Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

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Dissipative mechanisms
in finite quantum systems

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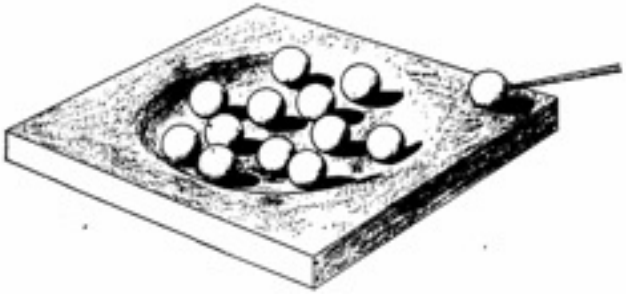
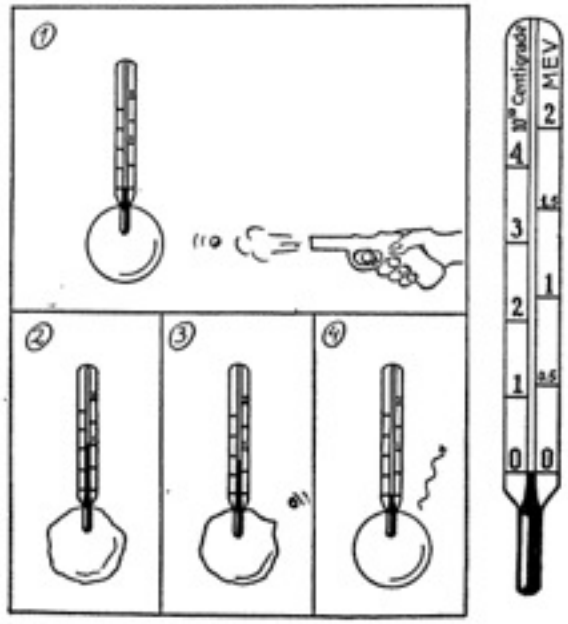
An old story…

neutron on nucleus





N. Bohr, Science, 1937

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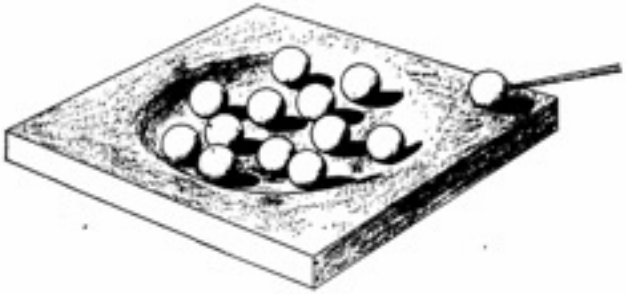

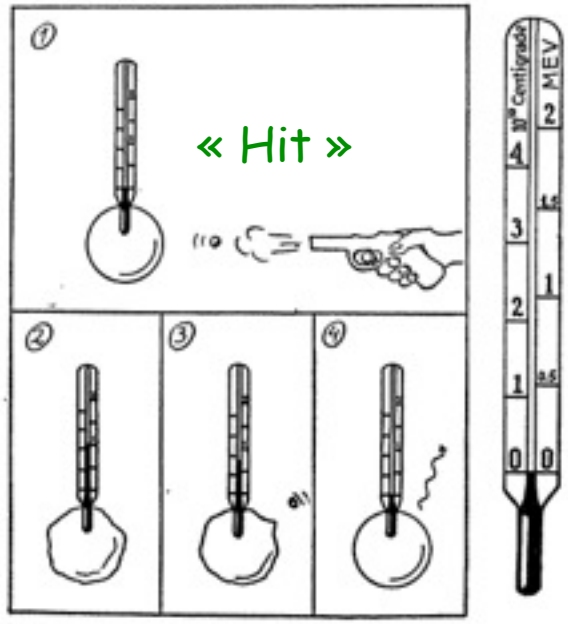

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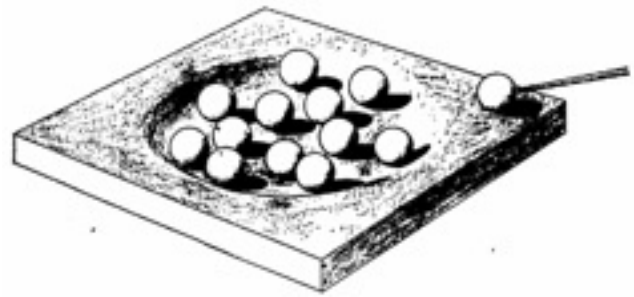

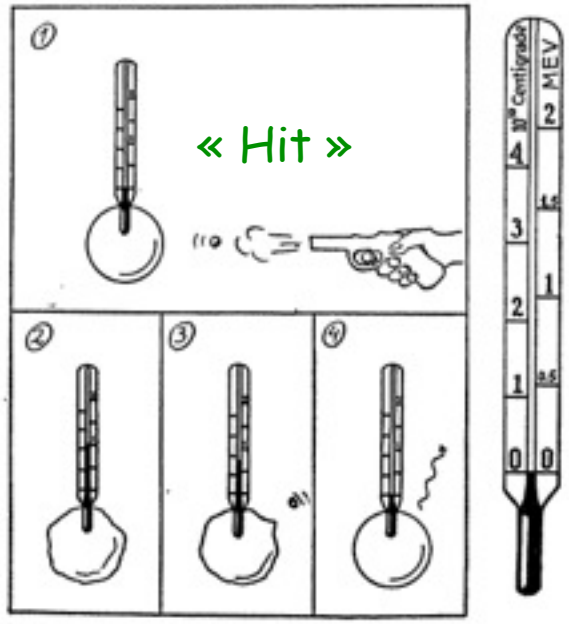

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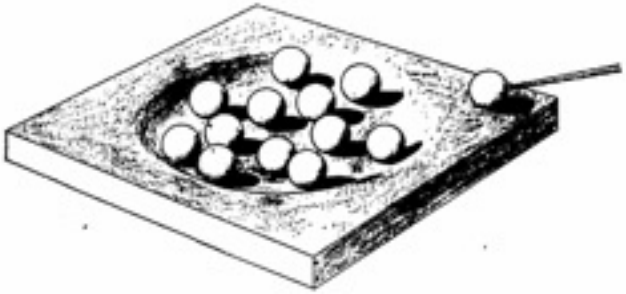

