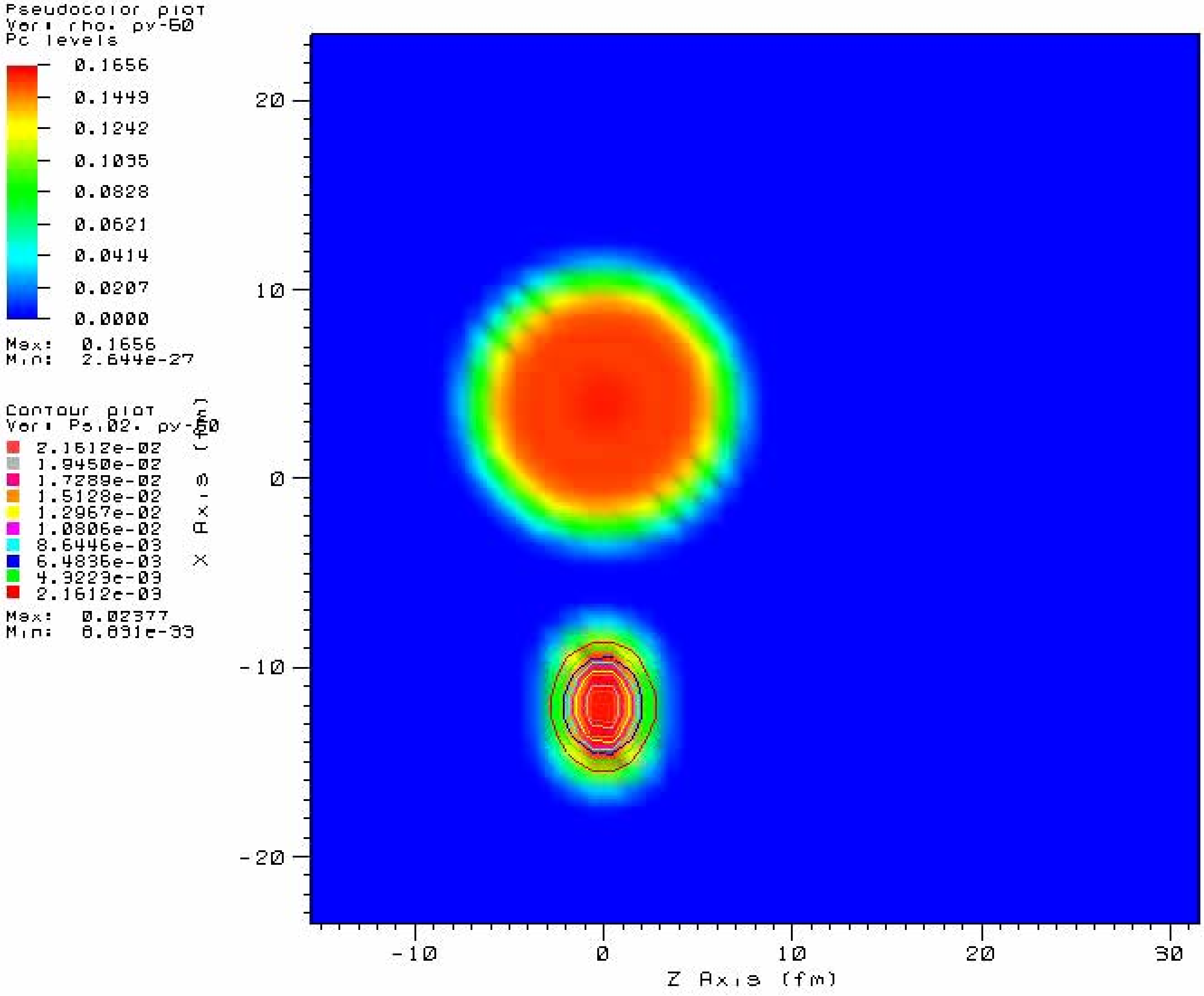






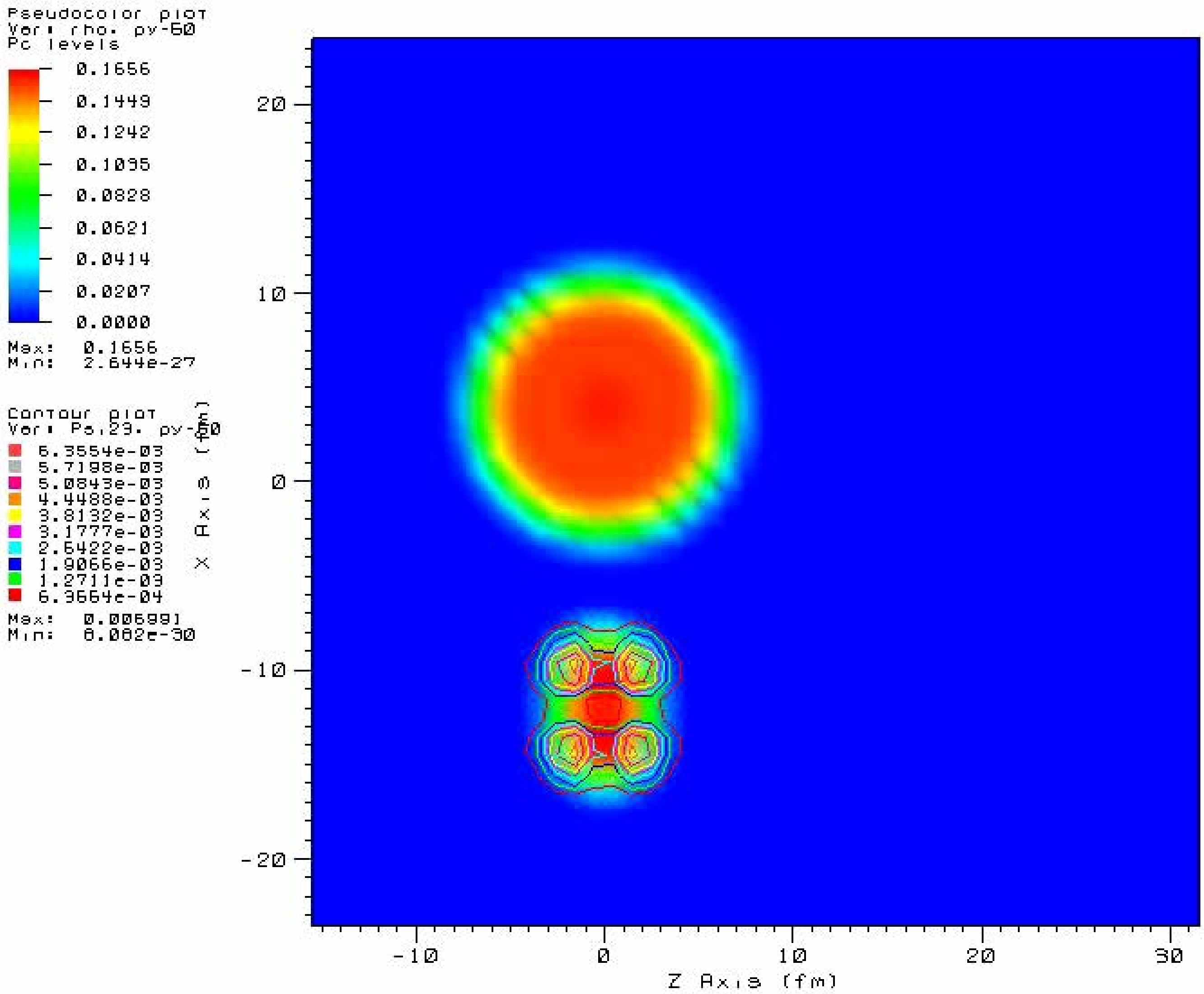
Mg
Wave
Function
#1

350 MeV
8.8 fm



Mg
Wave
Function
#23

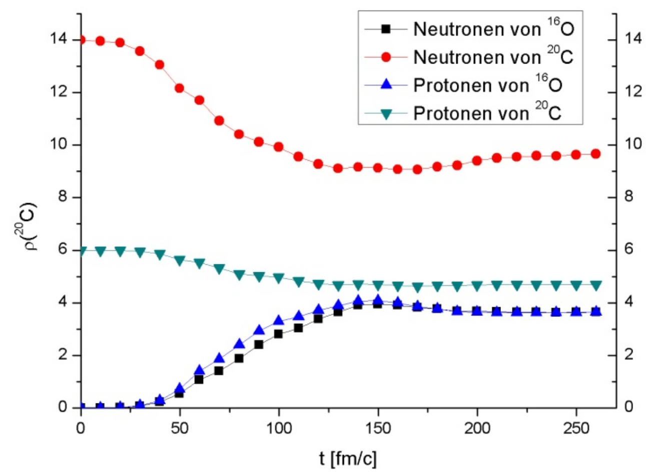
350 MeV
8.8 fm

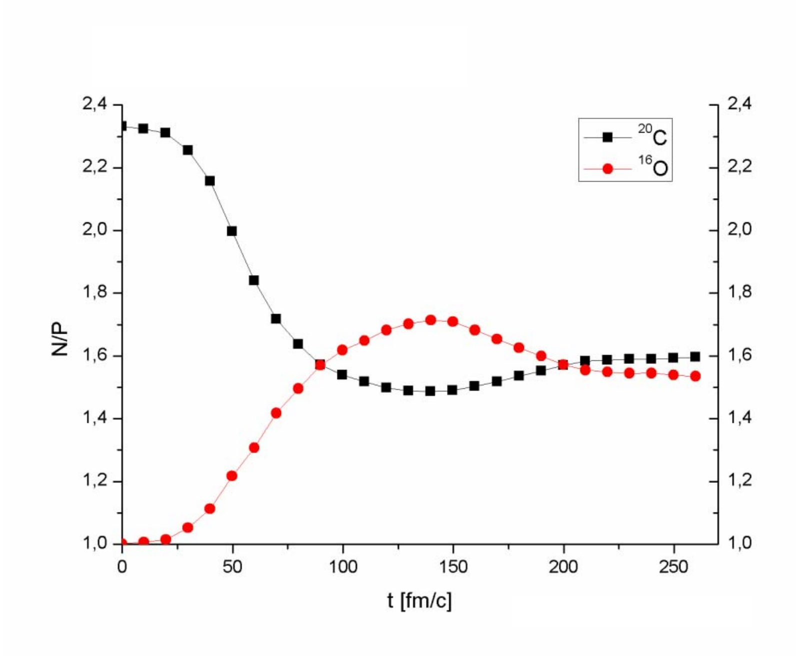


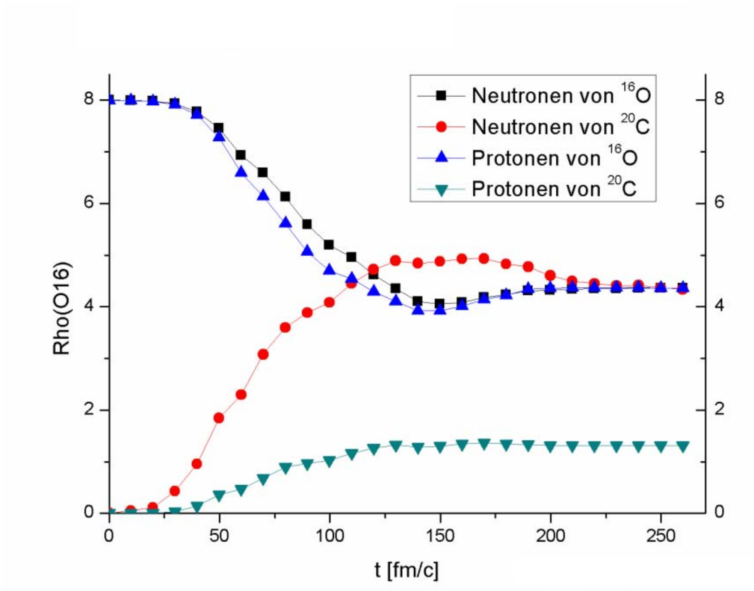
Lower Energy, Light System

$^{16}O+^{20}C$, 100 MeV, 5.8 fm

B. Schütrumpf
Bachelor Thesis



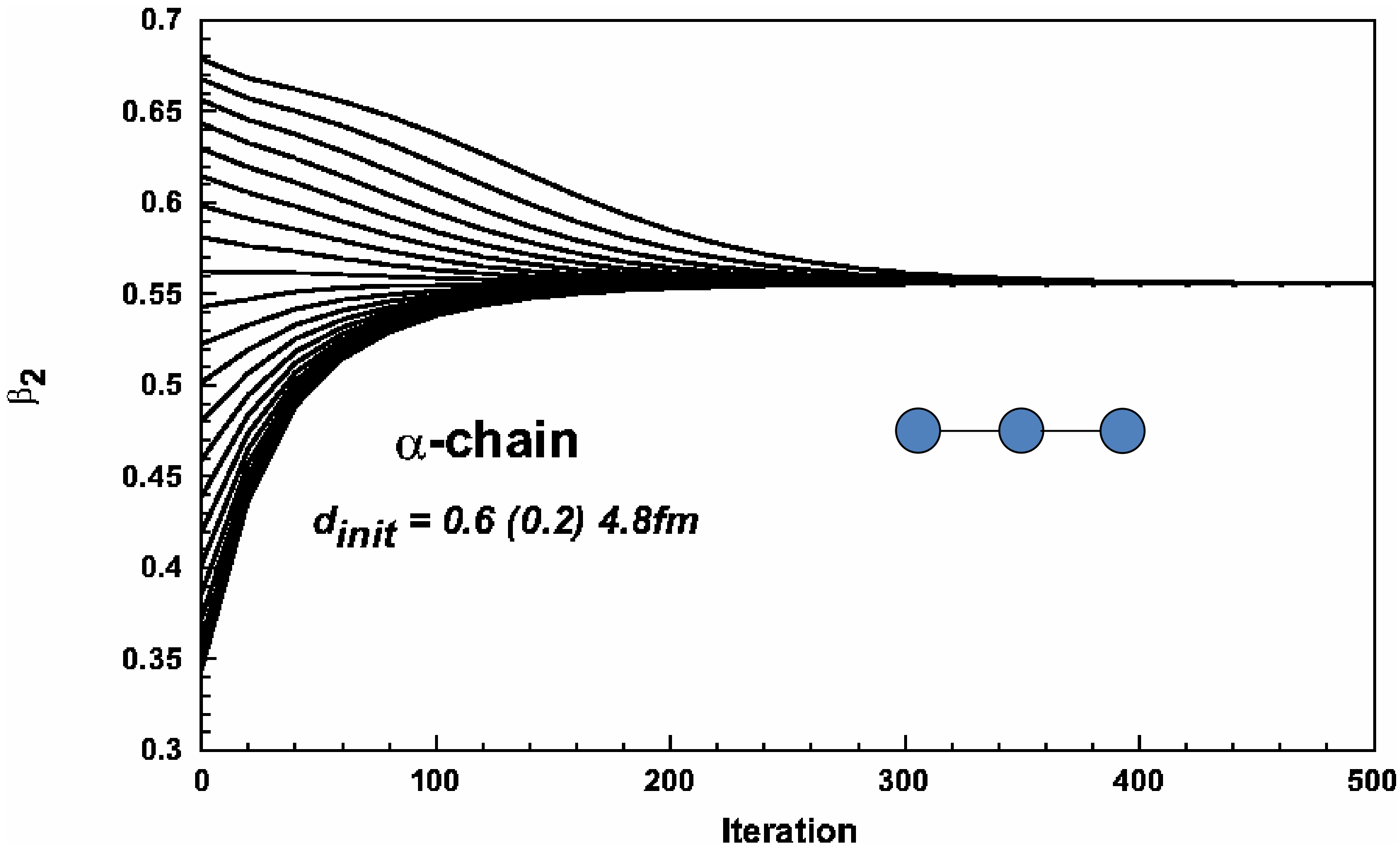




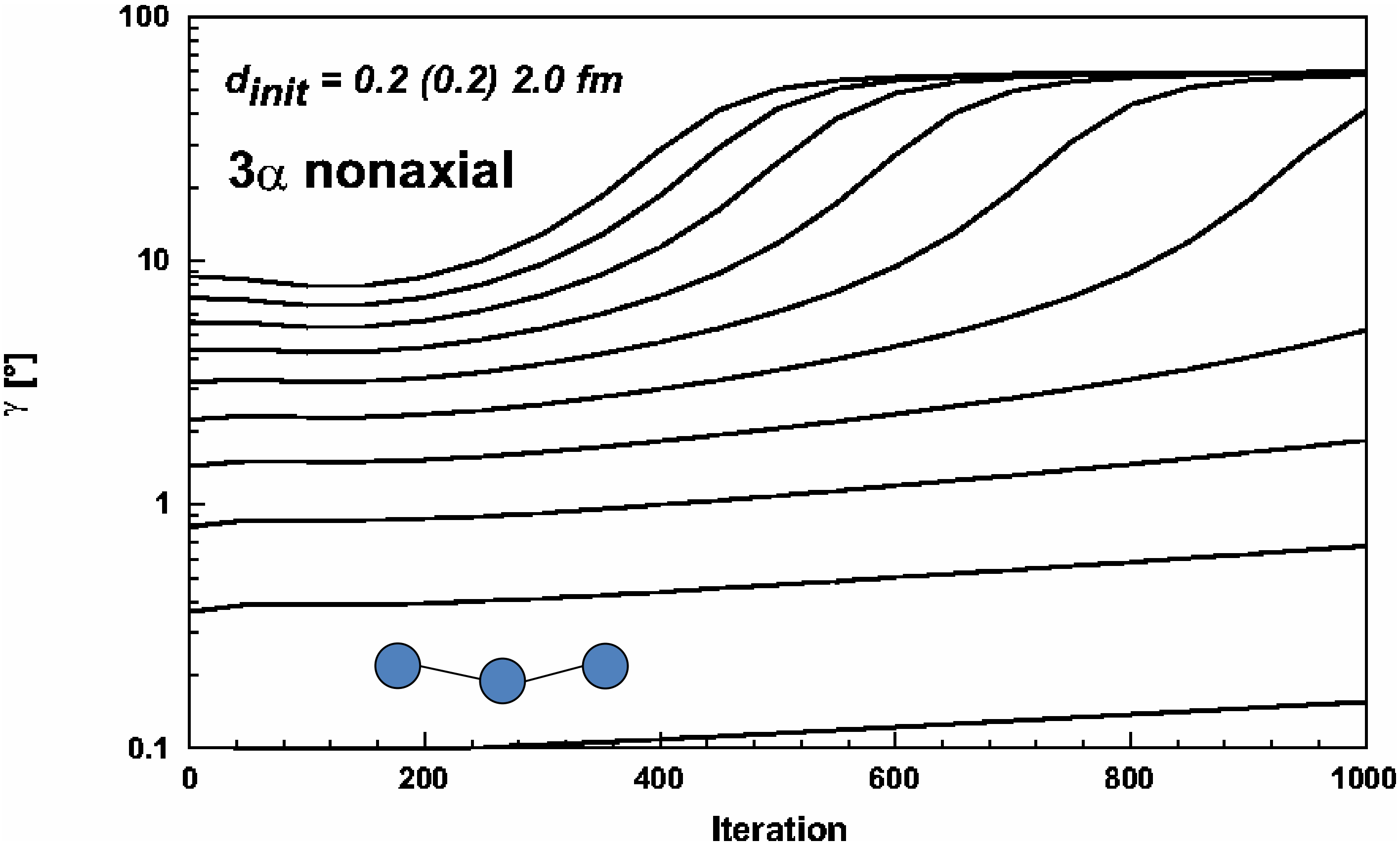
Conclusions

- The exchange of wave functions starts extremely rapidly
- The process of mixing appears to be statistic: no evidence for oscillations
- The „single-particle dissipation“ mechanism appears to be very effective – no need for NN-collisions *in the early stage of the collision*
- Transparency for central collisions may still be unphysical: special symmetry makes dissipation slower
- To understand the physics, it will be useful to look at the details of TDHF calculations

3-α Chain for ^{12}C



Three-α-Chain Nonaxial



Initialization for ^{16}C

- For three α-clusters Gaussians at z=0, -d, and +d, with d usually 3 fm. Width 1.8 fm.
- σ-state neutrons added as distorted Gaussians (3 times larger width in z-direction) multiplied by z(z-d)
- π-state neutrons similar with factor (x+isry). s for spin direction, r for regular (r=1) π' and irregular (r=-1) π.
- δ-states use factor (x+isy)z.
- In the results, π' have $j_z=\pm 1/2$, π have $j_z=\pm 3/2$
- Both for time-reversal invariant and other states, HF-3D produces the angular-momentum quantization very well.

