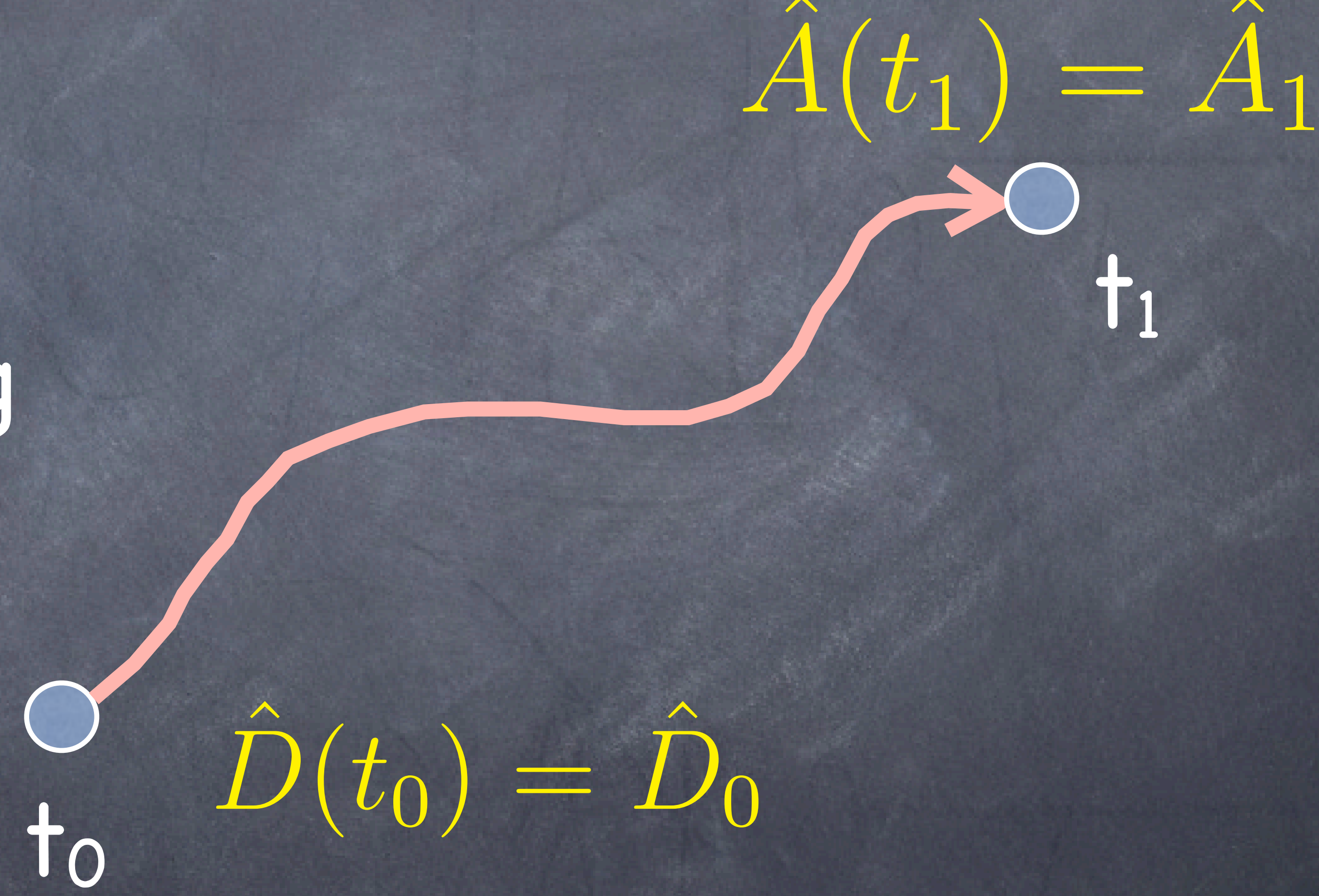
Particle number *fluctuations* and *correlations* with the Balian-Vénéroni variational principle

Cédric Simenel
CEA/Saclay, IRFU/SPhN (France)

Balian-Vénéroni variational principle

Boundary conditions

Expectation value of A_1 at t_1 knowing the state D_0 at t_0



R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Balian-Vénéroni variational principle

Boundary conditions $\hat{D}(t_0) = \hat{D}_0$ $\hat{A}(t_1) = \hat{A}_1$

Action-like quantity

$$J = \mathrm{Tr}\left[\hat{A}(t_1)\hat{D}(t_1)\right] - \int_{t_0}^{t_1} dt\ \mathrm{Tr}\left[\hat{A}(t)\left(\frac{d\hat{D}(t)}{dt} + i\left[\hat{H}(t), \hat{D}(t)\right]\right)\right]$$

$$\delta_A J = 0 \quad \Rightarrow \quad i\frac{d\hat{D}(t)}{dt} = \left[\hat{H}, \hat{D}(t)\right]$$

Schrödinger equation

R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Balian-Vénéroni variational principle

Variational spaces

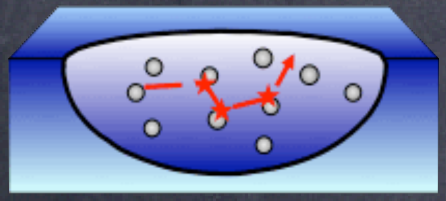
1-body observables $\delta_A \hat{A}(t) \equiv \hat{a}^\dagger \hat{a}$

R, P, E_{kin}, L, N...

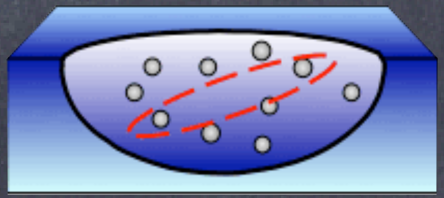
Independent particles $\hat{D}(t) = |\phi(t)\rangle\langle\phi(t)|$

Neglected correlations:

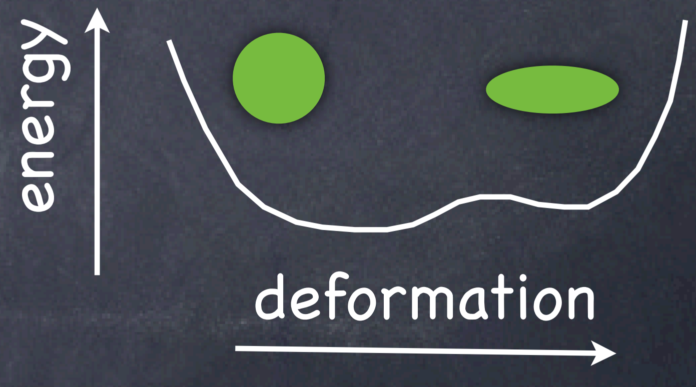
collision term



pairing



configuration mixing



R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Balian-Vénéroni variational principle

Time-dependent Hartree-Fock (TDHF) equation

$$i\hbar\frac{d}{dt}\rho = [h[\rho],\rho]$$

1-body density matrix $\rho_{\alpha\beta} = \mathrm{Tr}\left[\hat{D}\hat{a}^\dagger_\beta\hat{a}_\alpha\right]$

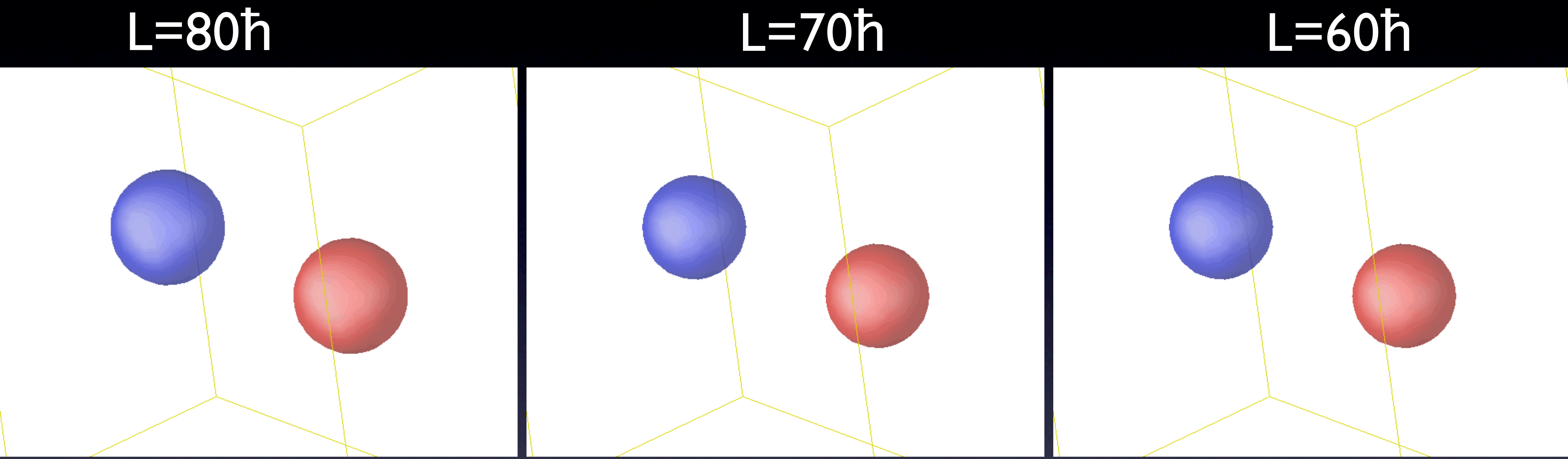
HF single-particle Hamiltonian $h[\rho]_{\alpha\beta} = \frac{\delta\langle\hat{H}\rangle}{\delta\rho_{\beta\alpha}} = \frac{\delta E[\rho]}{\delta\rho_{\beta\alpha}}$

with energy density functional (EDF) E[ρ]