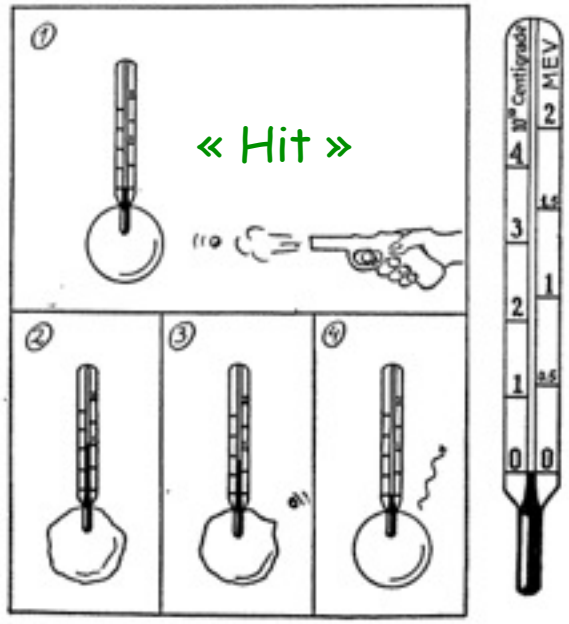

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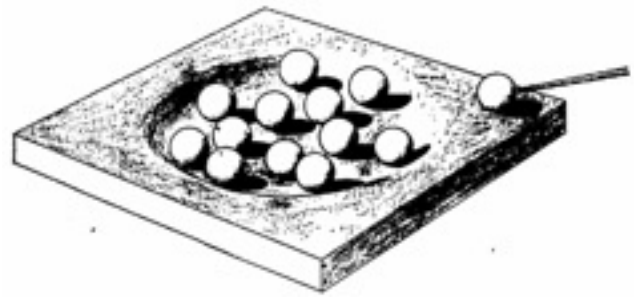

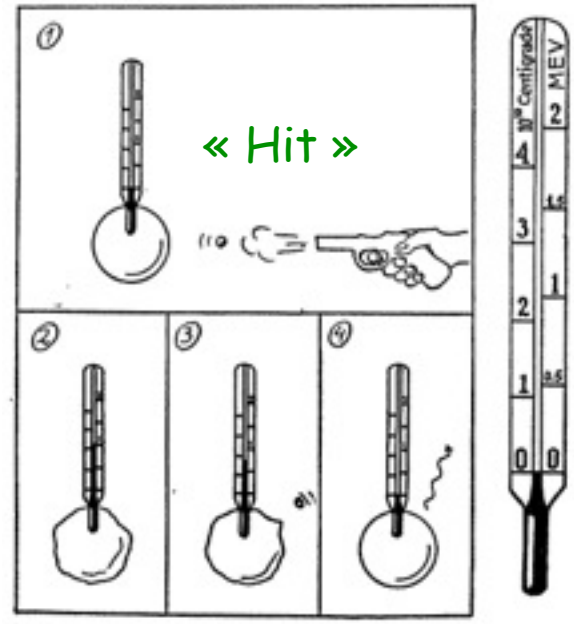

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Dissipation

Dynamical picture

Microscopic description

Finite systems

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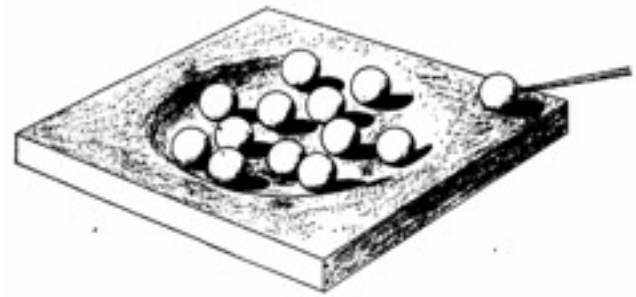

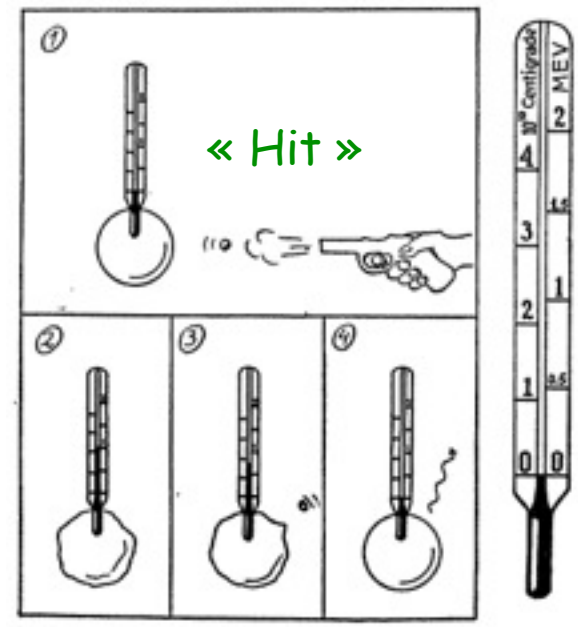

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Nuclei at finite temperature