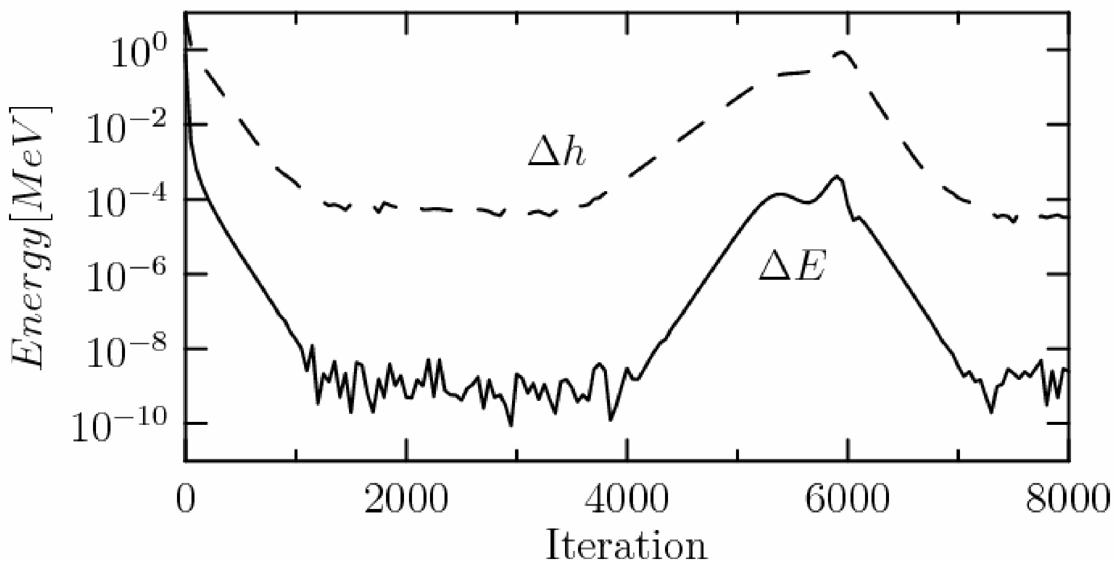
Initial		**Final**
Name	Spins	States
$\pi^2\sigma^2$	+ - + -	$\pi^2\pi'^2$
$\pi^2\sigma\pi$	+ - + -	$\pi^2\sigma\pi'$
$\pi^2\sigma\pi'$	+ - + +	$\pi^2\pi'^2$
$\pi^2\delta^2$	+ - + -	$\pi^2\delta^2$
$\pi^2\delta\pi$	+ - + -	$\pi^2\delta\pi'$
$\pi^2\delta\pi'$	+ - + +	$\pi^2\delta\pi''$

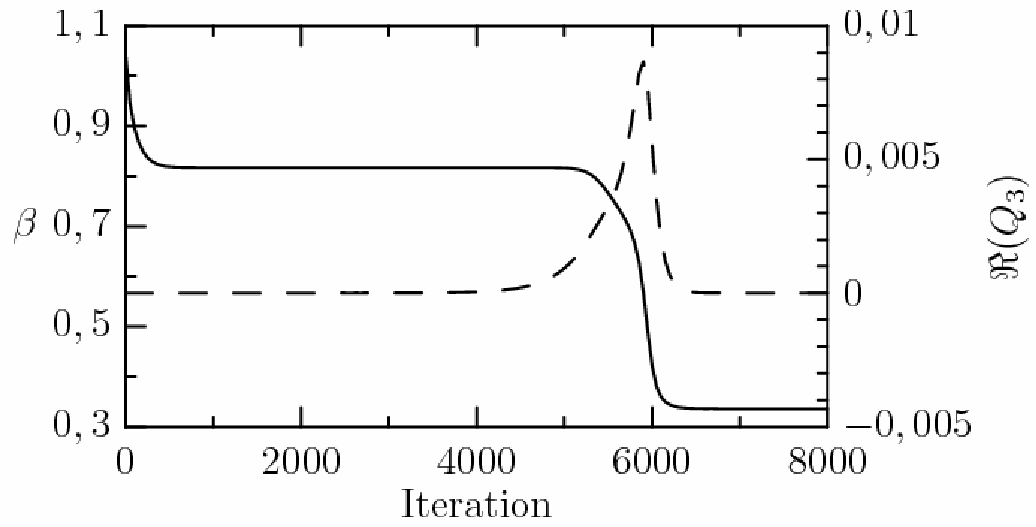
Convergence Behavior

An excited quasistable (?) state appears as an apparently converged configuartion for 1000's of iterations. Sometimes convergence indicators are as good as for the ground state.

$$\Delta h = \frac{1}{A}\sum_{k=1}^{A}\sqrt{\langle \phi_k \,|\, \hat{h}^2 \,|\, \phi_k \rangle - \langle \phi_k \,|\, \hat{h} \,|\, \phi_k \rangle^2}$$

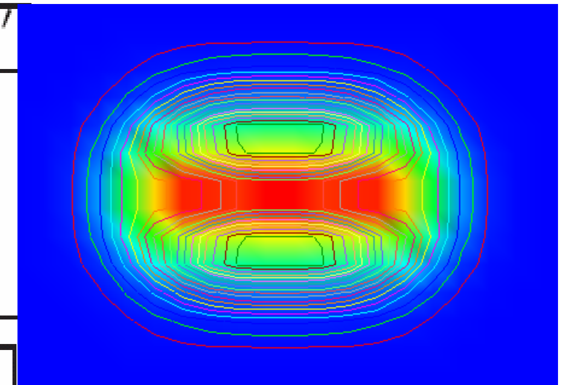
Subsequently, there is rapid conversion to the ground state via triaxial shapes.





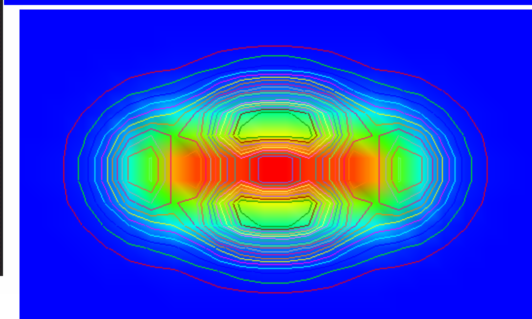
Observed states: contain 2/3 probability for 3-a chain

Force	E_B	$\pi^2\delta^2$	$\pi^2\pi'^2$	$\pi^2\delta\pi'$	$\pi^2\sigma\pi'$	$\pi^2\delta\pi''$
SkI3	101.5	19.5	14.5	17.0	19.1	17.5
SkI4	100.8	19.9	15.7*	17.6	19.7	18.0
Sly6	100.6	18.9	15.4*	17.0	19.0	17.3
SkM*	115.0	17.5	16.4*	16.9	19.7	17.0

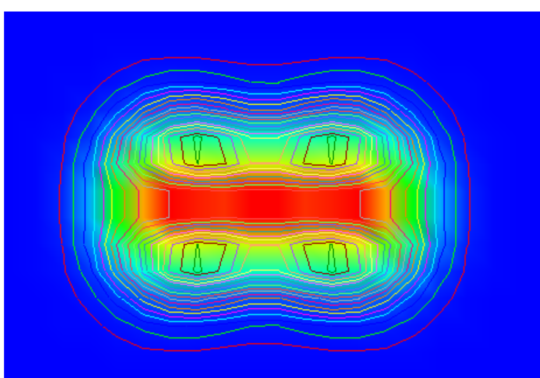


$K^\pi=1^-$

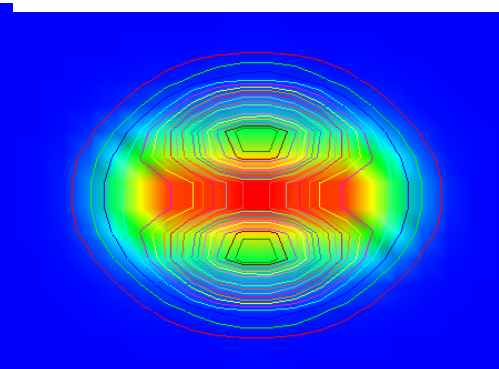
Force	$\beta_{g.s.}$	$\pi^2\delta^2$	$\pi^2\pi'^2$	$\pi^2\delta\pi'$	$\pi^2\sigma\pi'$	$\pi^2\delta\pi''$
SkI3	0.34	0.82	0.69	0.76	0.88	0.76
SkI4	0.33	0.80	0.68*	0.75	0.86	0.74
Sly6	0.32	0.81	0.68*	0.75	0.87	0.75
SkM*	0.28	0.79	0.66*	0.73	0.85	0.73



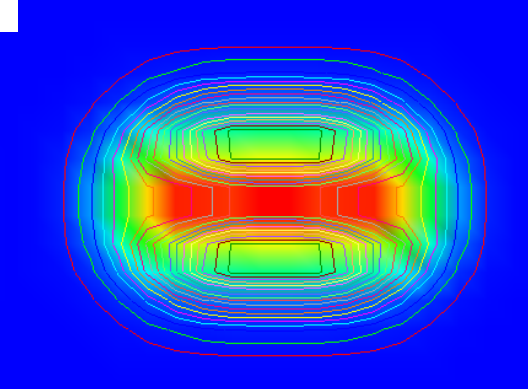
$K^\pi=1^+$



$K^\pi=0^+$



$K^\pi=0^+$



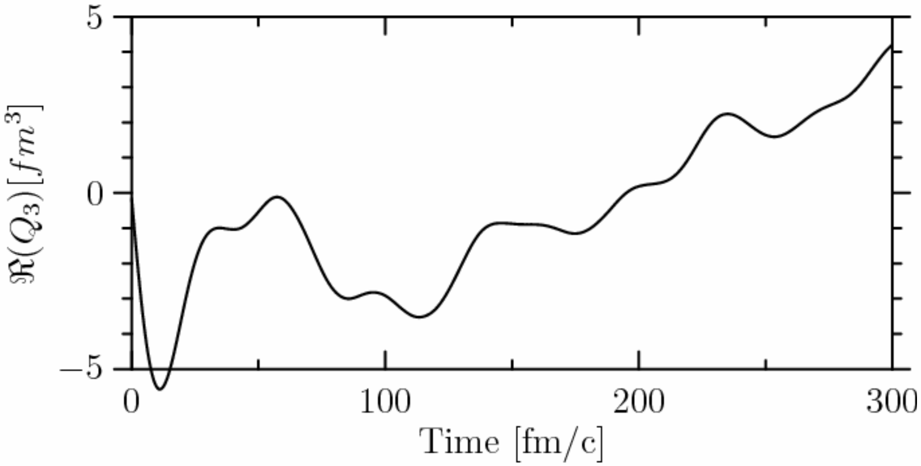
$K^\pi=2^+$

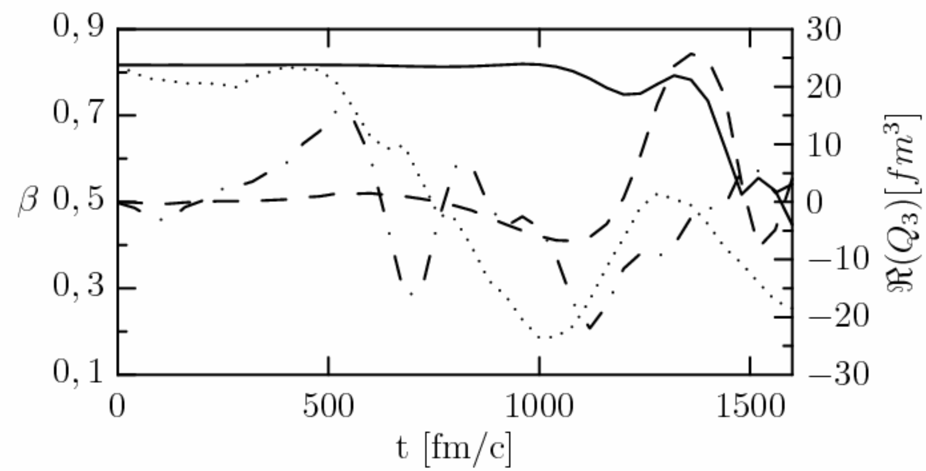
Dynamic Stability

Give wave functions an initial boost factor
with r=3fm, α=1fm
Then do time-dependent calculation.
Result shows long-term return to ground state, but some oscillations before.