R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

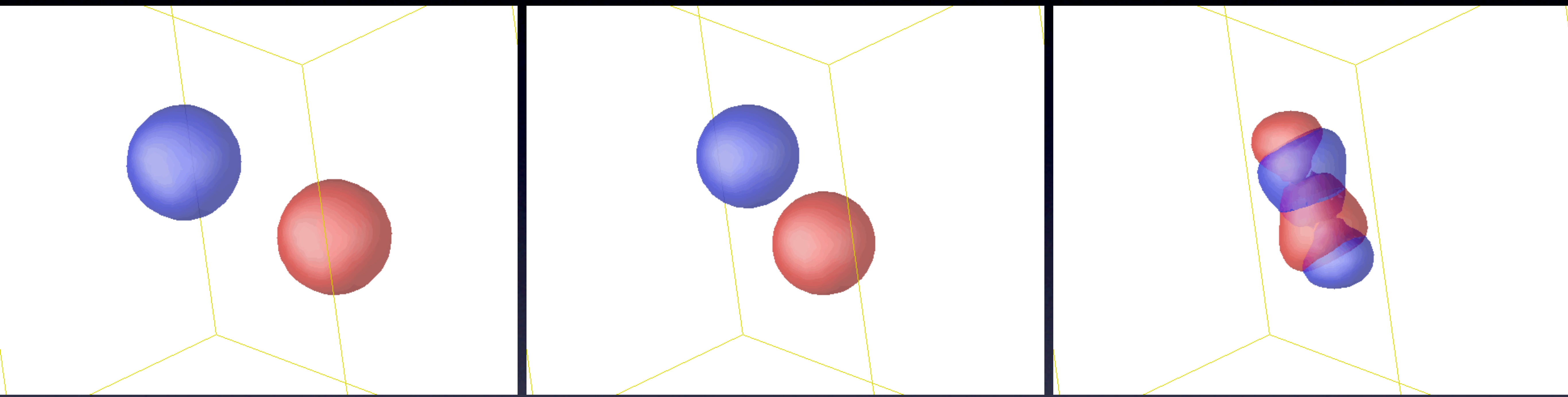


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

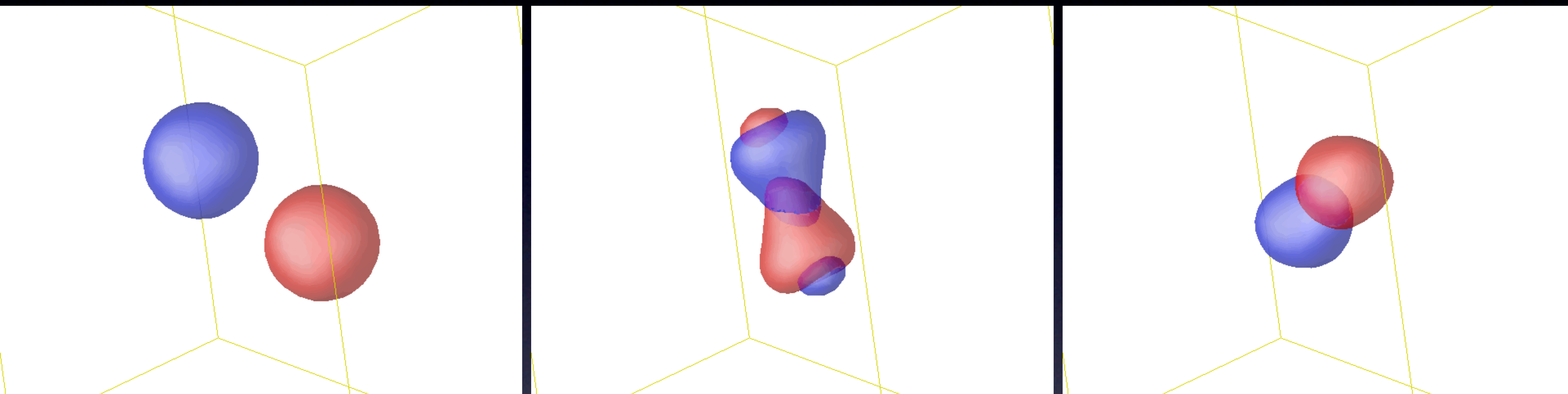


C.S., PRL 2011

Deep-inelastic collisions

^{40}Ca+^{40}Ca at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

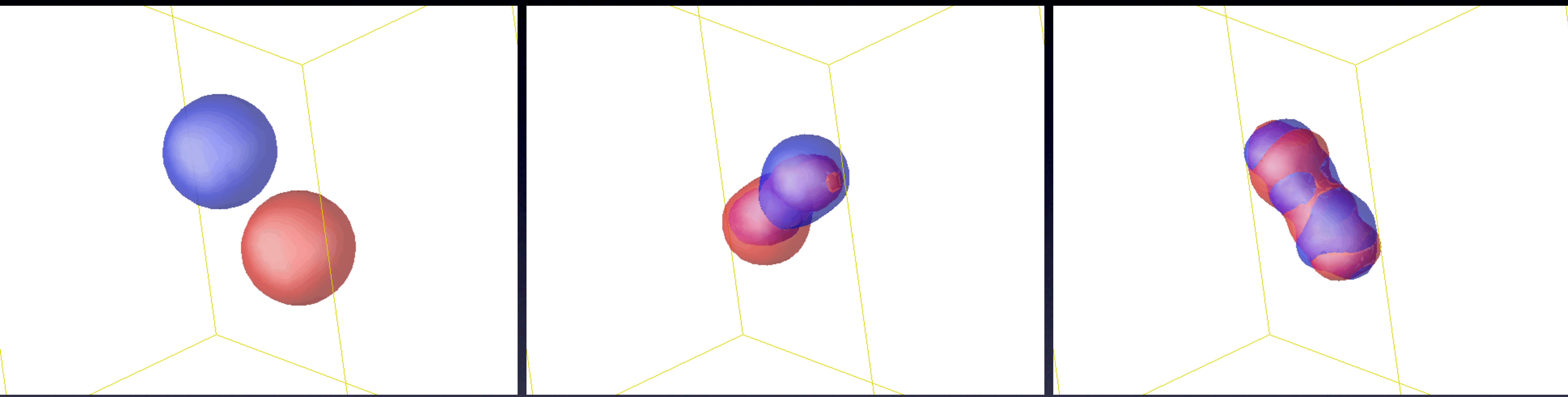


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

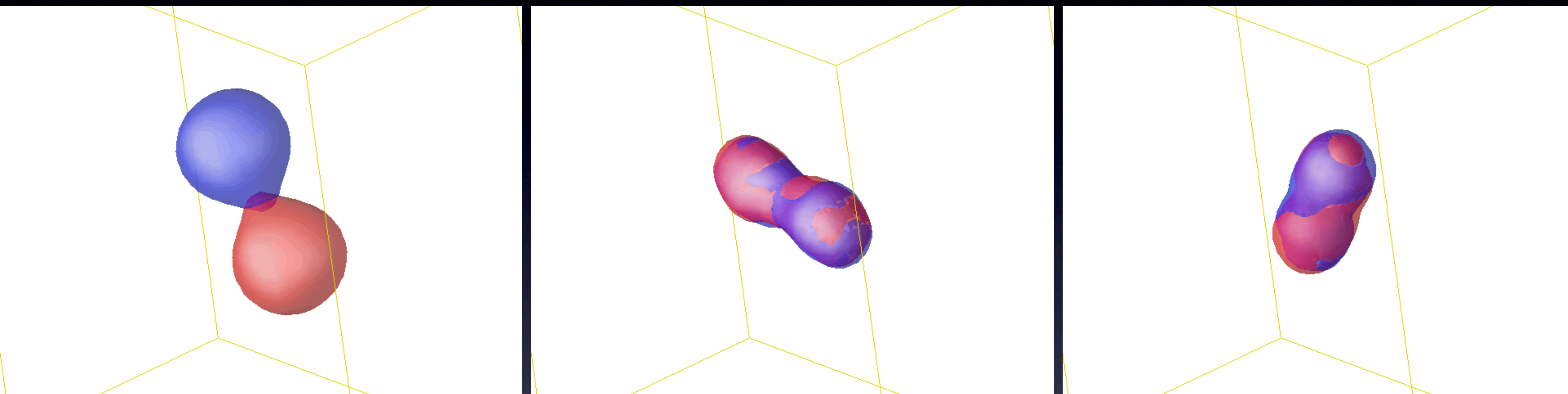


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca + ^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