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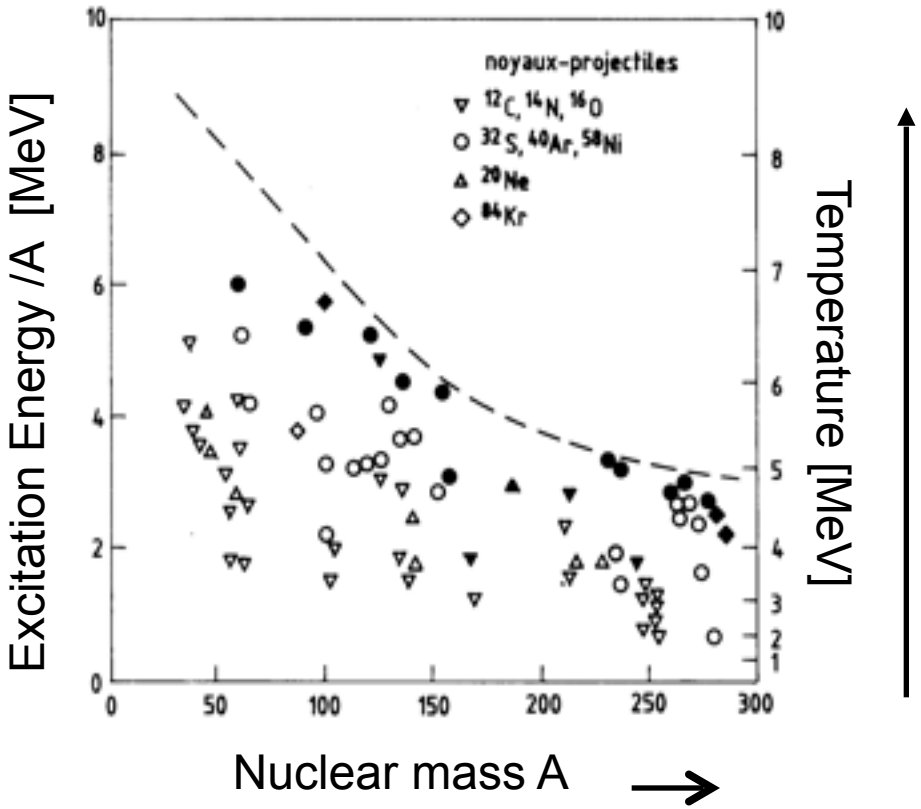

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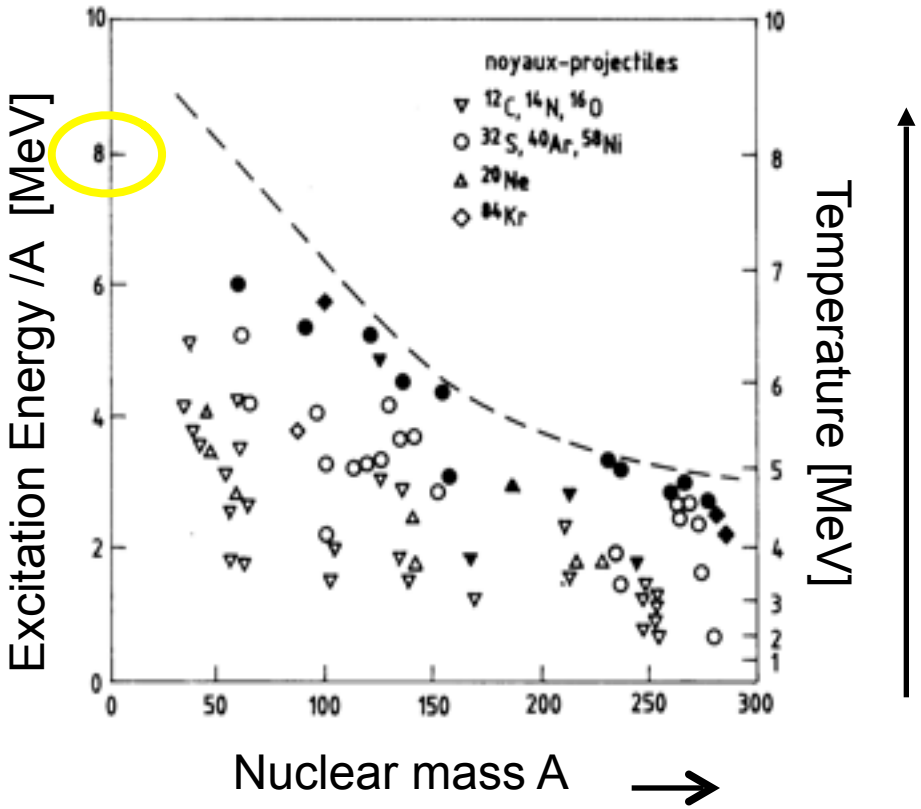

$$T/S_n \lesssim 0.5 - 1$$

$$T/\varepsilon_F \lesssim 0.1 - 0.2$$

Temperature in clusters and molecules

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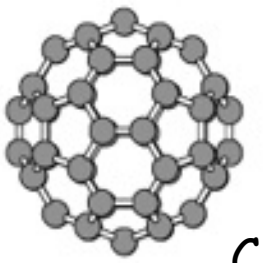