$$A\frac{\exp e^{iQ(\vec{r})}}{1+e^{(r-r_0)/\alpha}}$$

Sample calculations for 0.04 and 2.83 MeV excitation energy

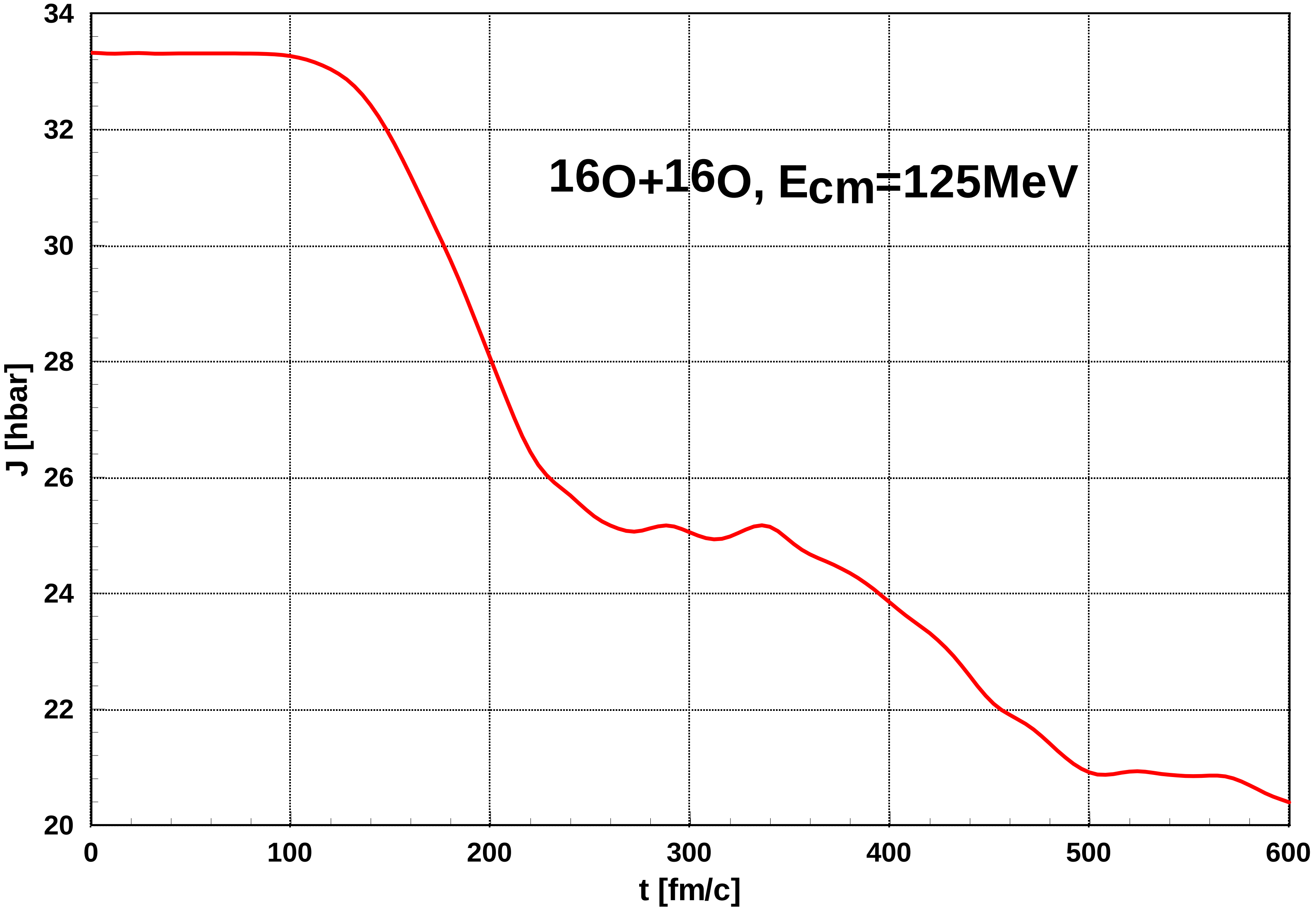




Summary

- Static Hartree-Fock seems to yield metastable states as well
- Stability crucially dependent on symmetries
- In ^{16}C the superdeformed chain-type states are unstable for sausage deformation, but may be present as resonances
- TDHF and constrained Hartree-Fock may be used to test stability

Angular Momentum Not Conserved?



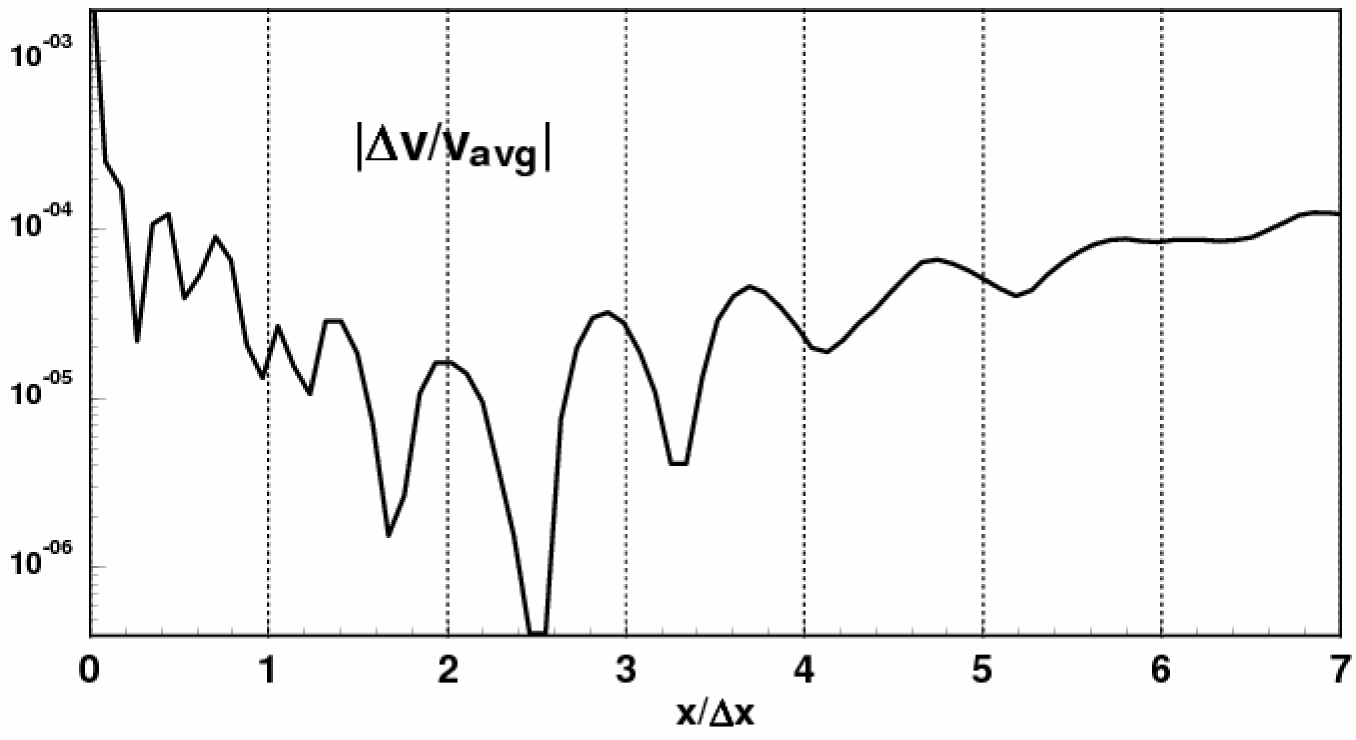
Conserved Quantities

Quantity	Periodic Boundary Conditions (no Coulomb)	„Reflecting“ Boundary Conditions
Particle Number	Per-cell value strictly conserved. In practice good to 10^{-4}	Not conserved when matter interacts with boundary
Total energy	Per-cell value strictly conserved. In practice good to 10^{-4}	Not conserved when matter interacts with boundary
Momentum	Per-cell value strictly conserved. In practice good to 10^{-4}	Not conserved when matter interacts with boundary
Angular momentum	Not conserved when matter leaves cell, because defined relative to specific cell center	Not conserved when matter interacts with boundary

Note that conservation is physically incorrect if particles leave the cell but are spuriously reentered by boundary conditions!

Momentum Conservation

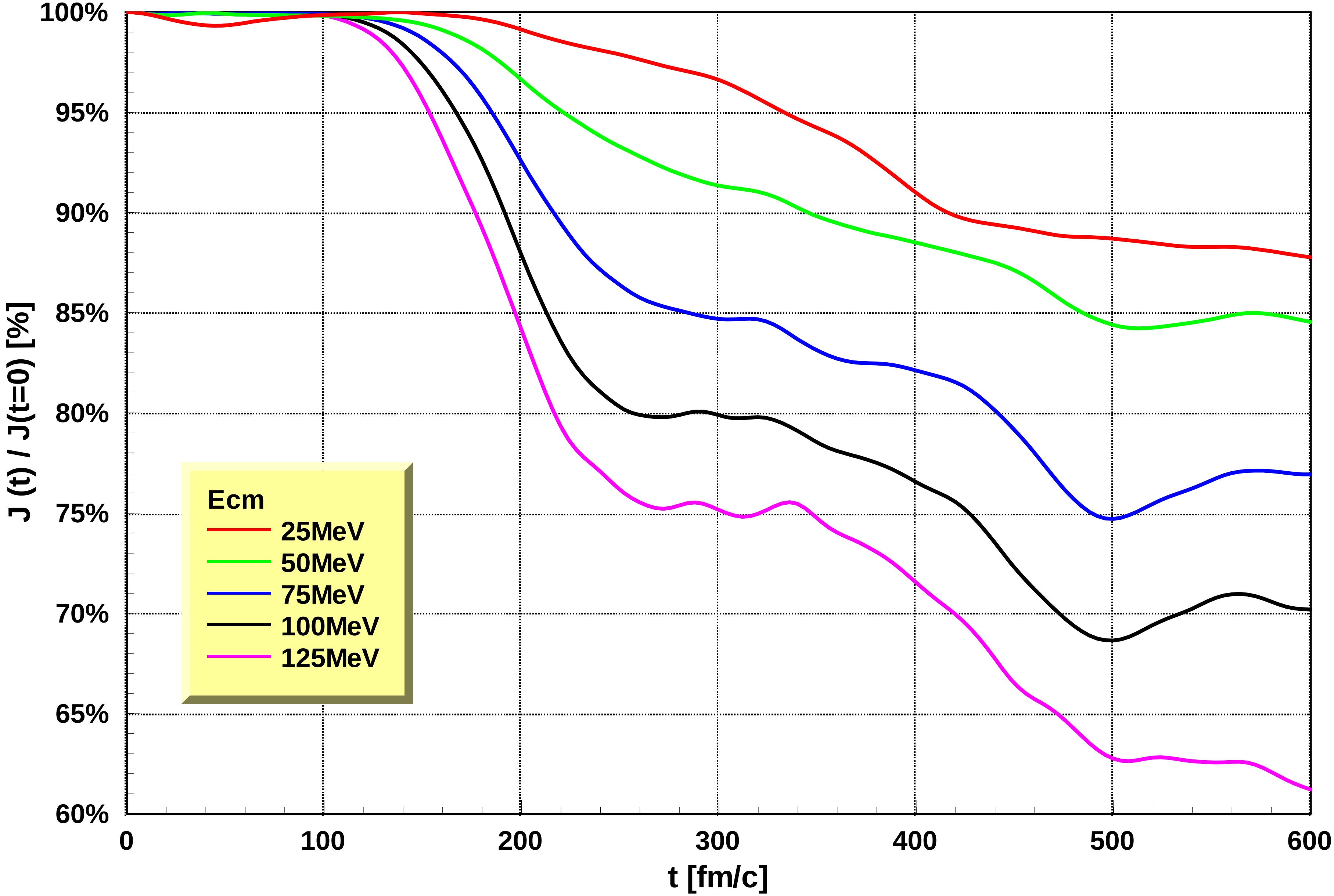
Free translation of ^{16}O through a numerical mesh
Kinetic energy 48 MeV/c