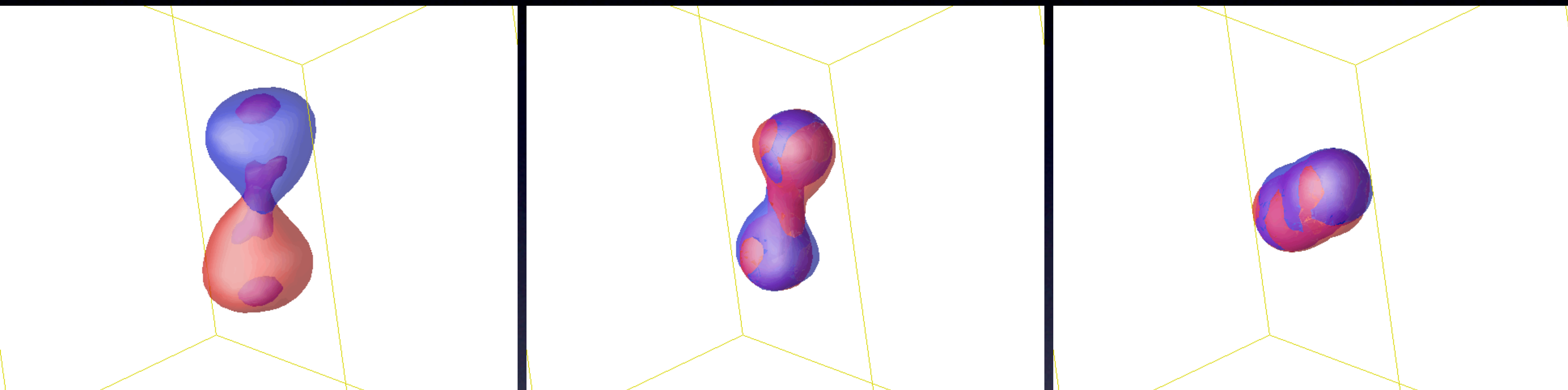


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at $E_{cm}=128$ MeV

$L=80\hbar$ $L=70\hbar$ $L=60\hbar$

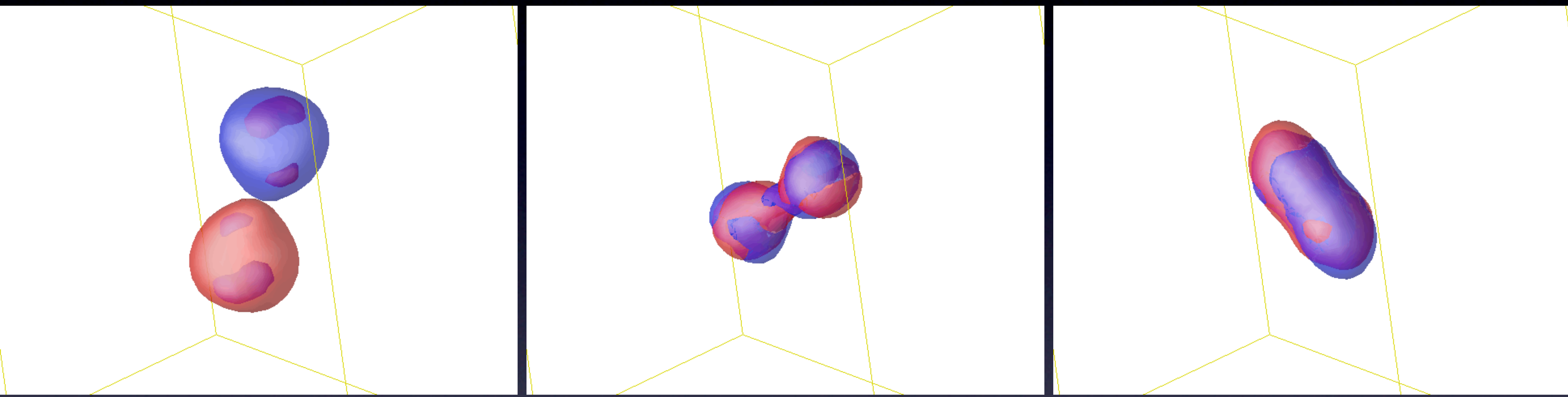


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

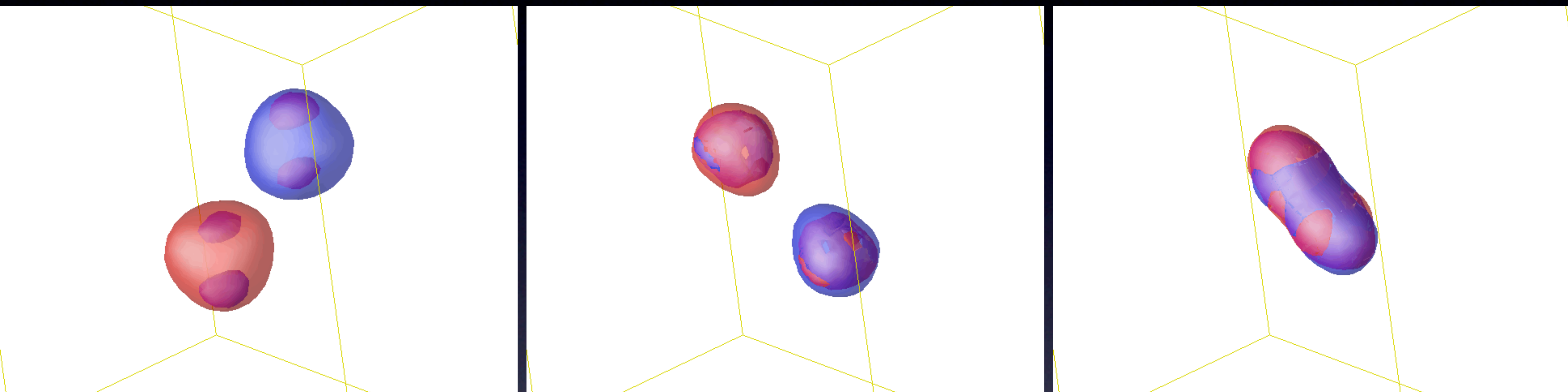


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

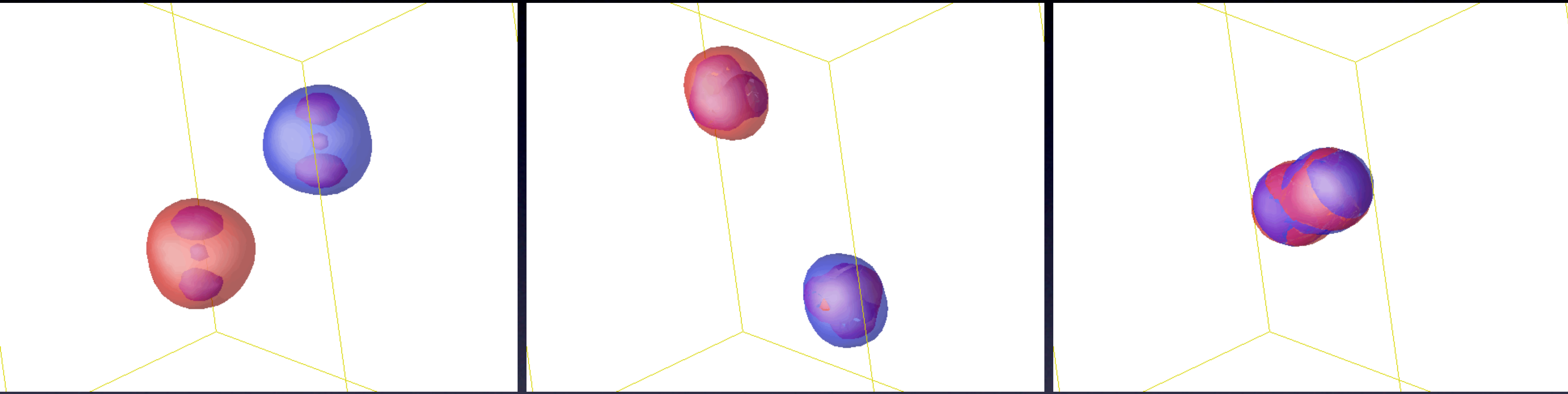


C.S., PRL 2011

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=80ħ L=70ħ L=60ħ

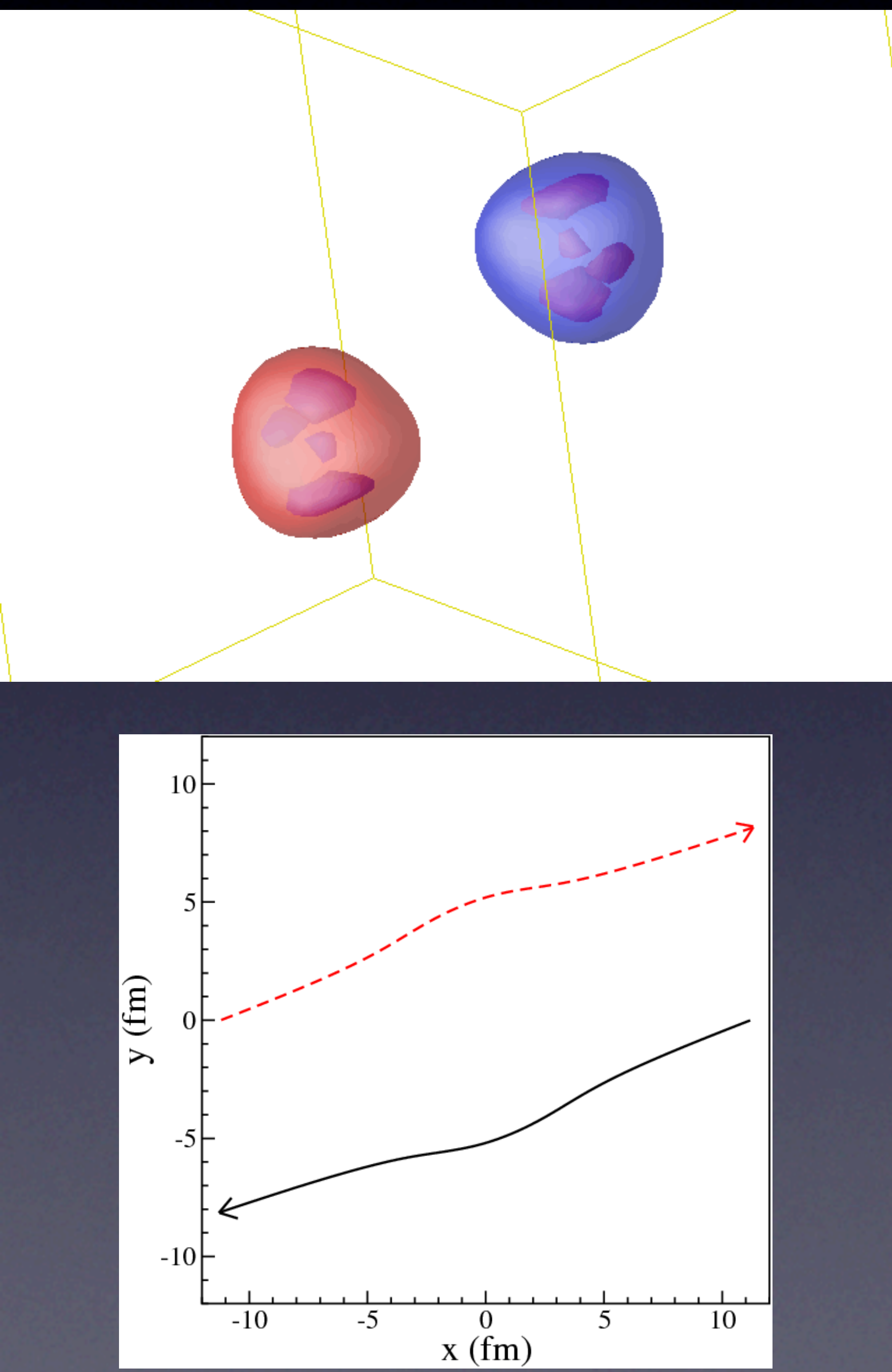


C.S., PRL 2011

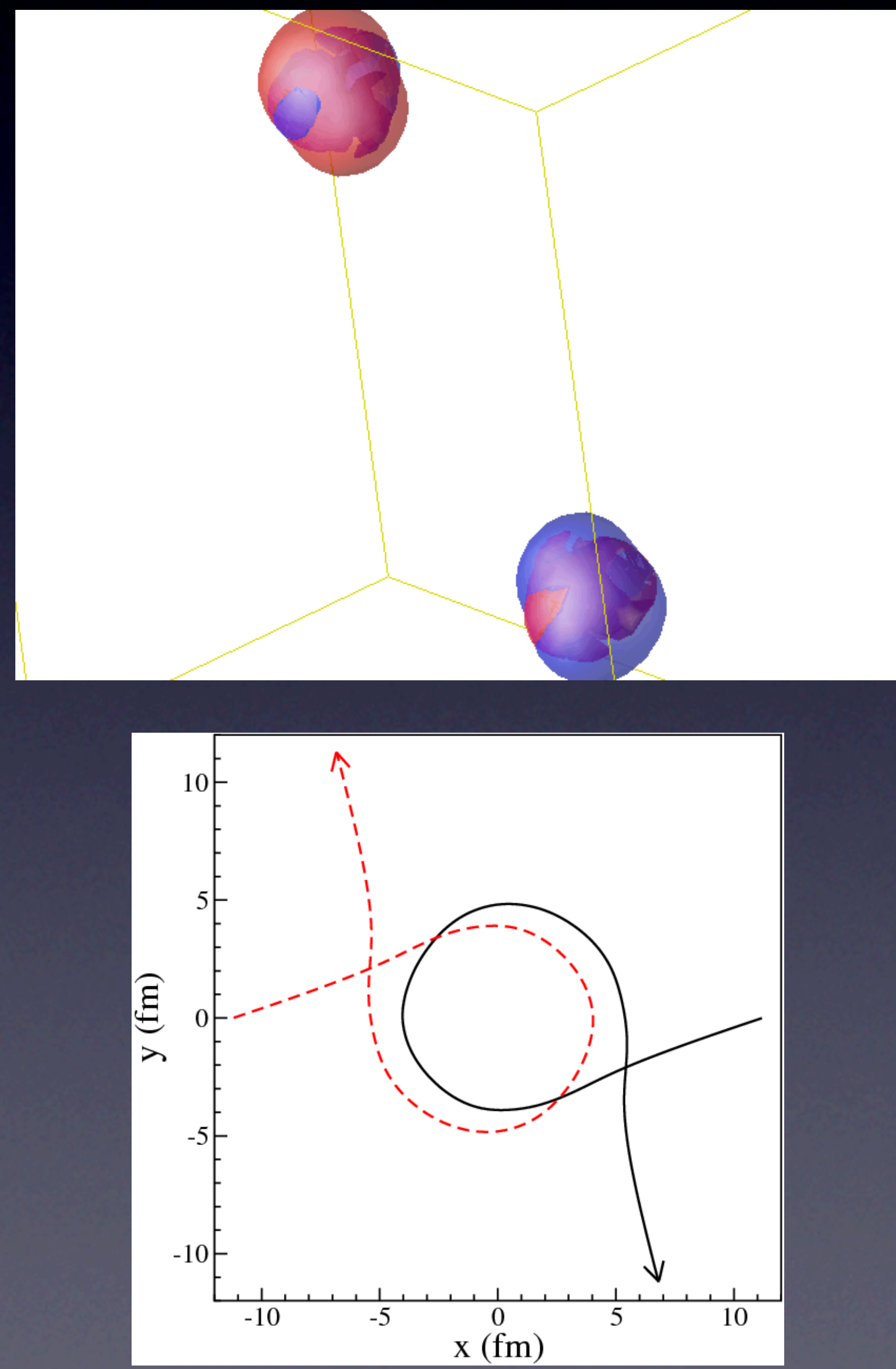
Deep-inelastic collisions

$^{40}Ca + ^{40}Ca$ at E_{cm}=128 MeV

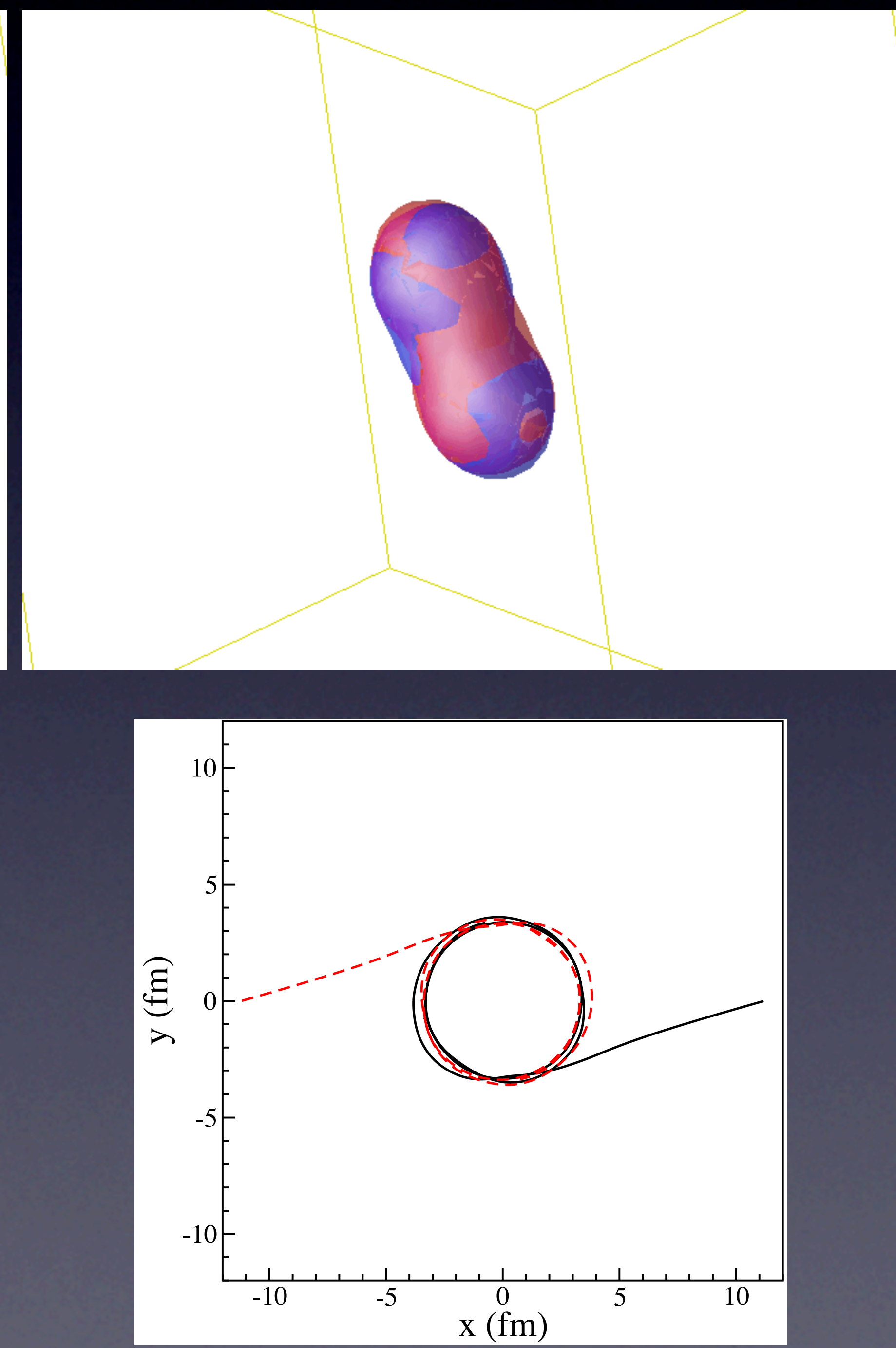
L=80ħ



L=70ħ



L=60ħ

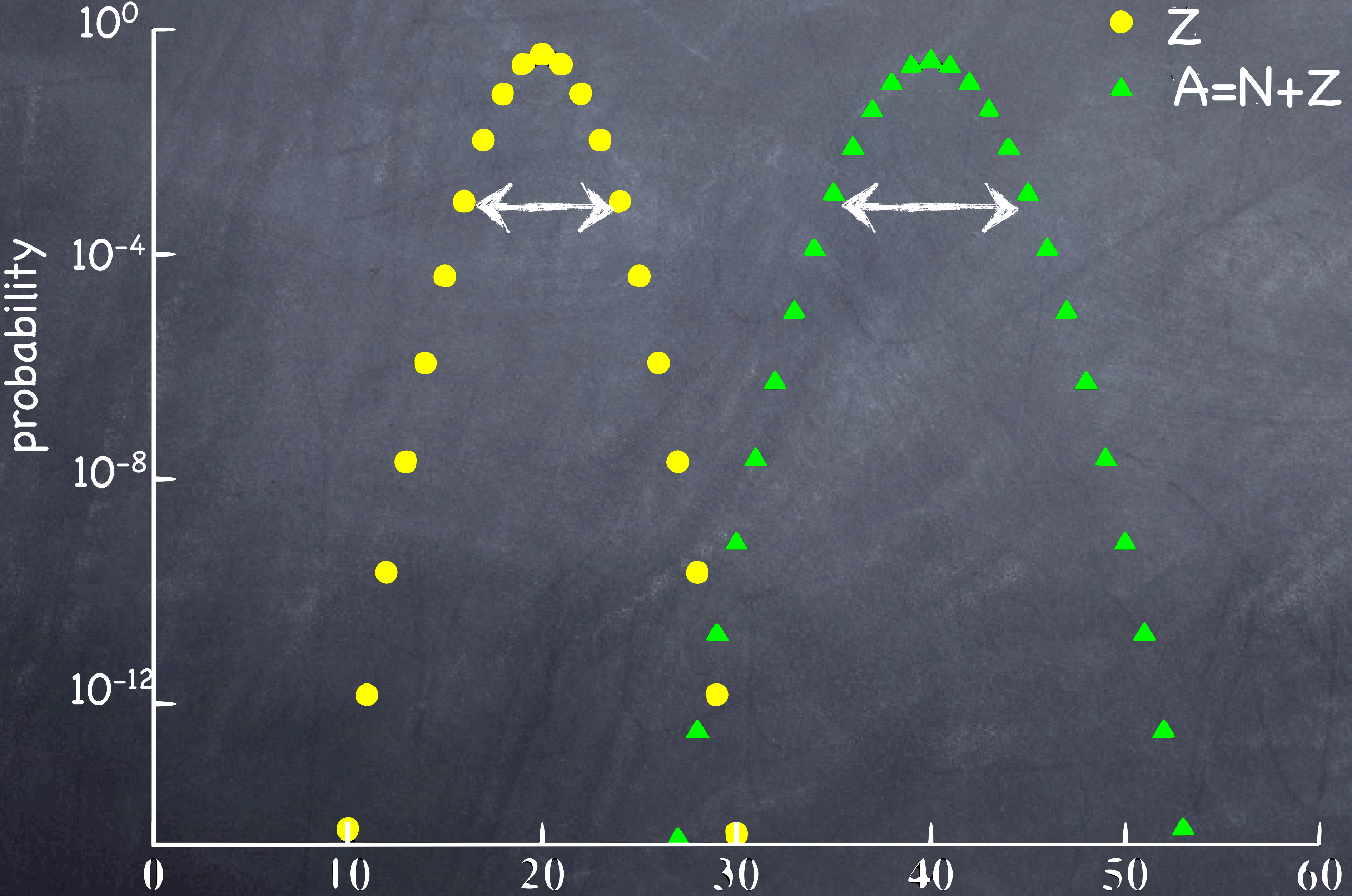


C.S., PRL 2011

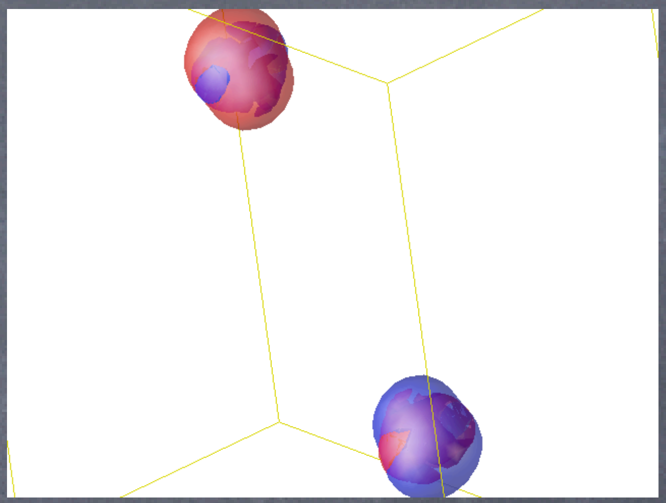
Deep-inelastic collisions

Mass and charge distributions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV



L=70ħ



$$\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2}$$

$\Delta A_{TDHF} \approx 1.5$

$\Delta Z_{TDHF} \approx 1.1$

$\Delta A_{exp} \approx 11$ (*)

$\Delta Z_{exp} \approx 5$

C.S., PRL 2010, PRL 2011