C_{60}

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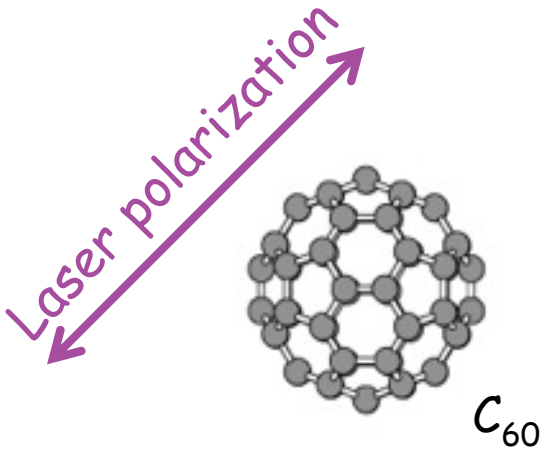

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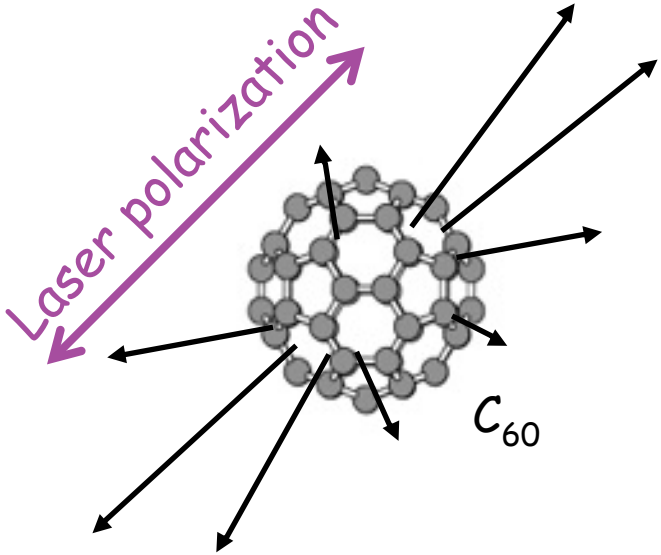

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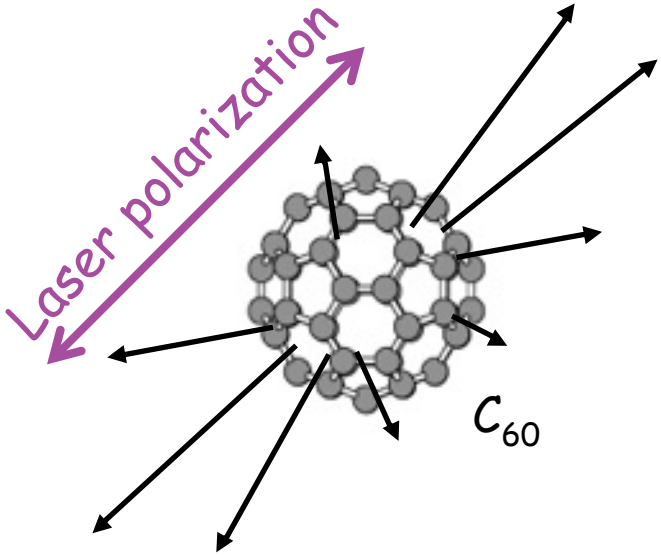

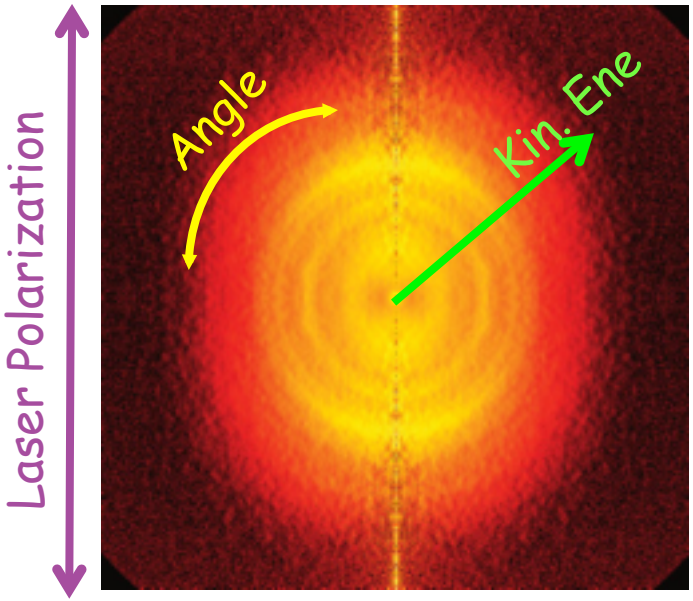

Exp: Campbell 2010

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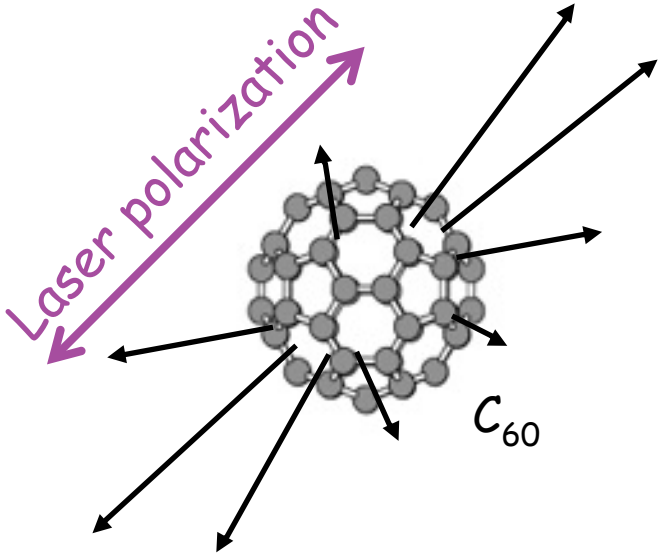