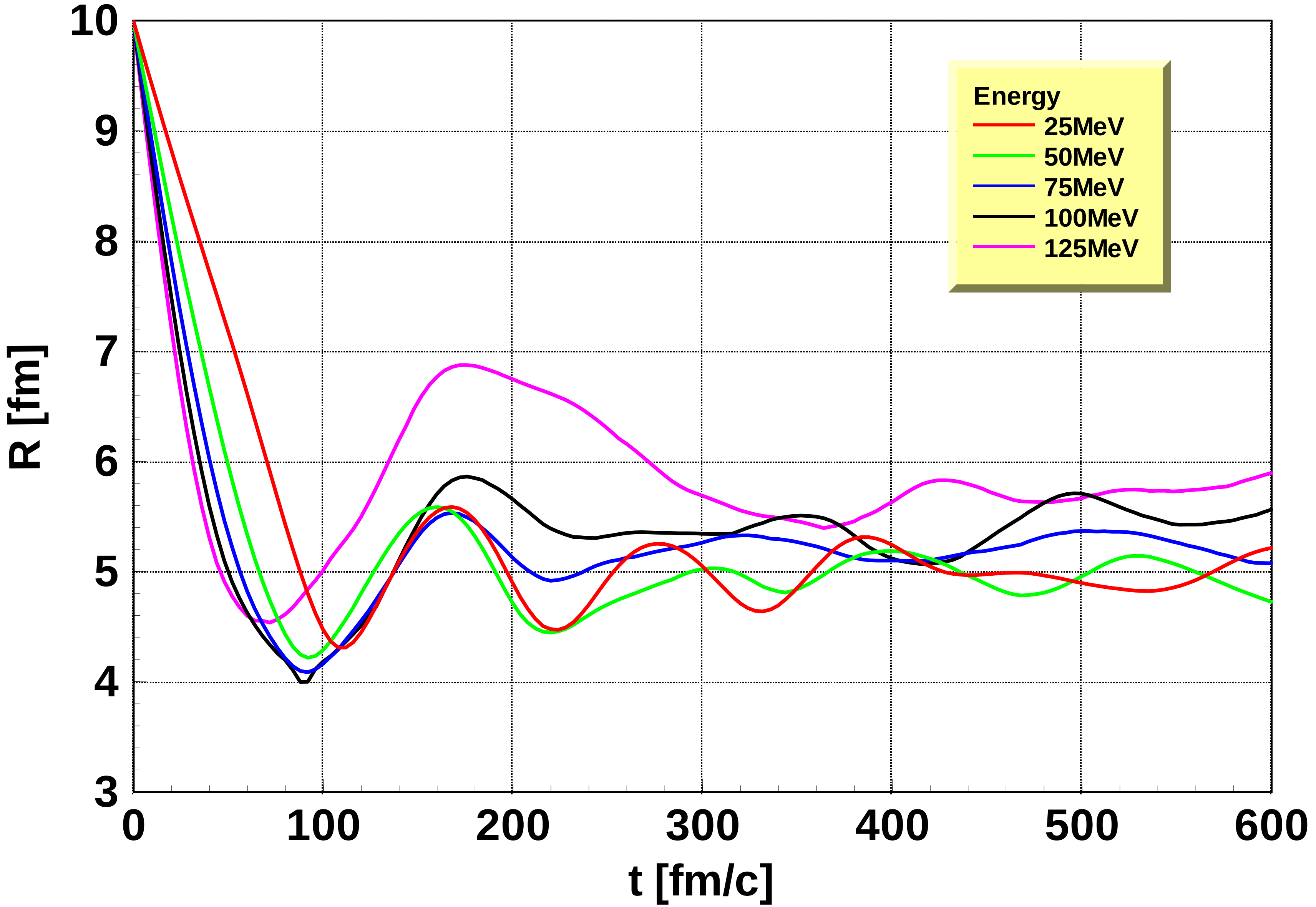
Test Case for Rotation

- ^{16}O on ^{16}O at E_{cm} from 25 through 125 MeV
- Grid spacing 1 fm, size 32×24×32
- Full Skyrme SkI3 or Sly6
- Initial spacing 10 fm
- b(E) varied to keep minimum distance constant

To the best of our knowledge, angular momentum conservation in 3D TDHF was never investigated – or not published?



100%
95%
90%
85%
80%
75%
70%
65%
60%
J (t) / J(t=0) [%]
0
100
200
300
400
500
600
t [fm/c]
Ecm
25MeV
50MeV
75MeV
100MeV
125MeV

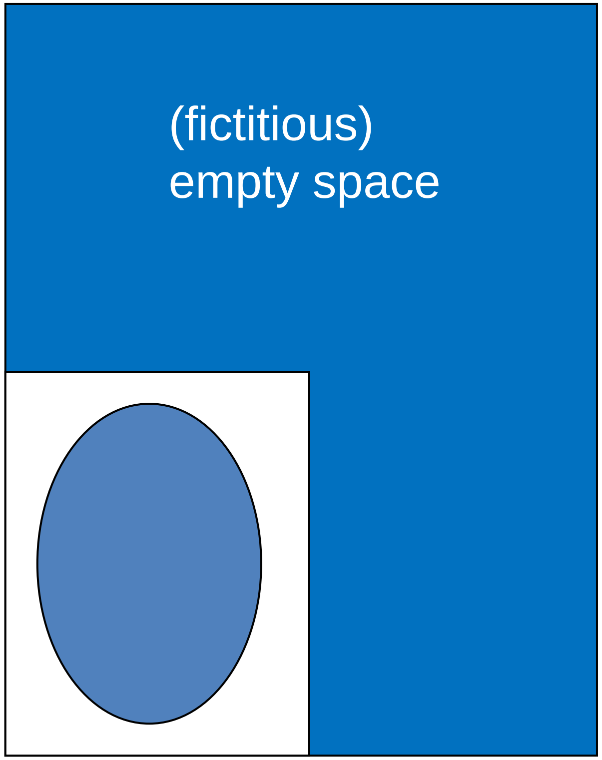

R [fm]
10
9
8
7
6
5
4
3
0
100
200
300
400
500
600
t [fm/c]
Energy
25MeV
50MeV
75MeV
100MeV
125MeV

Principal Questions

- Rotating wave functions on a Cartesian grid means stretching and shrinking the spacing by a factor $\sqrt{2}$. How accurately can rotation be described?
- There should be a *physical loss* of angular momentum of the compound system by emission of particles
- Particles crossing the boundary can add *spurious* loss, because the numerical boundary conditions are not correct. This problem is known from giant resonance calculations (P.-G. Reinhard, P. D. Stevenson, D. Almehed, J. A. Maruhn, and M. R. Strayer, Phys. Rev. E **73**, 036709 (2006)).
- Problems from the Coulomb field should appear only when particles approach the boundary