(*) data from Roynette et al., PLB 1977 and Evans et al., NPA 1991

Balian-Vénéroni variational principle

Variational spaces

Independent particles $\hat{D}(t) = |\phi(t)\rangle\langle\phi(t)|$

1-body observables $\delta_A \hat{A}(t) \equiv \hat{a}^\dagger \hat{a}$

=> TDHF

R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Balian-Vénéroni variational principle

Variational spaces

Independent particles $\hat{D}(t) = |\phi(t)\rangle\langle\phi(t)|$

exp(1-body observables) $\hat{A}(t) = \exp(-\varepsilon \hat{a}^\dagger \hat{a})$

R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Balian-Vénéroni variational principle

R. Balian and M. Vénéroni, PRL 1981; PLB 1984

Observable $\hat{Q} = \exp(-\epsilon\hat{X})$

with X = one-body operator

small ε => fluctuations $\sigma_X = \sqrt{\langle\hat{X}^2\rangle - \langle\hat{X}\rangle^2}$

indeed $\ln\langle\exp(-\epsilon\hat{X})\rangle \simeq -\epsilon\langle\hat{X}\rangle + \frac{\epsilon^2}{2}\sigma_X^2$

Variational principle $\delta S_{BV} = 0$ + independent particles

=> BV prescription $\sigma_X^2(t_1) = \lim_{\epsilon\rightarrow 0} \frac{\mathrm{tr}\{[\rho(t_0) - \rho_X(t_0,\epsilon)]^2\}}{2\epsilon^2}$