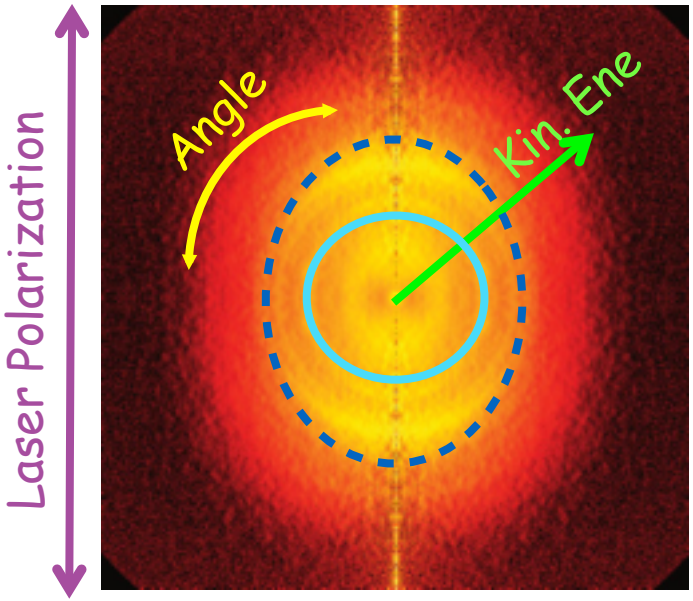

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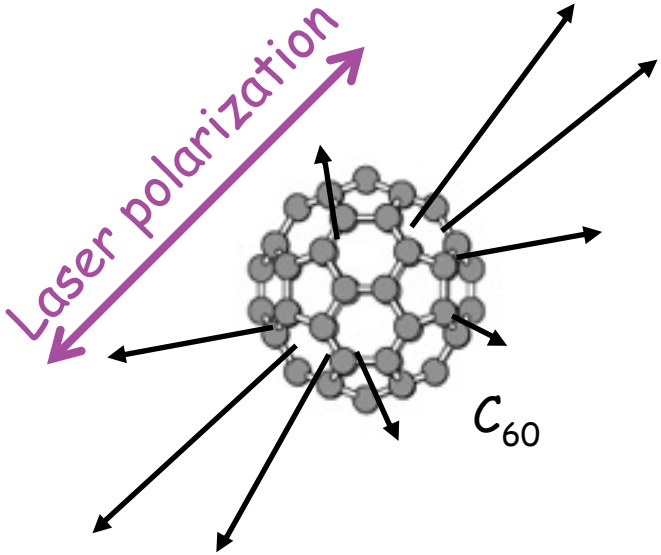

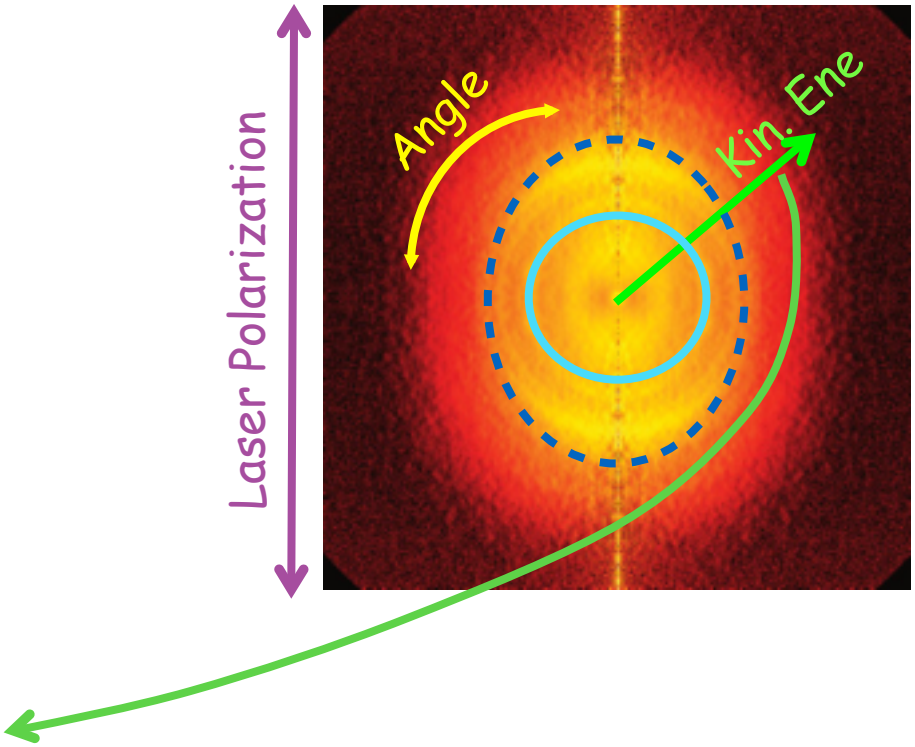

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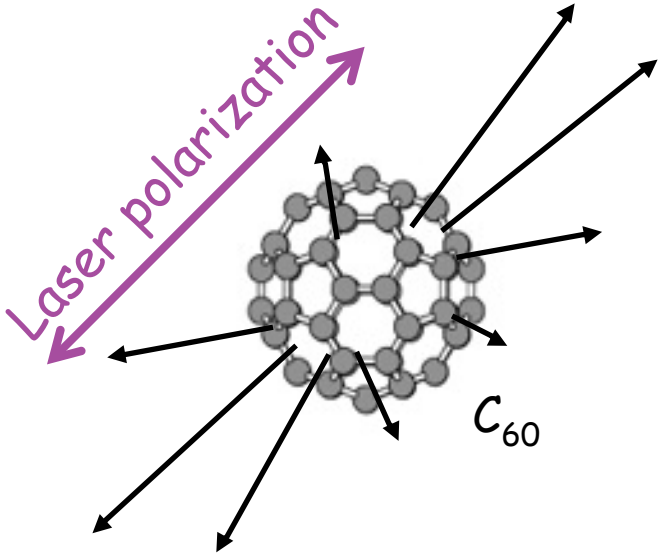