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



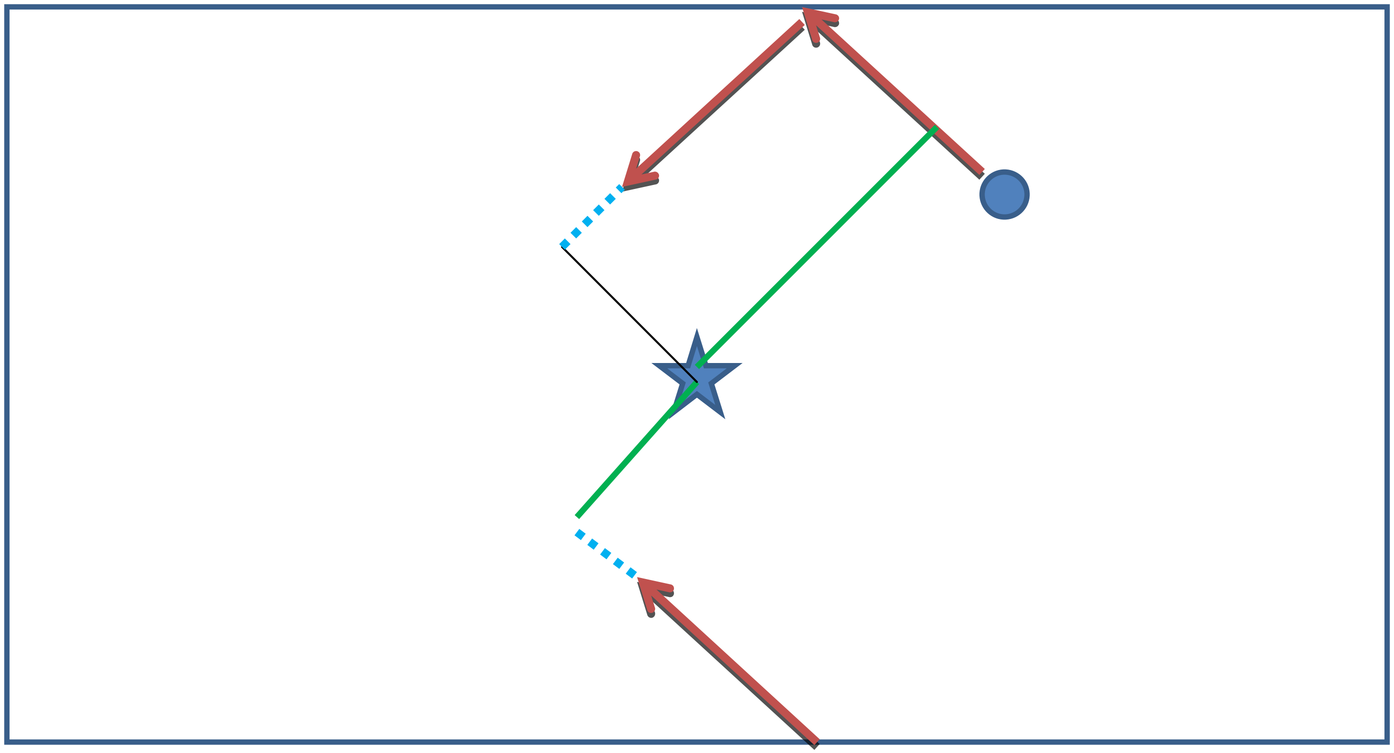
The solution constructed via

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

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

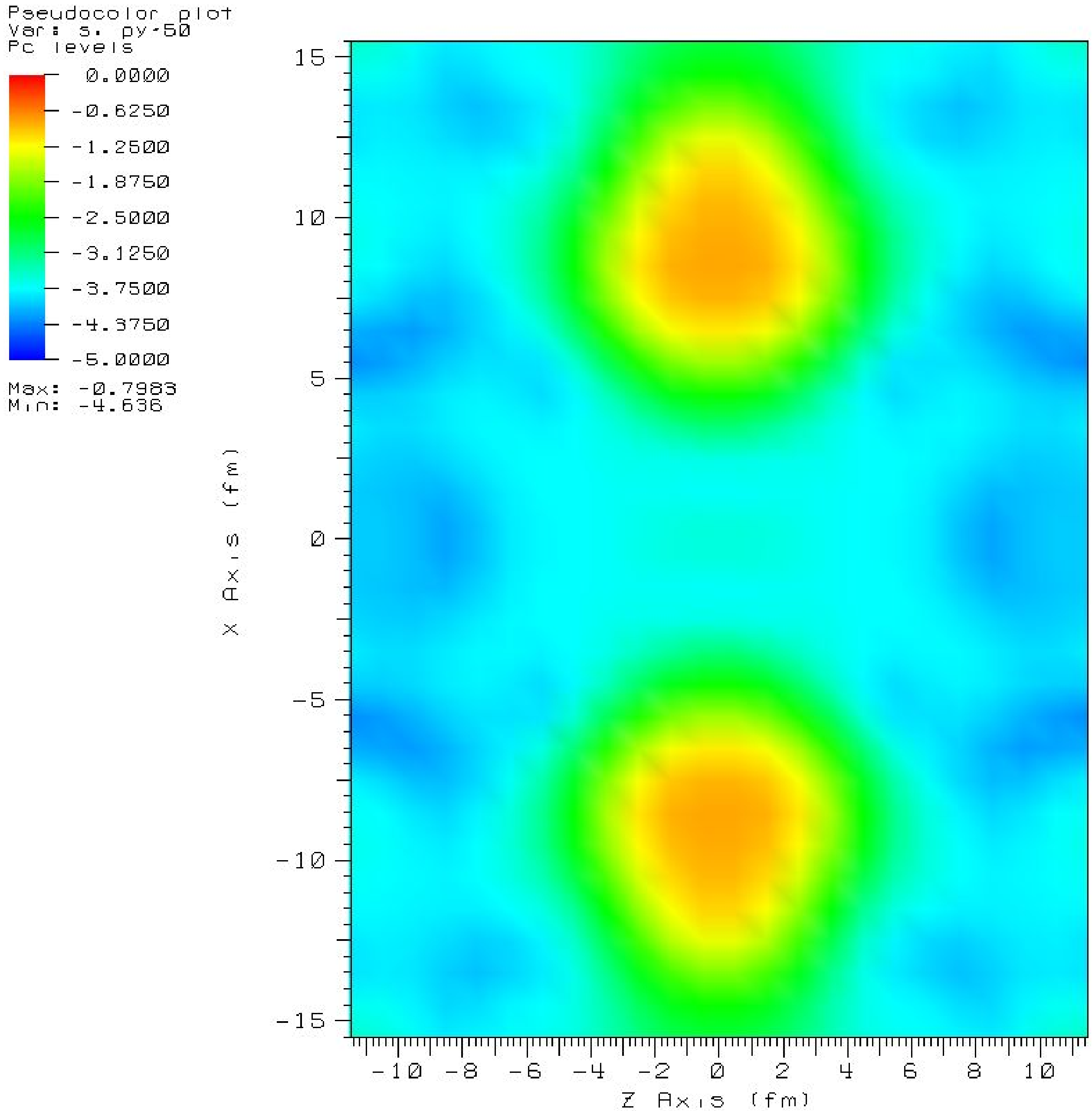
J.W. Eastwood and D.R.K. Brownrigg, J. Comp. Phys. **32**, 24 (1979)

Both periodic and reflecting boundary conditions can change the angular momentum drastically!



Emission and Reflection in

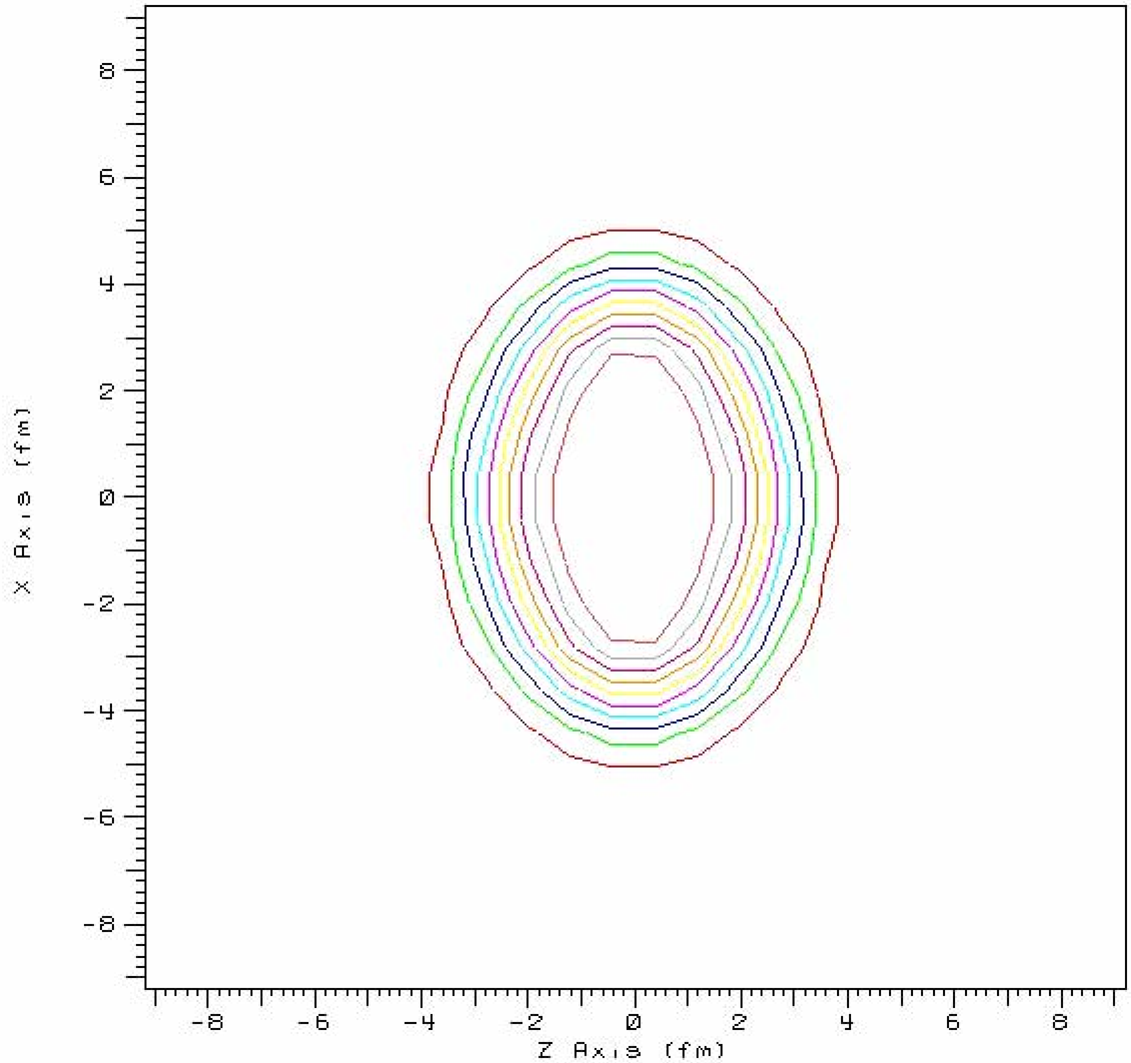
Log (ρ)