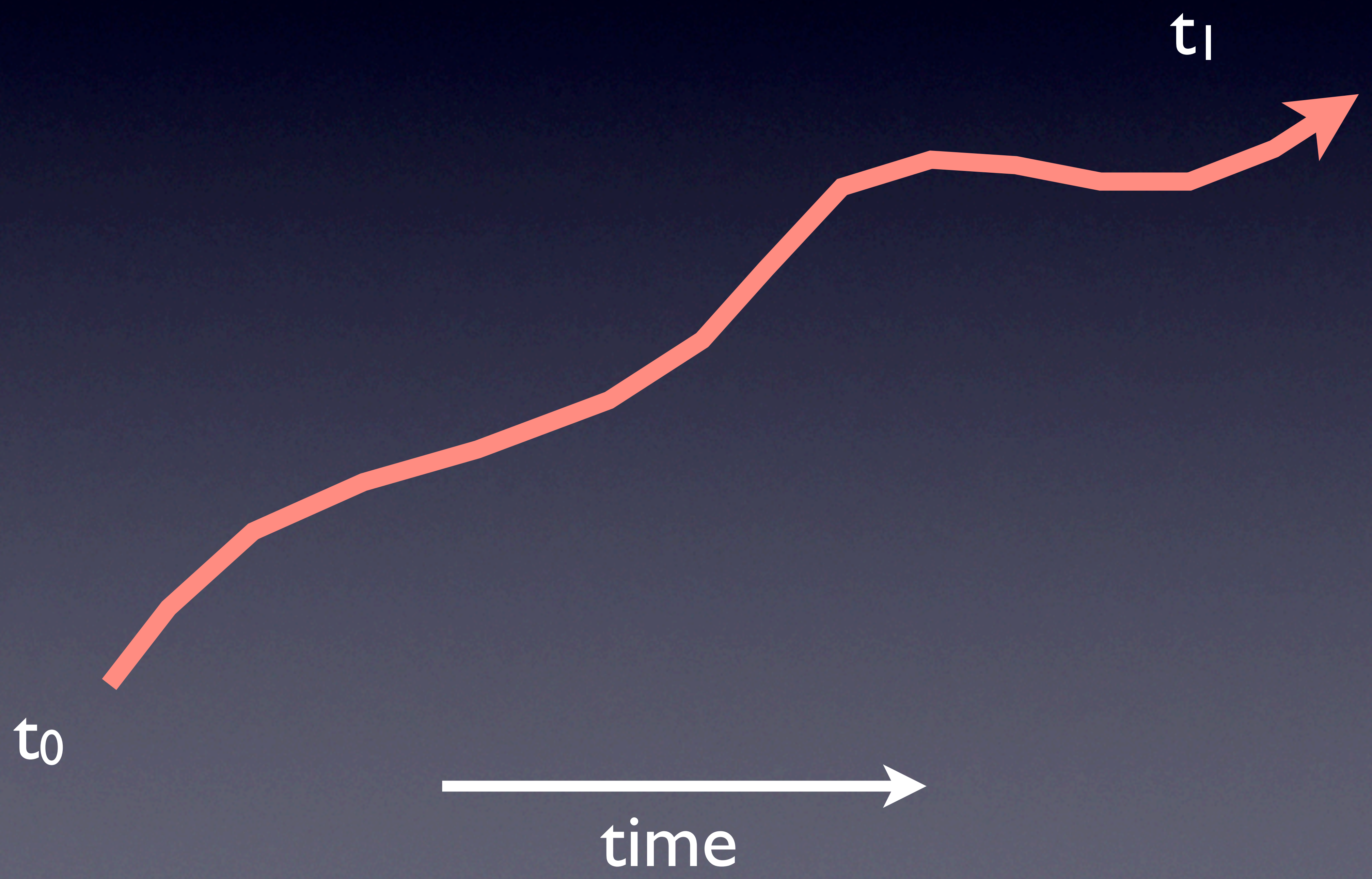
with $\rho_X(t_1,\epsilon) = e^{i\epsilon X}\,\rho(t_1)\,e^{-i\epsilon X}$

=> needs backward TDHF evolution to get $\rho_X(t_0,\epsilon)$

Numerical application of the BV prescription

standard forward TDHF

Troudet and Vautherin, PRC 1985
Bonche and Flocard, NPA 1985
Marston and Koonin, PRL 1985
Broomfield and Stevenson, JPG 2008
C.S., PRL 2011



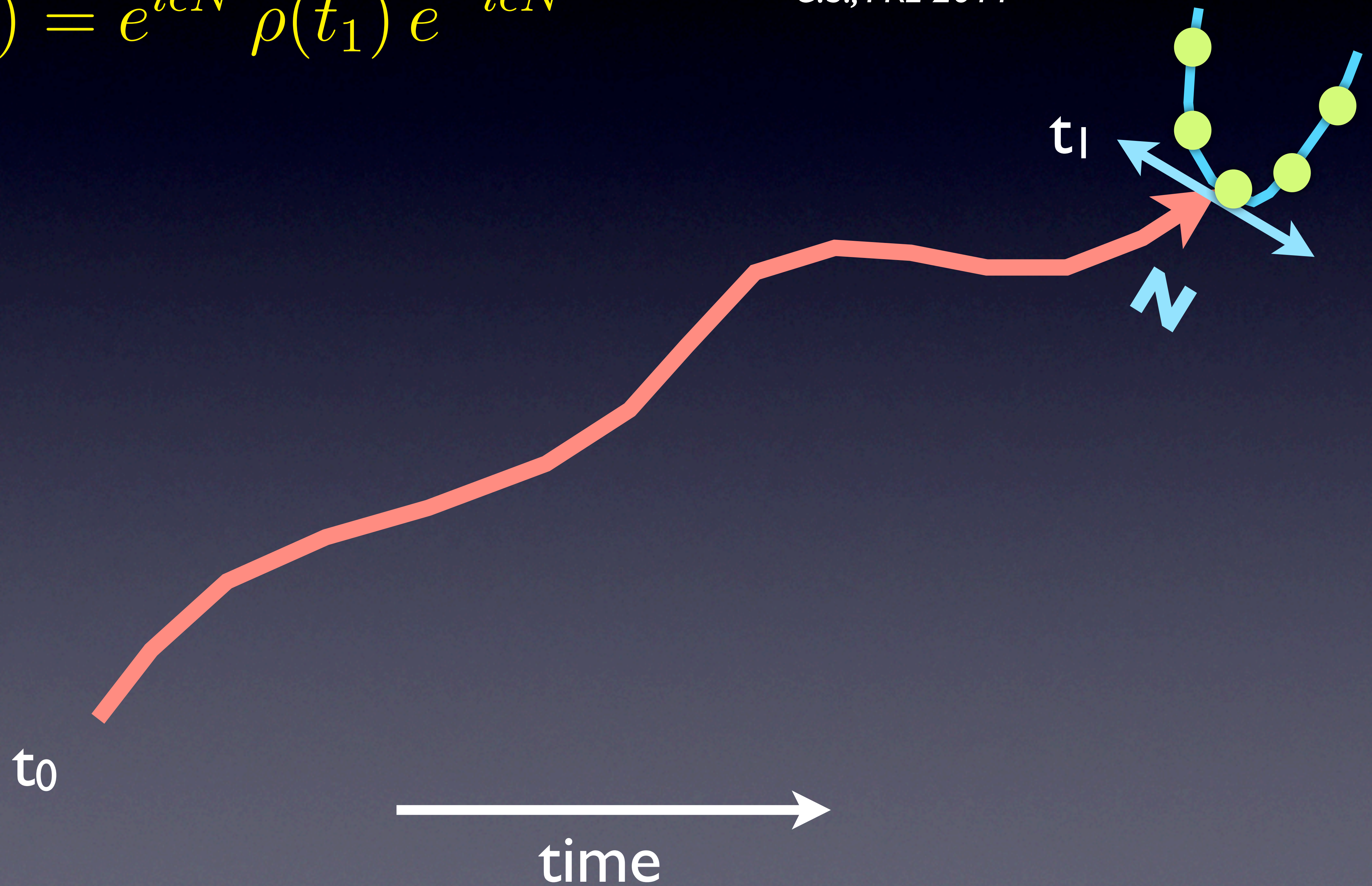
Numerical application of the BV prescription

standard forward TDHF

fluctuations of N at t_1

$$\rho_N(t_1,\epsilon) = e^{i\epsilon N}\,\rho(t_1)\,e^{-i\epsilon N}$$

Troudet and Vautherin, PRC 1985
Bonche and Flocard, NPA 1985
Marston and Koonin, PRL 1985
Broomfield and Stevenson, JPG 2008
C.S., PRL 2011



Numerical application of the BV prescription

standard forward TDHF

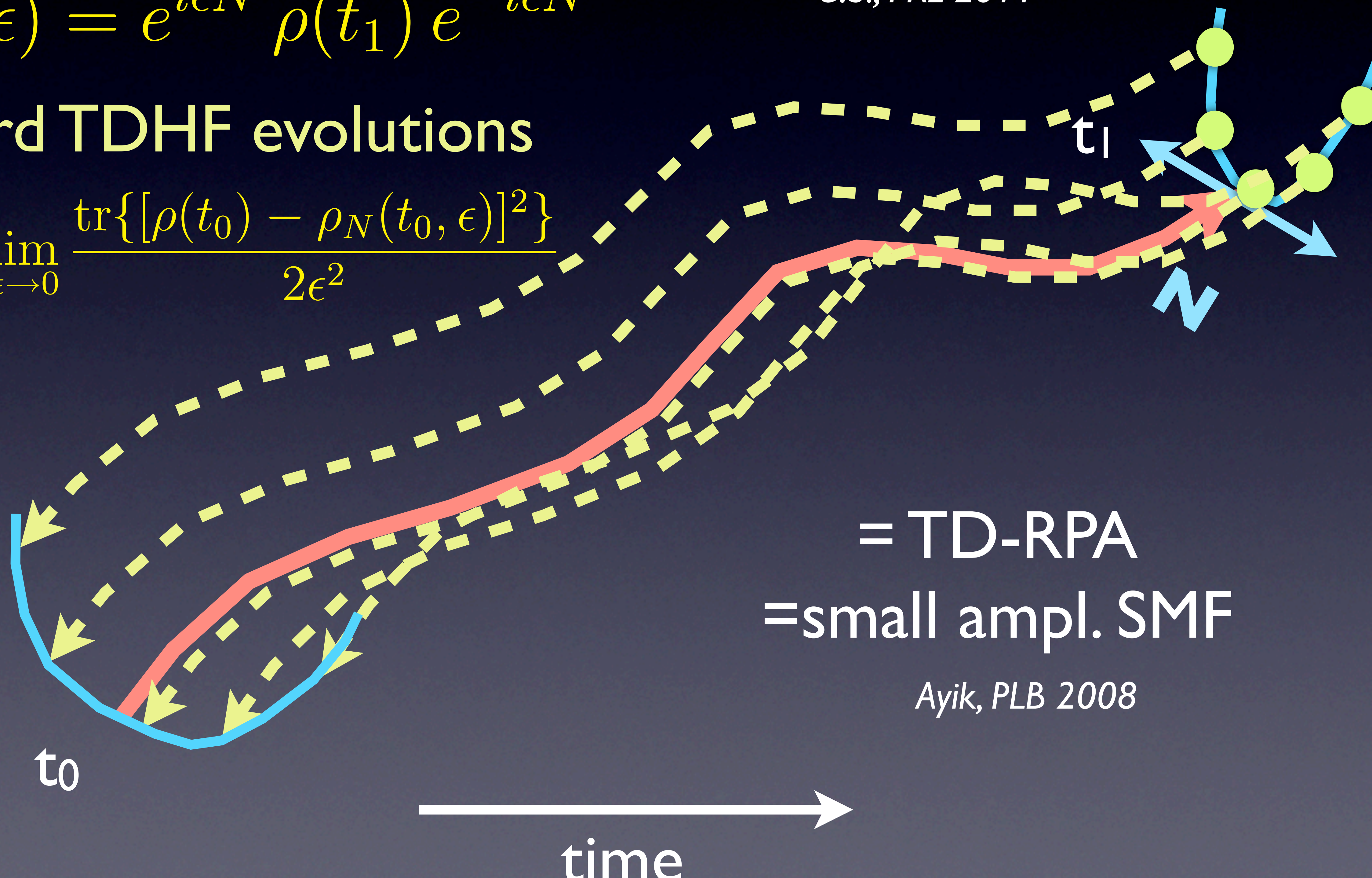
fluctuations of N at t_1

$$\rho_N(t_1,\epsilon) = e^{i\epsilon N}\,\rho(t_1)\,e^{-i\epsilon N}$$

backward TDHF evolutions

$$\sigma_N^2(t_1) = \lim_{\epsilon\rightarrow 0}\frac{\mathrm{tr}\{[\rho(t_0)-\rho_N(t_0,\epsilon)]^2\}}{2\epsilon^2}$$