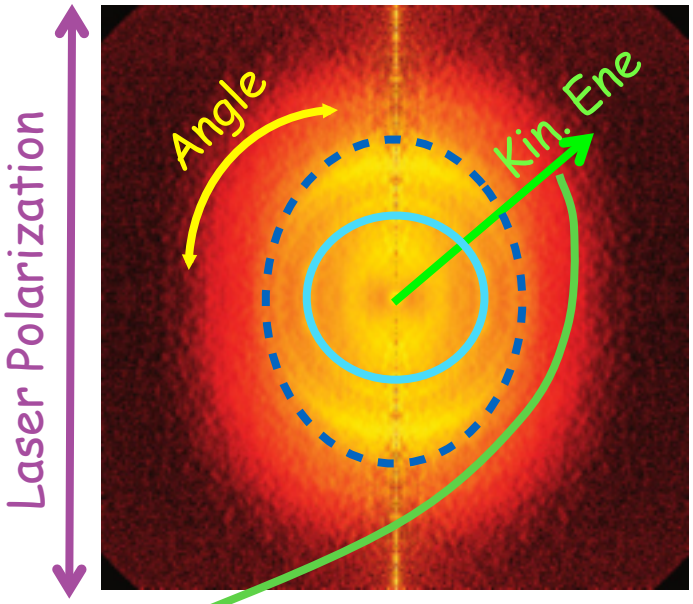

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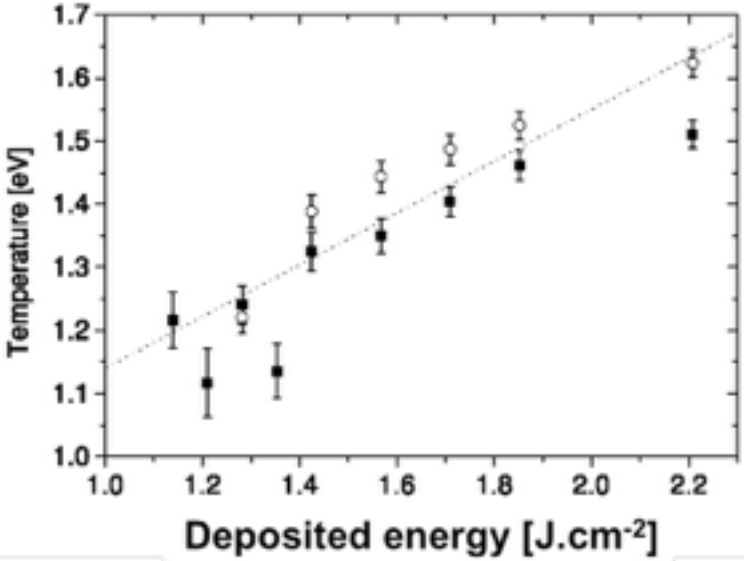

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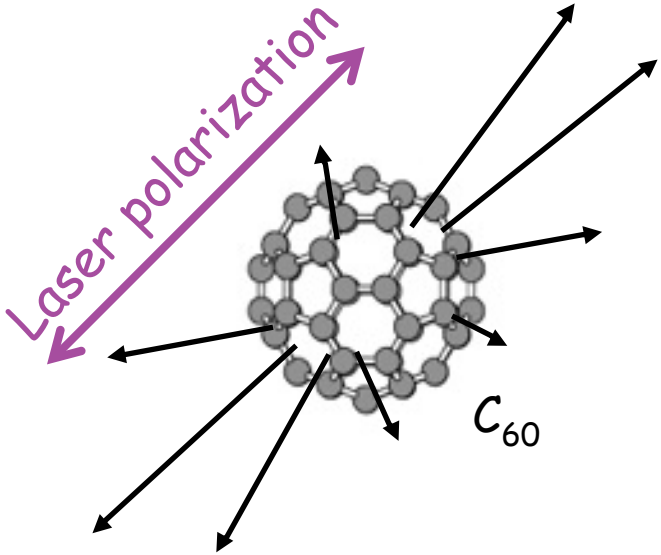