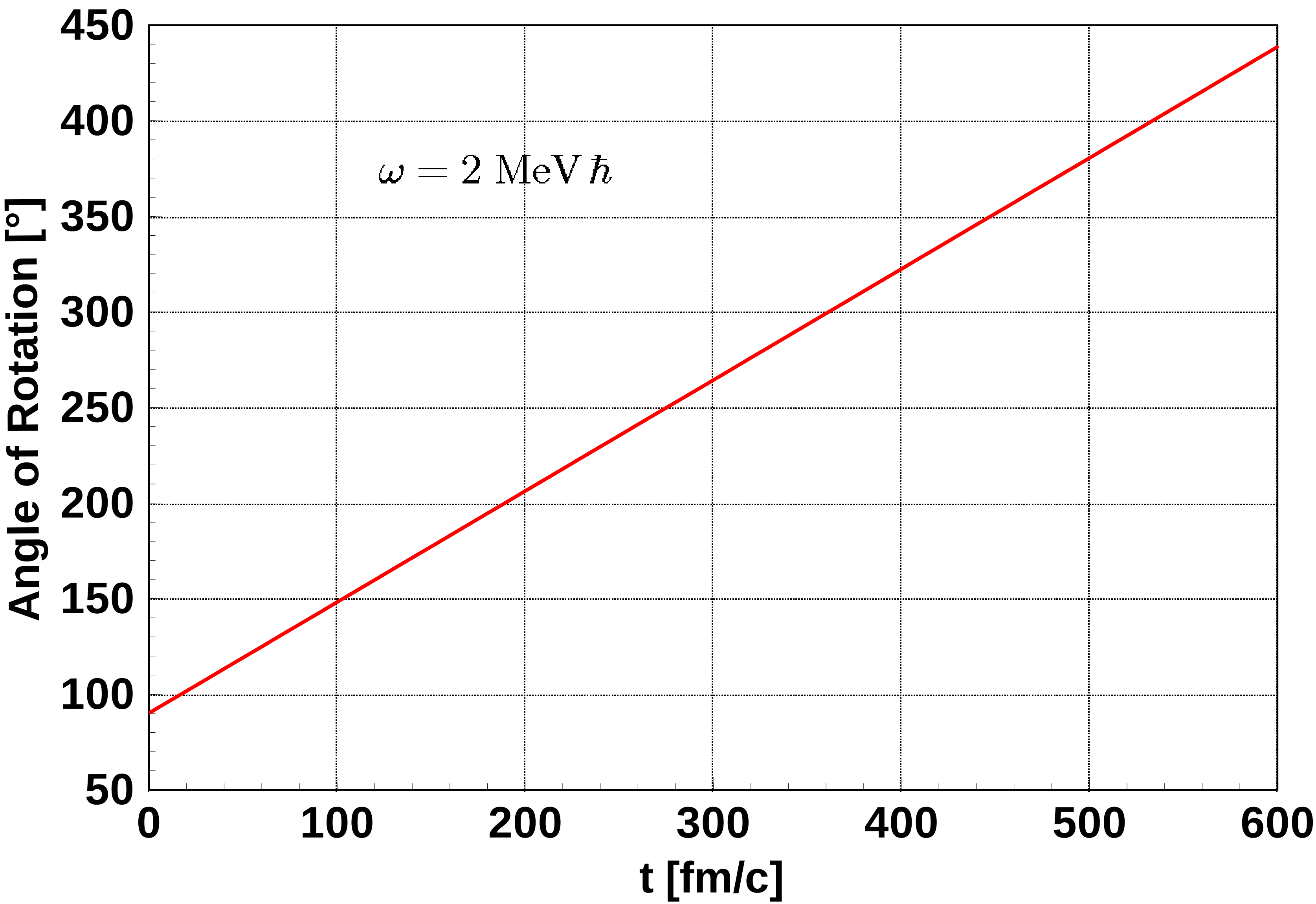
Rotation of a „Cranked“ Nucleus

- Obtain the static Hartree-Fock solution with an $\omega \hat{J}_z$ constraint
- Use this as the starting value for a time-dependent calculation *without* constraint term
- The result is a uniformly rotating nucleus in the 3-dimensional Cartesian grid
- This could be useful for studying unstable rotation

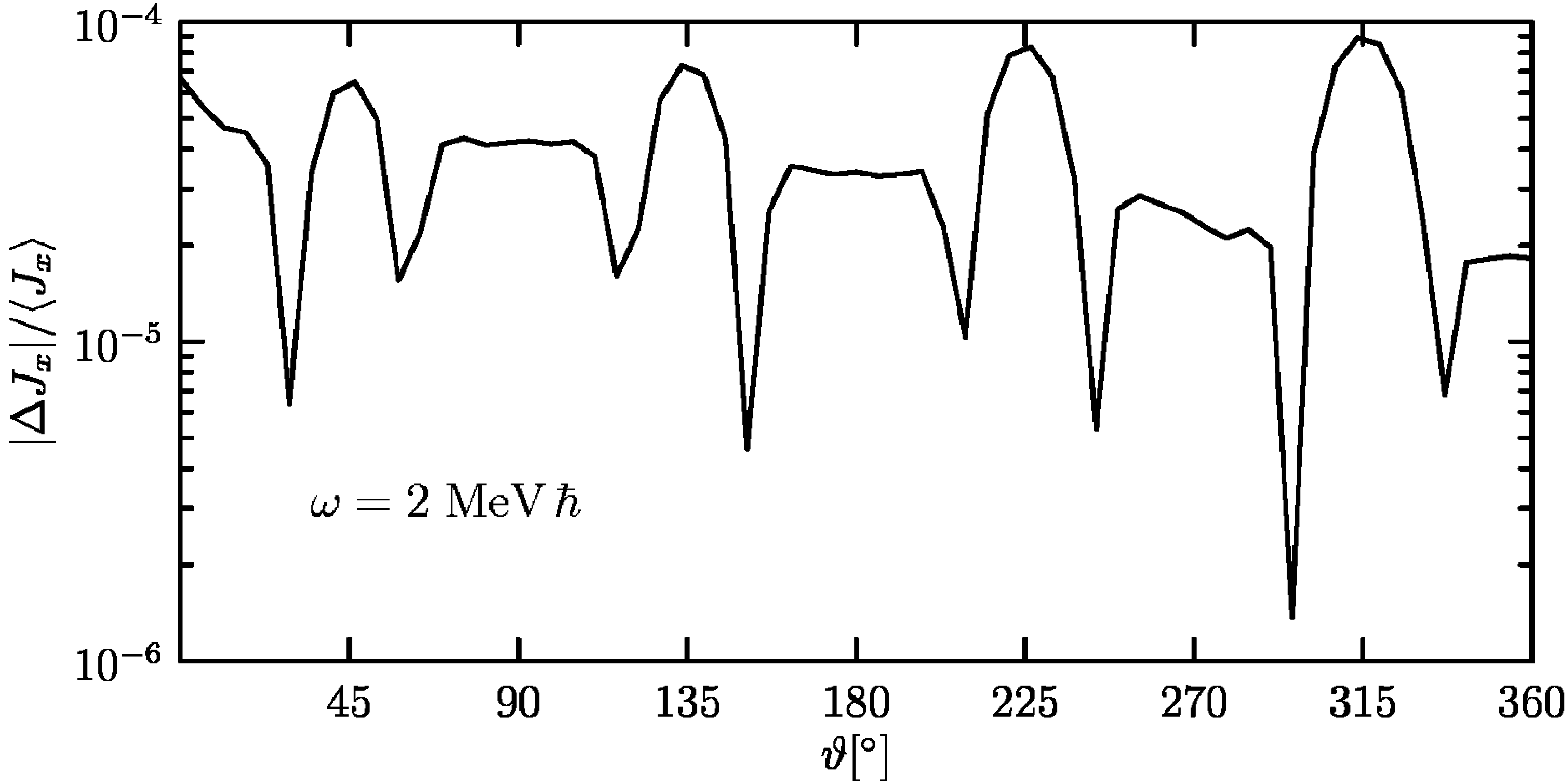
Rotation of Mg^{24}, full physics, ω=2 MeV/hbar



Rotation of Mg^{24}, full physics

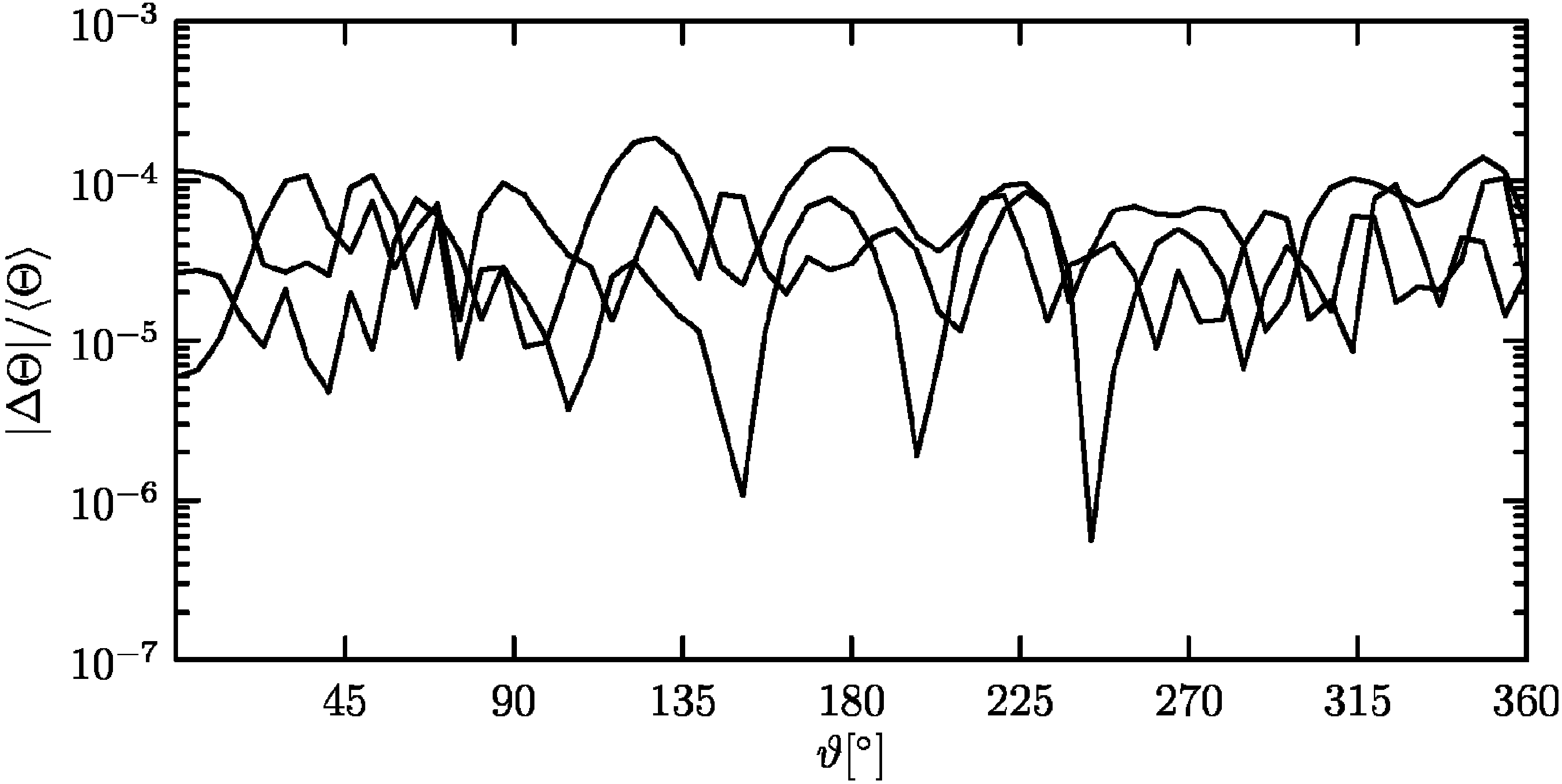


Rotation of Mg^{24}, full physics



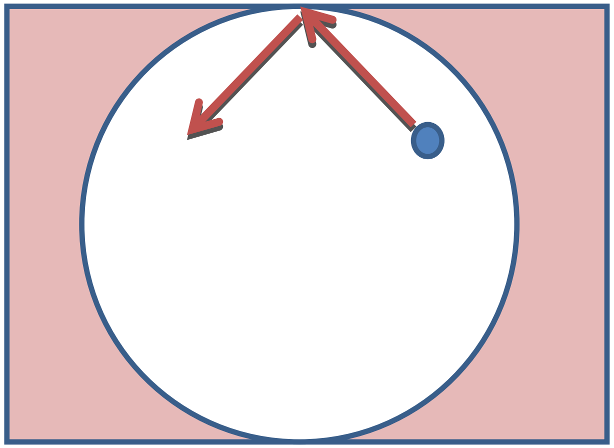
The changes in angular momentum are surprisingly small
and correlated with the rotation angle. In this case, the moment of inertia is very close to the rigid-body value.