Troudet and Vautherin, PRC 1985
Bonche and Flocard, NPA 1985
Marston and Koonin, PRL 1985
Broomfield and Stevenson, JPG 2008
C.S., PRL 2011



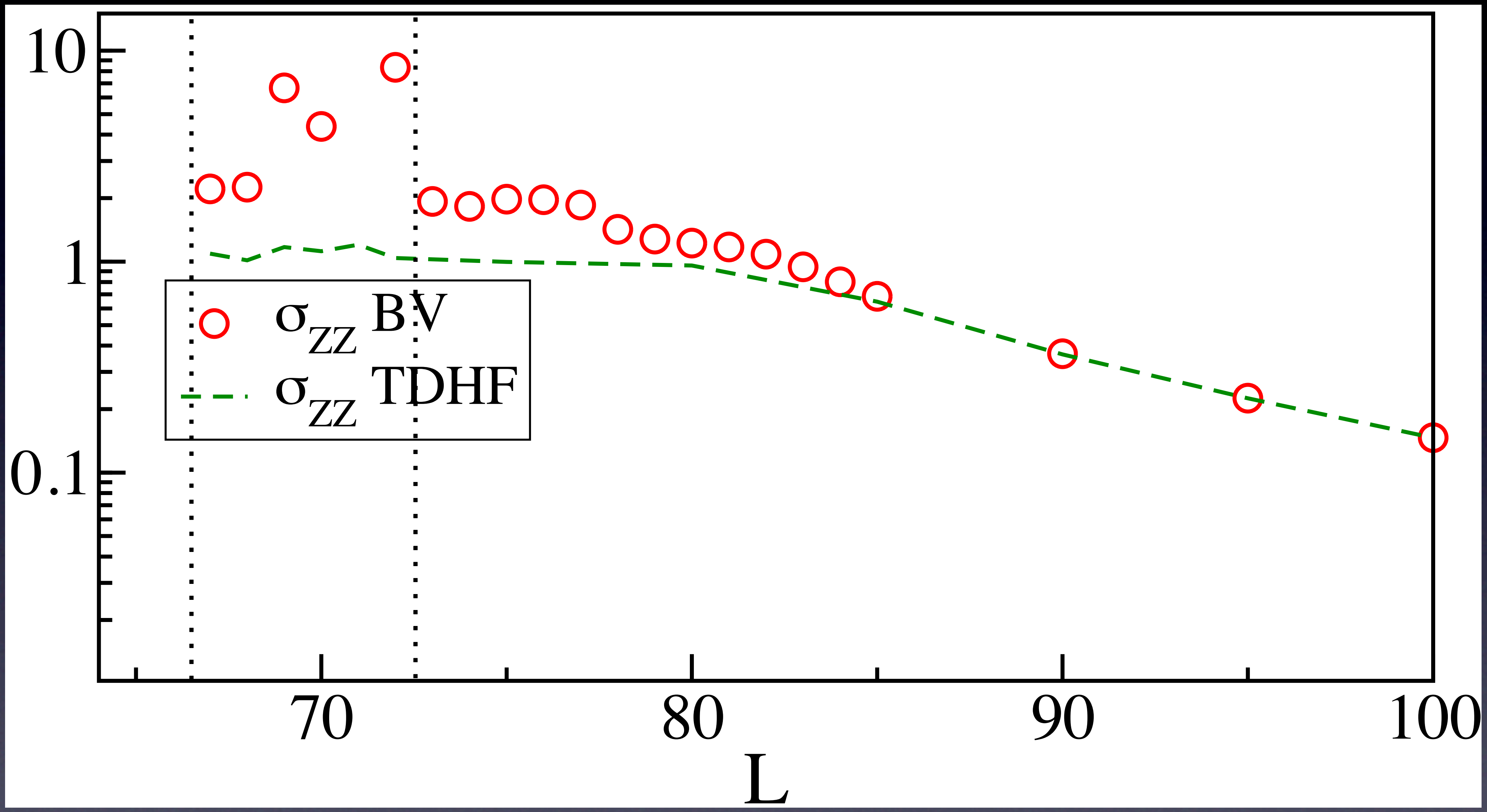
= TD-RPA

=small ampl. SMF

Ayik, PLB 2008

Deep-inelastic collisions

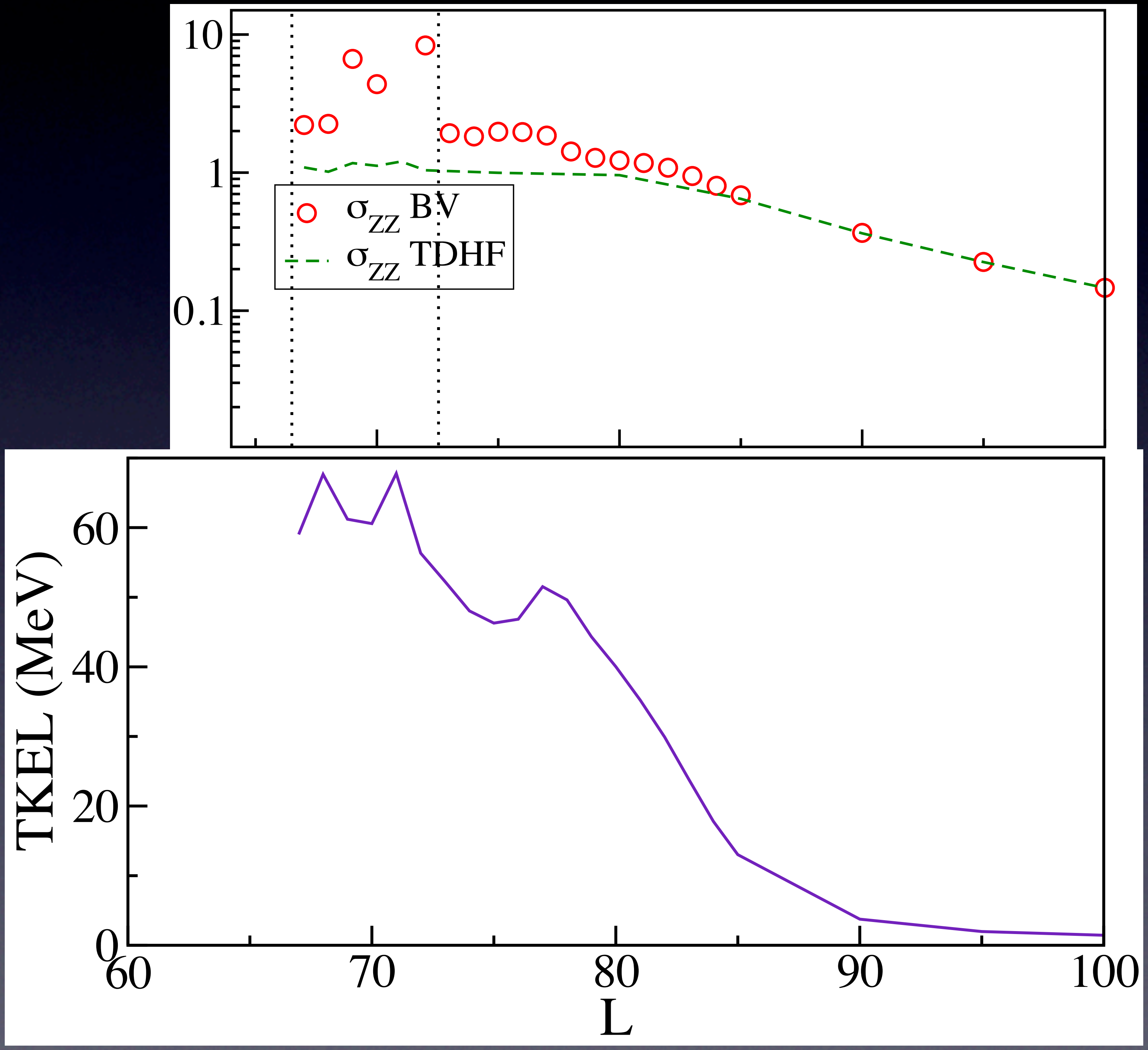
$^{40}Ca + ^{40}Ca$ at E_{cm}=128 MeV



C.S., PRL (2011)

Deep-inelastic collisions

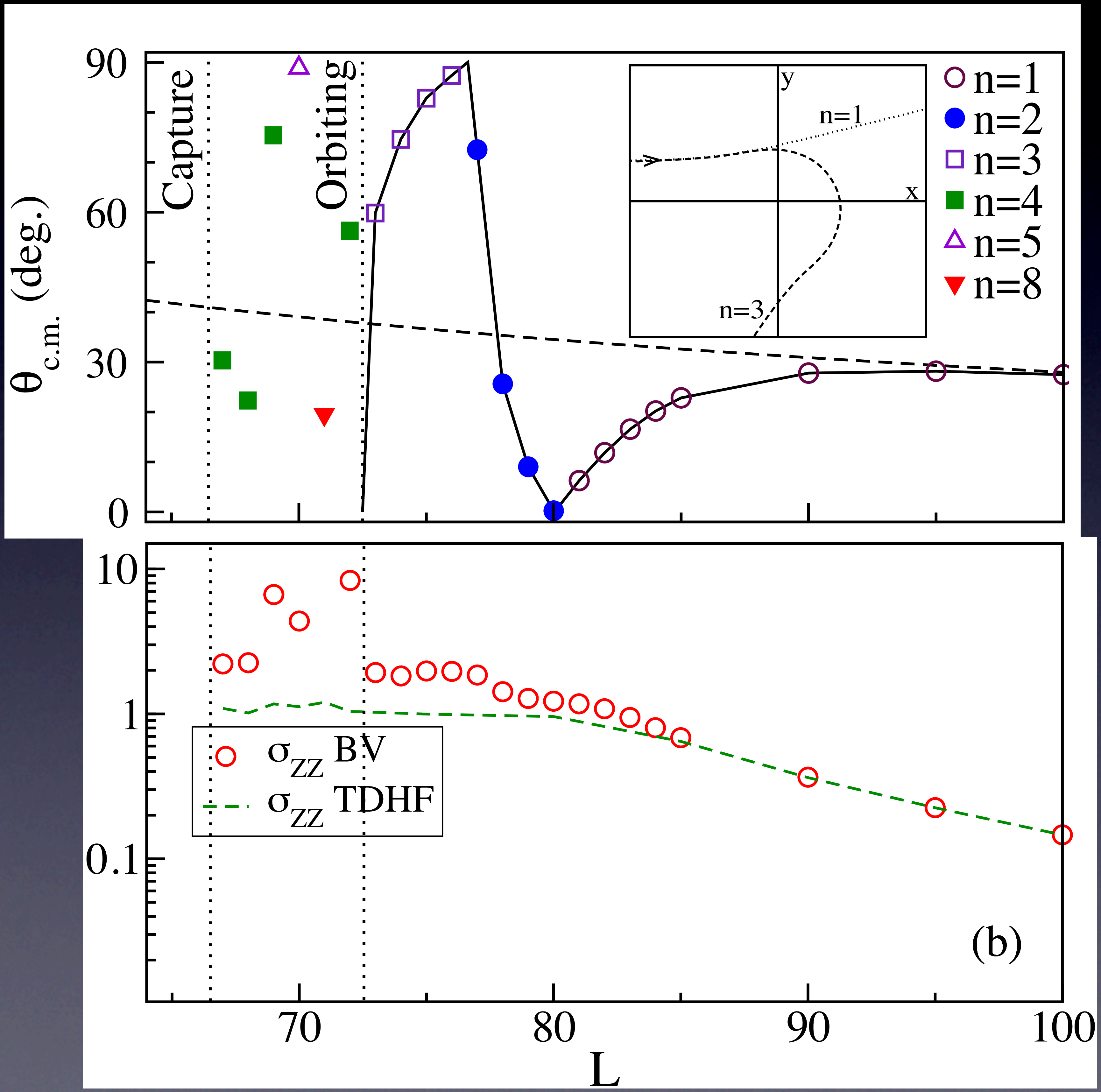
$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV