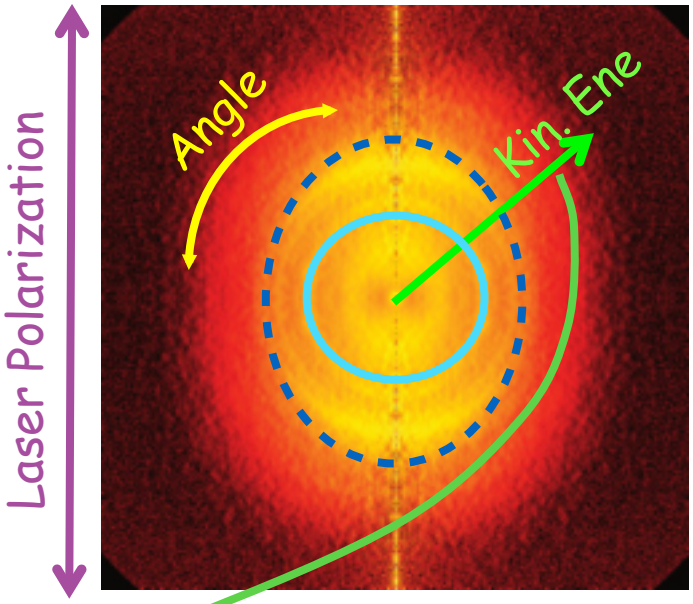

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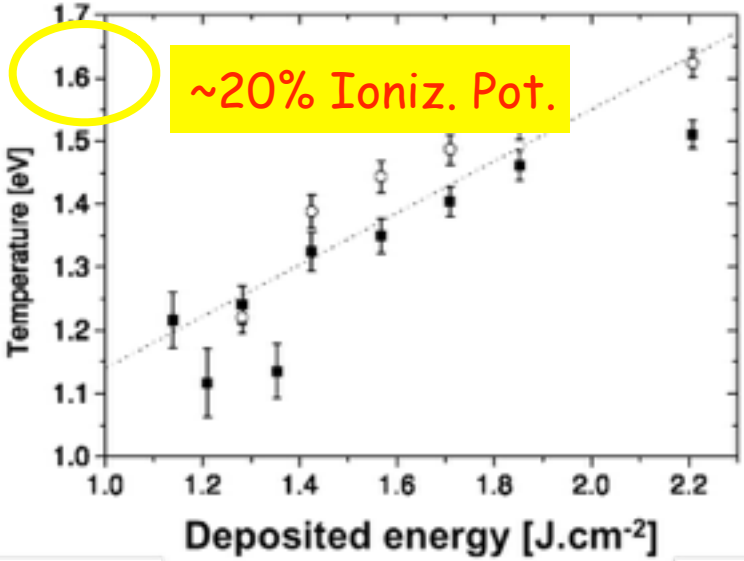

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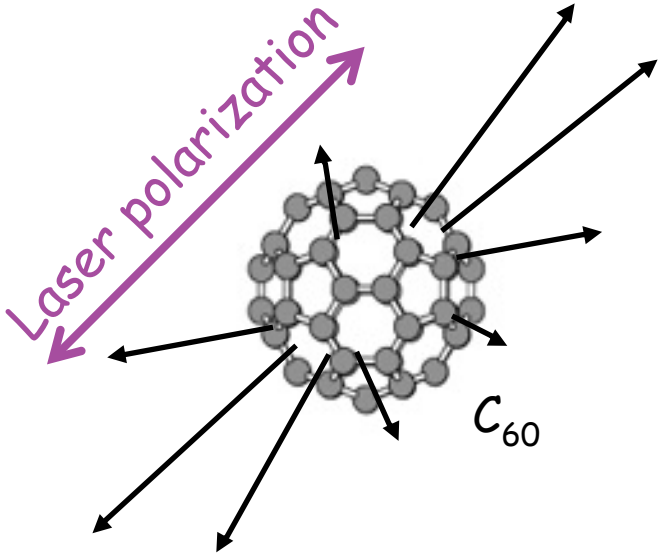