Rotation of Mg^{24}, full physics, ω=2 MeV/hbar

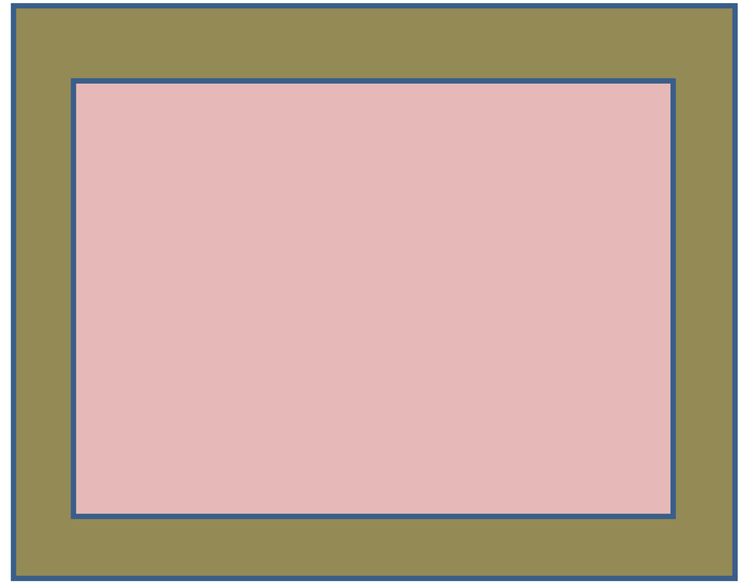


The moments of inertia show small excitations through the interaction with the grid, which are not correlated simply with the orientation angle.

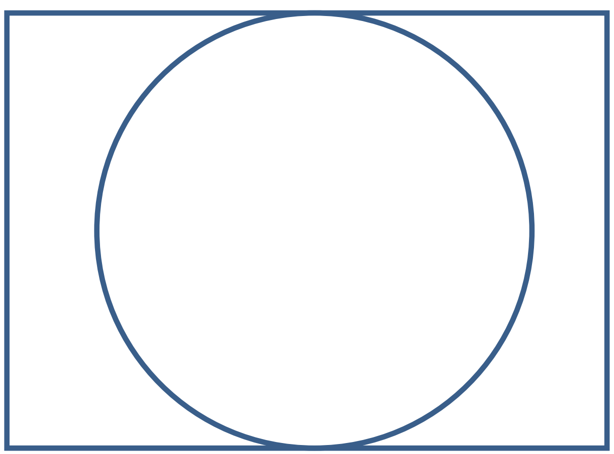
Tests and Correction Attempts



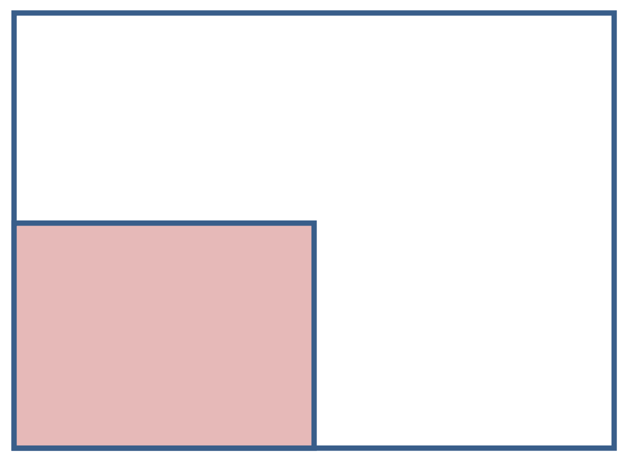
Spherical enclosing potential



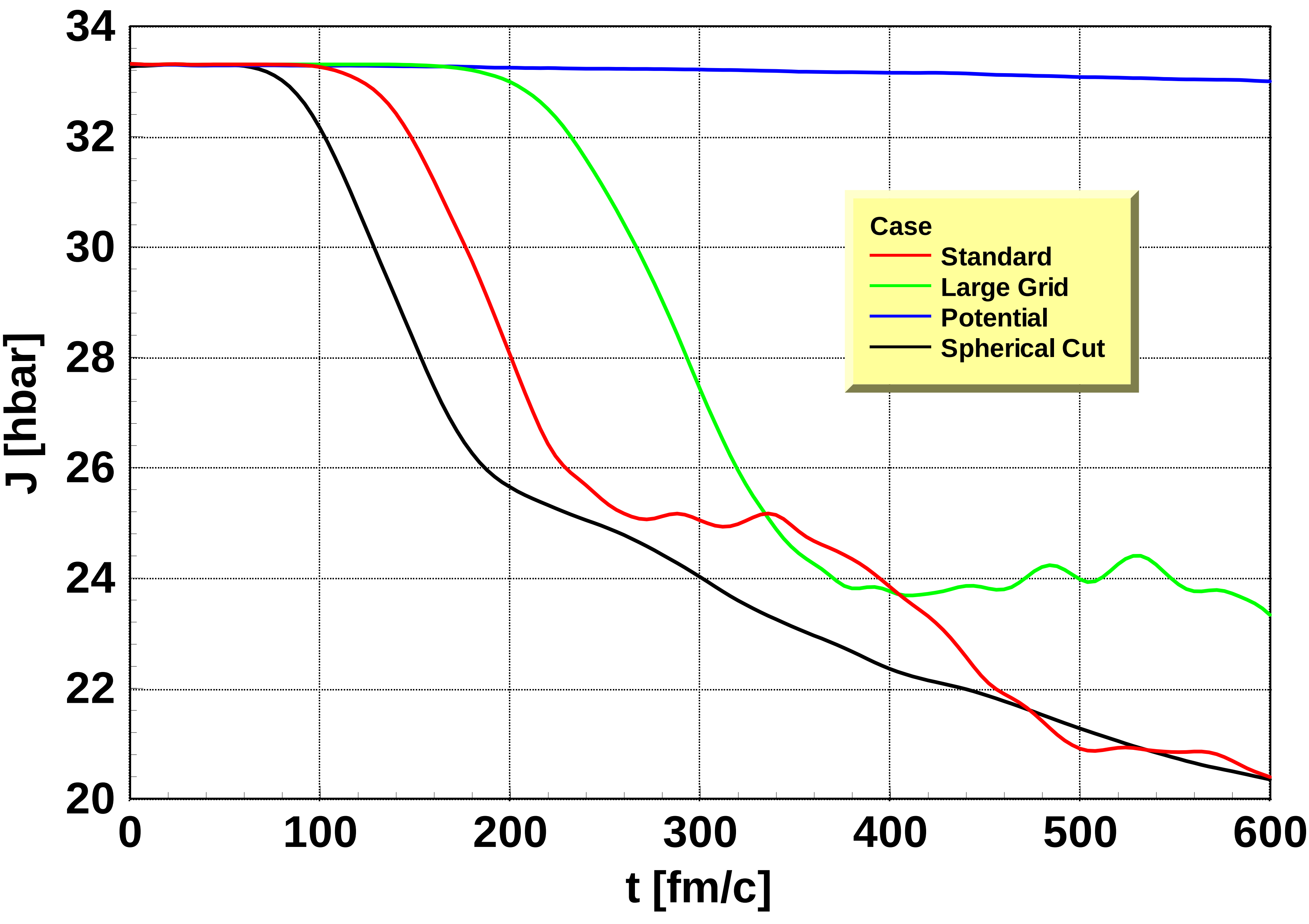
Enclosing absorbing potential



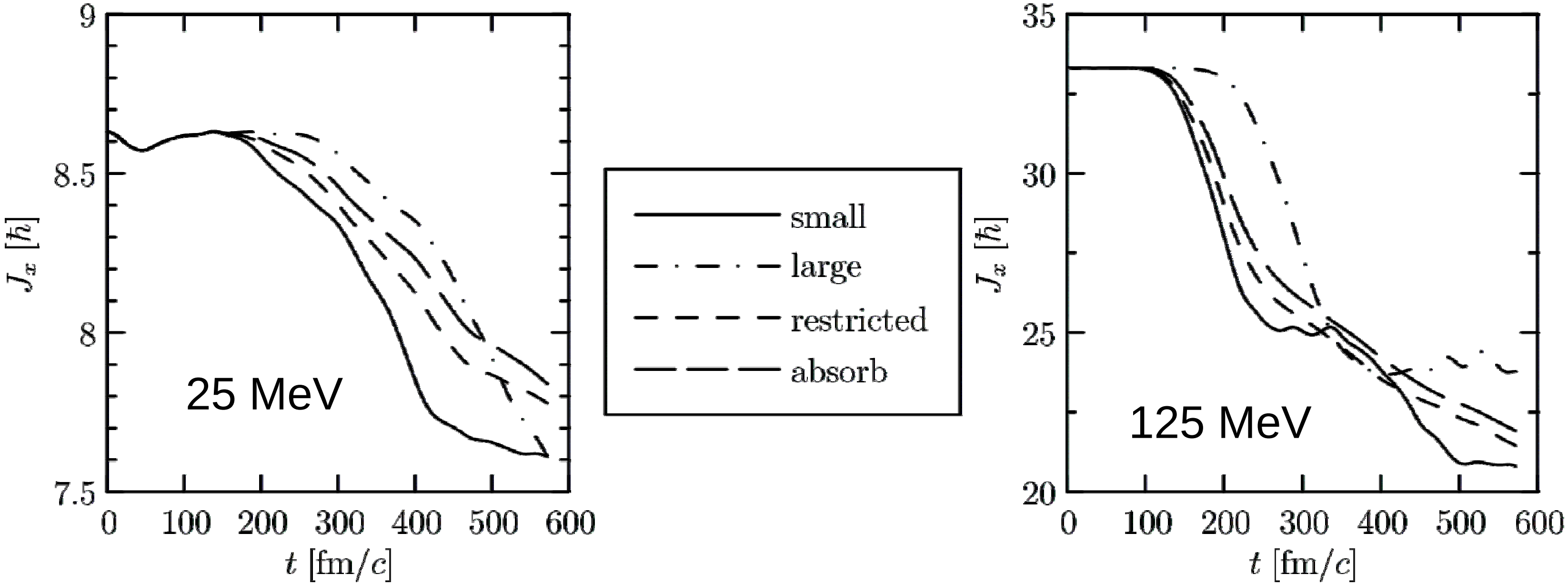
Spherical cutoff in J



Doubling the mesh


34
32
30
28
26
24
22
20
0
100
200
300
400
500
600
J [hbar]
t [fm/c]
Case
Standard
Large Grid
Potential
Spherical Cut

Attempt to determine the „correct“ loss



• „Restricted“ calculation: run in large box, but sum J only over small one. Should give proper physical loss for some time.

•The initial part of the reduction of angular momentum seems to be „physical“.

• This amounts to 2-3 rebounds, so that fusion studies may be correct.

Conclusions

- The interaction of emitted particles with the boundary causes major problems in TDHF.
- It corresponds to an additional *dissipation of collective energy.*
- The largest effects occur for angular momentum.
- The quality of rotation of an unexcited nucleus in the Cartesian grid is surprisingly good and could open new applications.
- For collisions, most of the loss in angular momentum appears to be „physical“ in the initial stages of the reactions.
- Longer-term calculations will need larger grids and/or absorptive layers: more expense.
- It remains to be seen to what extent the particle loss is physical.