C.S., PRL (2011)

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV



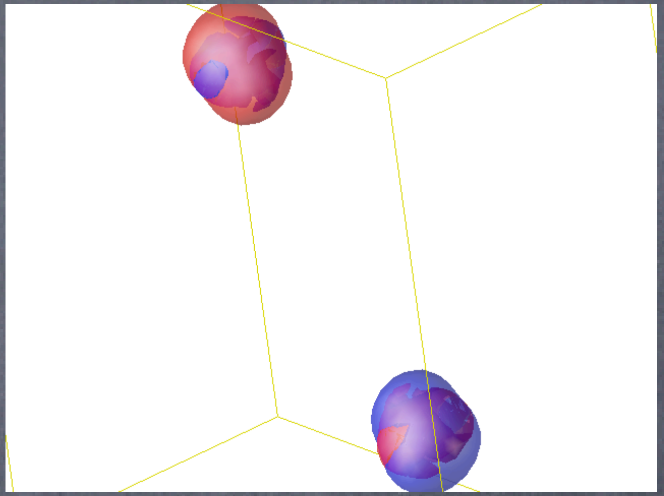
C.S., PRL (2011)

Deep-inelastic collisions

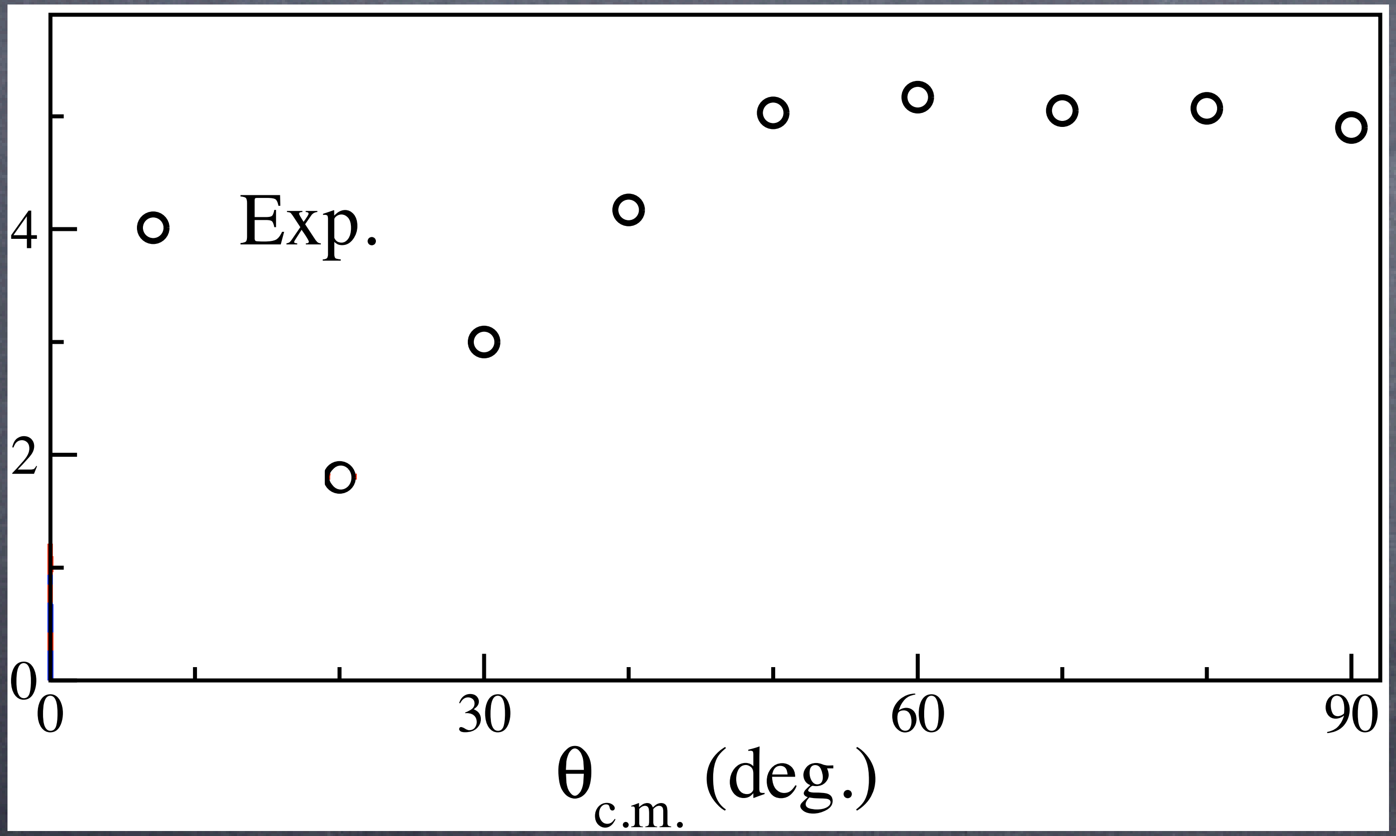
Charge fluctuations

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV

L=70ħ



σ_{ZZ}



data from Roynette et al., PLB 1977

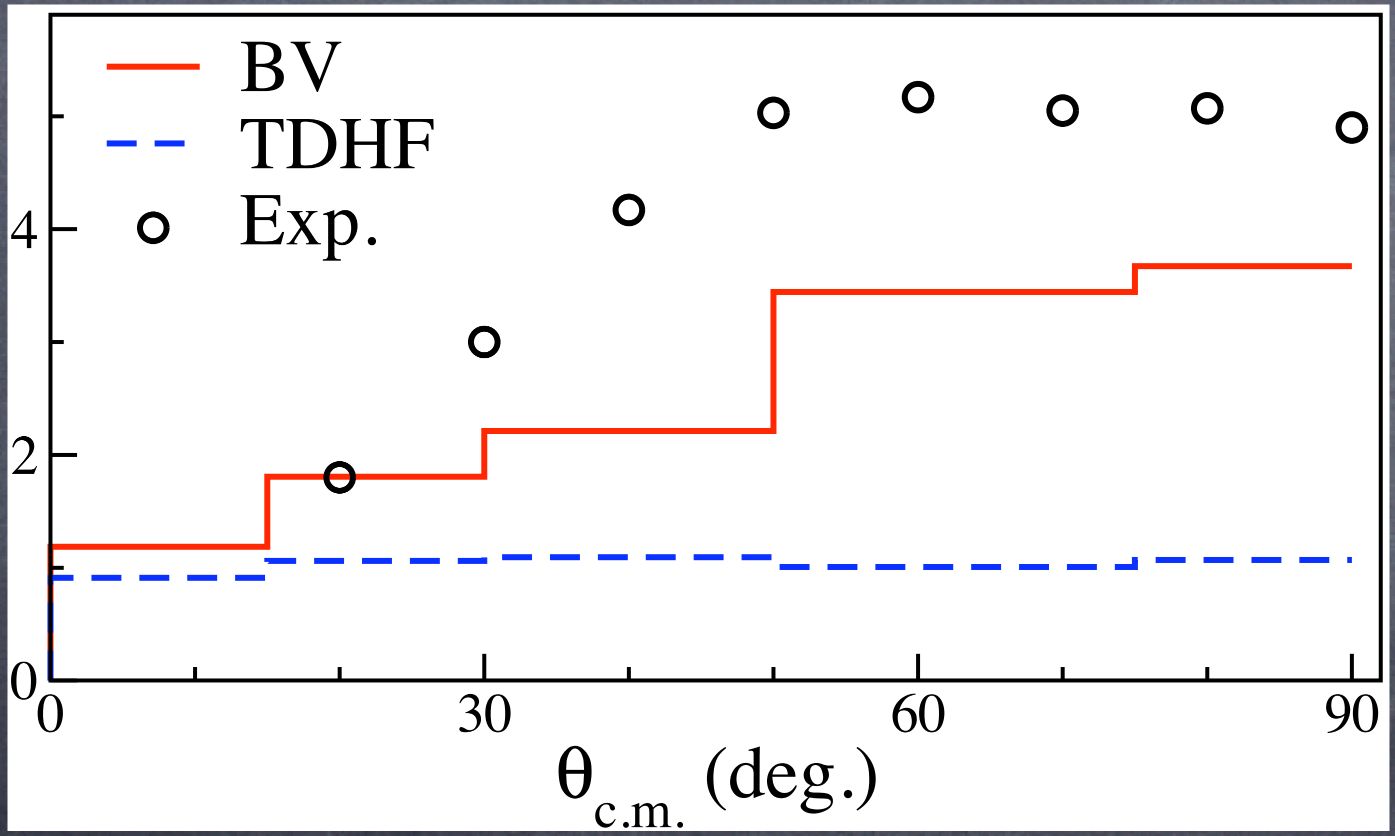
C.S., PRL 2011

Deep-inelastic collisions

Charge fluctuations

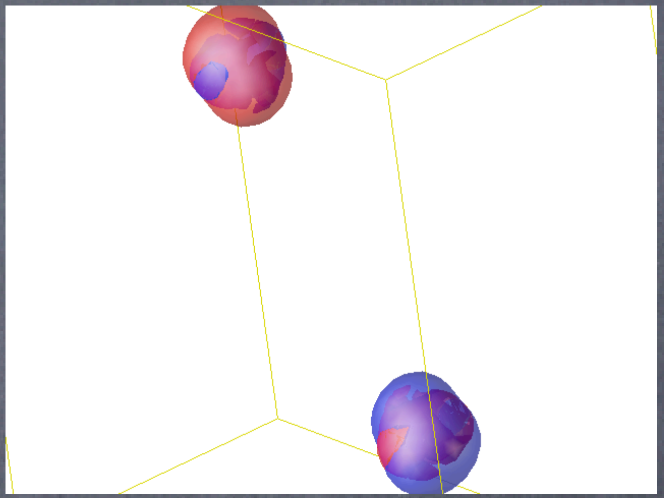
$^{40}Ca + ^{40}Ca$ at E_{cm}=128 MeV

σ_{ZZ}



data from Roynette et al., PLB 1977

L=70ħ



C.S., PRL 2011

Deep-inelastic collisions

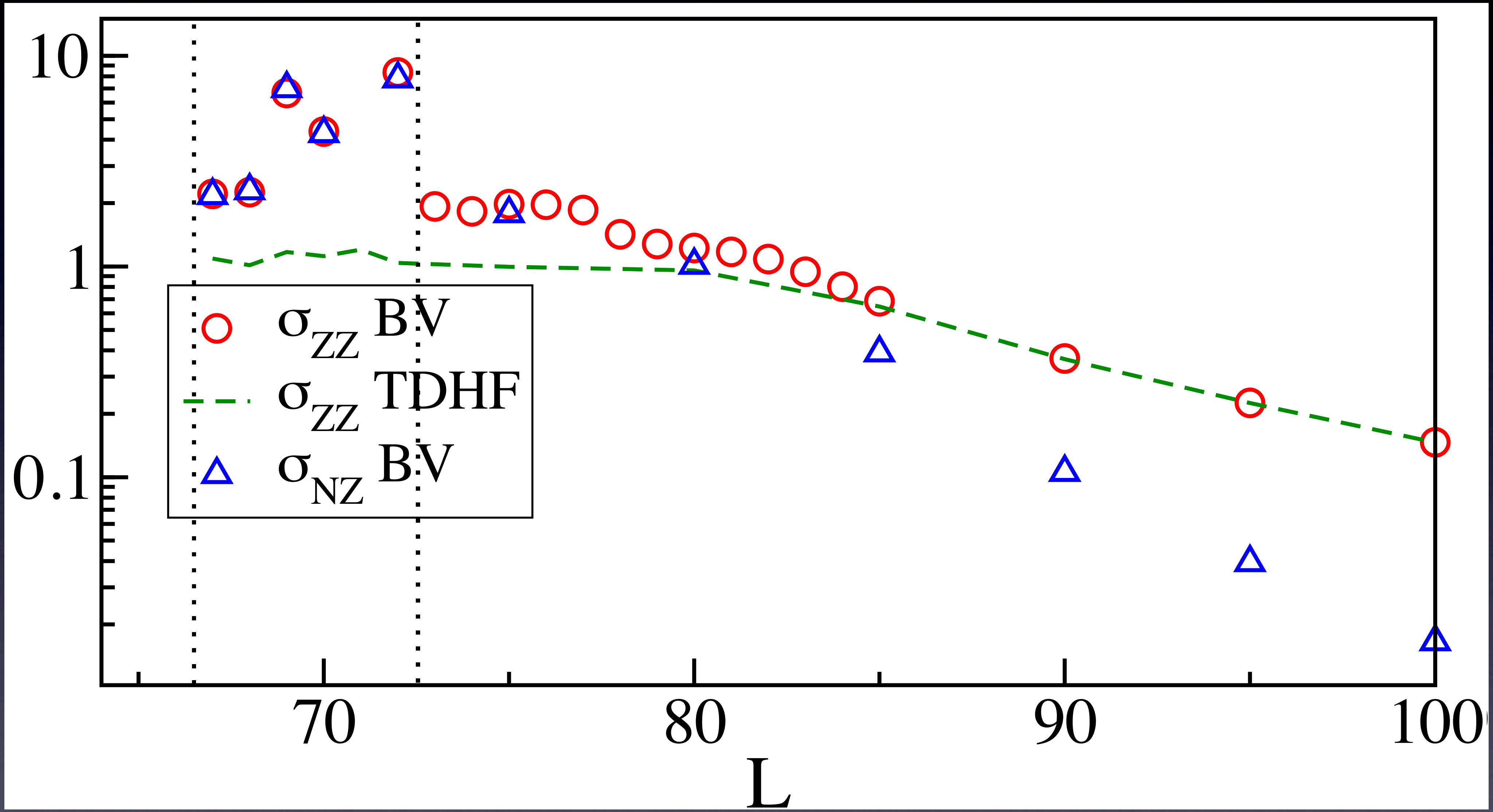
Correlations

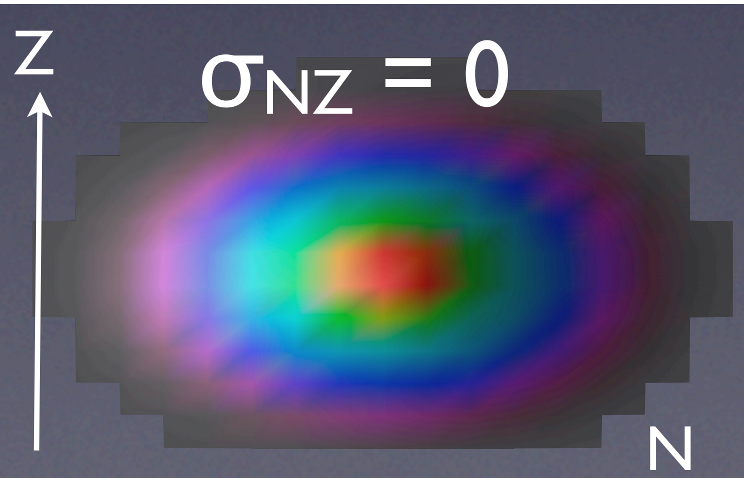
$\sigma_{NZ}^2 = \langle NZ \rangle - \langle N \rangle \langle Z \rangle$

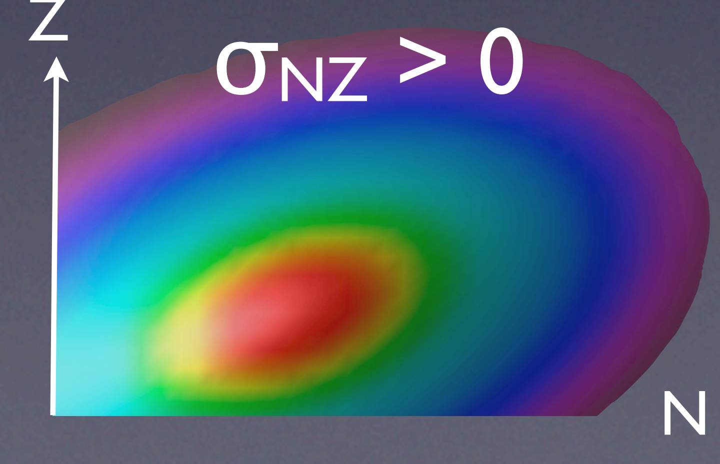
C.S., PRL (2011)

Deep-inelastic collisions

$^{40}Ca+^{40}Ca$ at E_{cm}=128 MeV







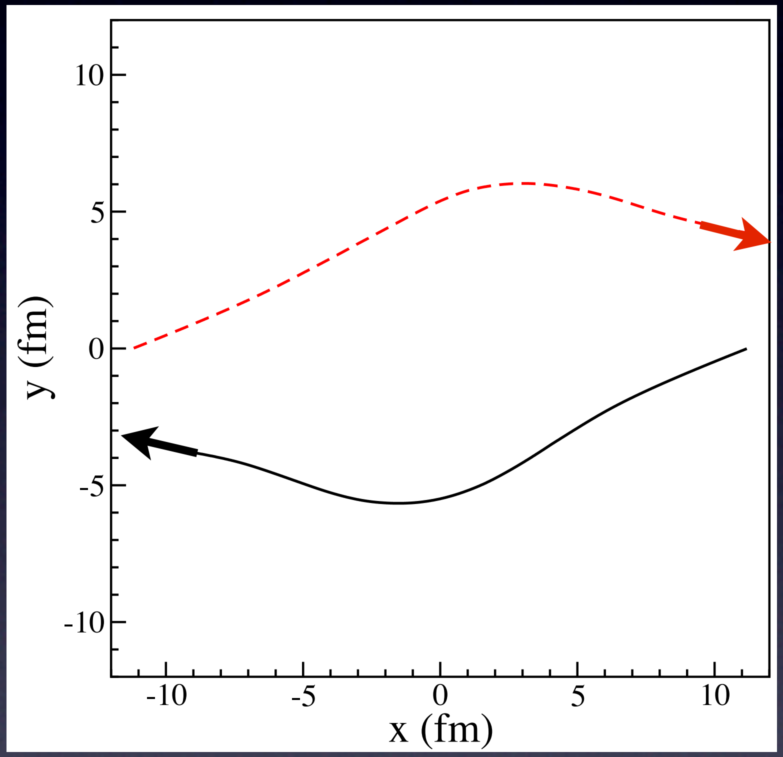
C.S., PRL (2011)

Deep-inelastic collisions

$^{80}Kr+^{90}Zr$ (N/Z= 1.22 and 1.25)

E/A = 8.5 MeV

L = 192 ħ



σ_{ZZ} = 5.3

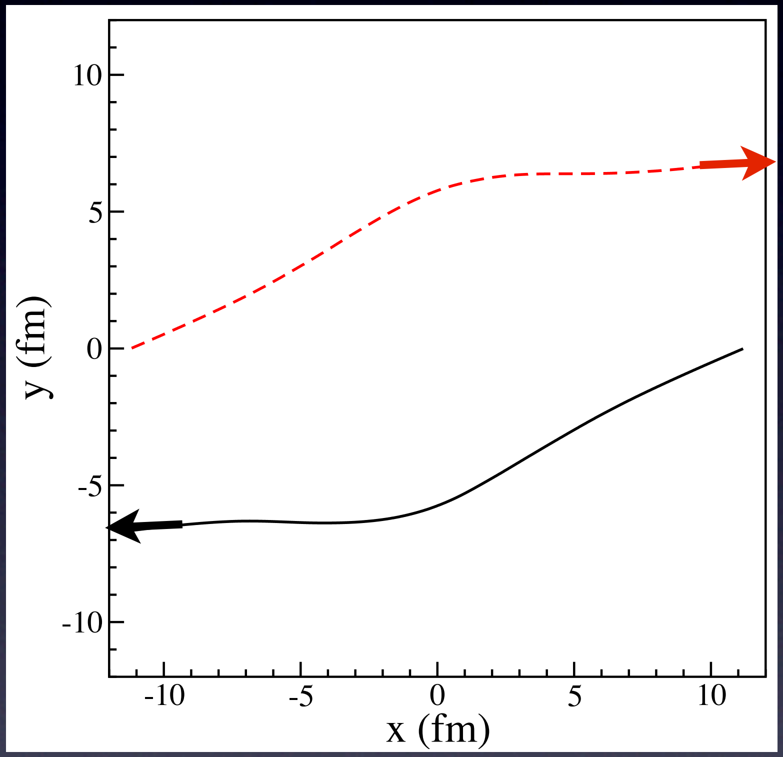
σ_{NN} = 7.1

σ_{NZ} = 5.7

$^{92}Kr+^{90}Zr$ (N/Z= **1.56** and 1.25)

E/A = 8.5 MeV

L = 223 ħ



σ_{ZZ} = 4.7

σ_{NN} = 8.4

σ_{NZ} = 8.5 (+50%)

C.S., PRL (2011)

Balian-Vénéroni variational principle

- Average of one-body observables: *TDHF*
- Their fluctuations and correlations: *BV prescription*