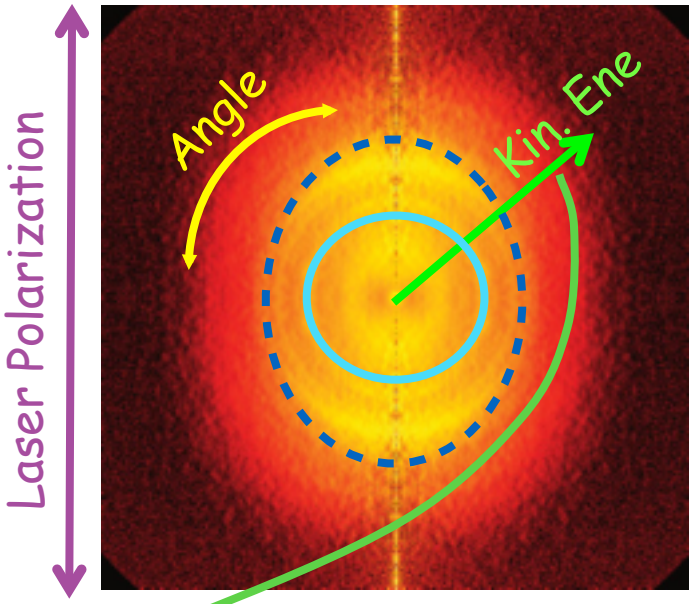

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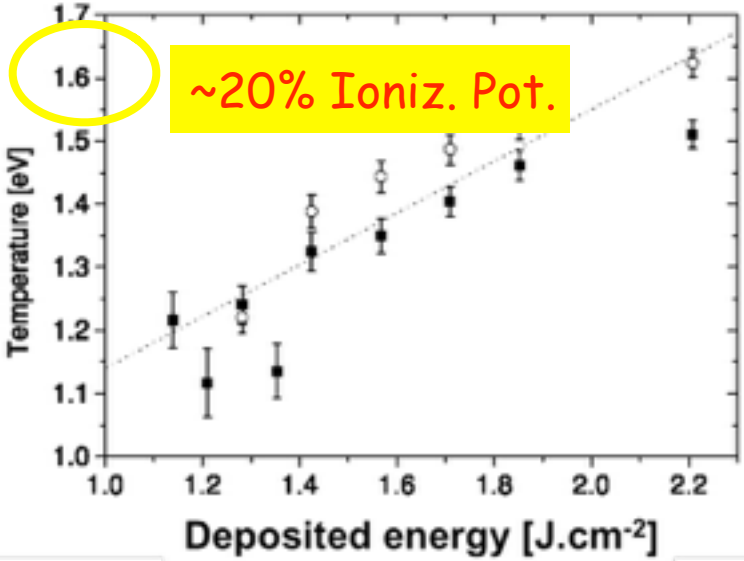
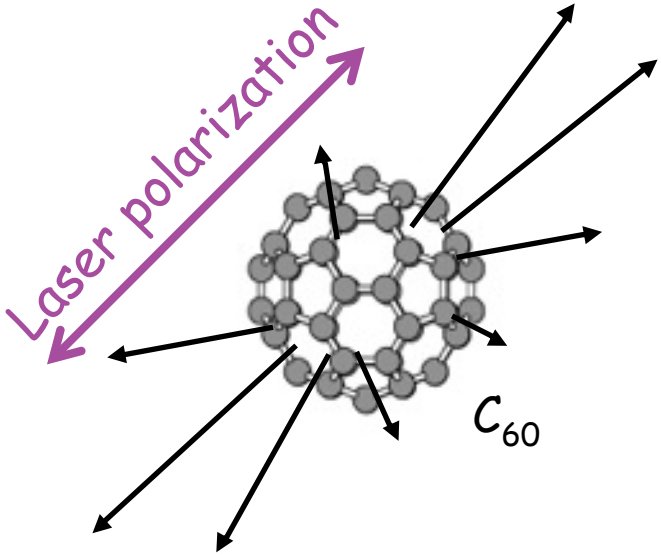


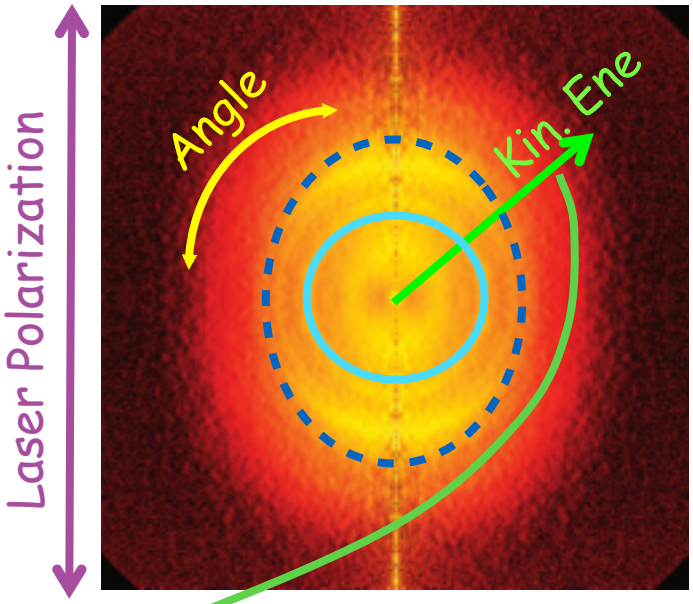
Thermalization

Dissipation:

collective (laser) → thermal

Temperature in clusters and molecules





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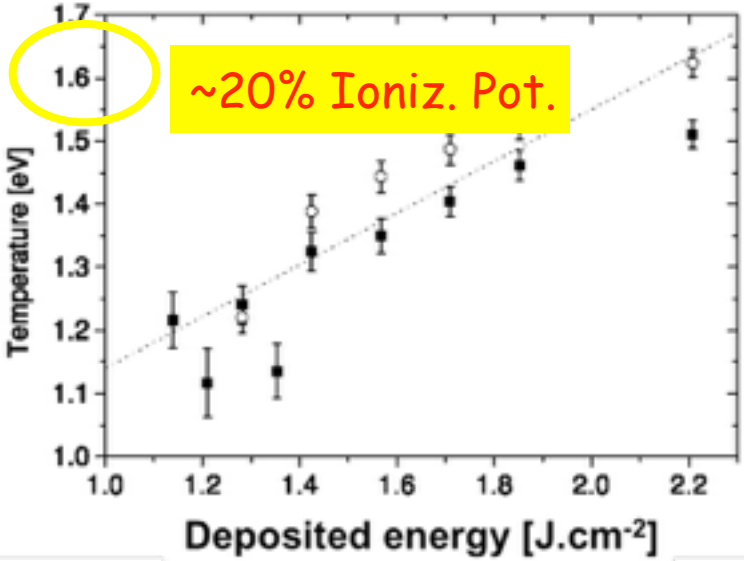

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- Strongly decreasing de Broglie wavelength in high energy dynamics
  Semi classics possible at high energy

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TDHF/TDDFT

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$\hat{\rho}, \hat{h} \xrightarrow[]{Wigner\ transform} f(\mathbf{r}, \mathbf{p}, t), h(\mathbf{r}, \mathbf{p}, t)$

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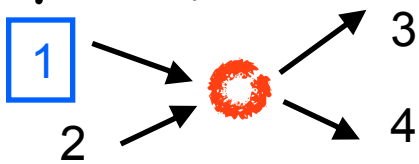

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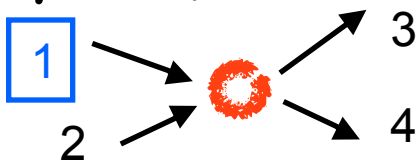

$$I_{coll}[f_1] \sim \int d\mathbf{p}_2 d\mathbf{p}_3 d\mathbf{p}_4 \delta(\sum \mathbf{p}_i)\delta(\sum \varepsilon_i)\frac{d\sigma}{d\Omega}[f_1 f_2(1-f_3)(1-f_4) - \ldots]$$

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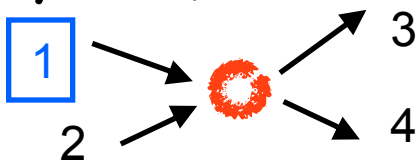

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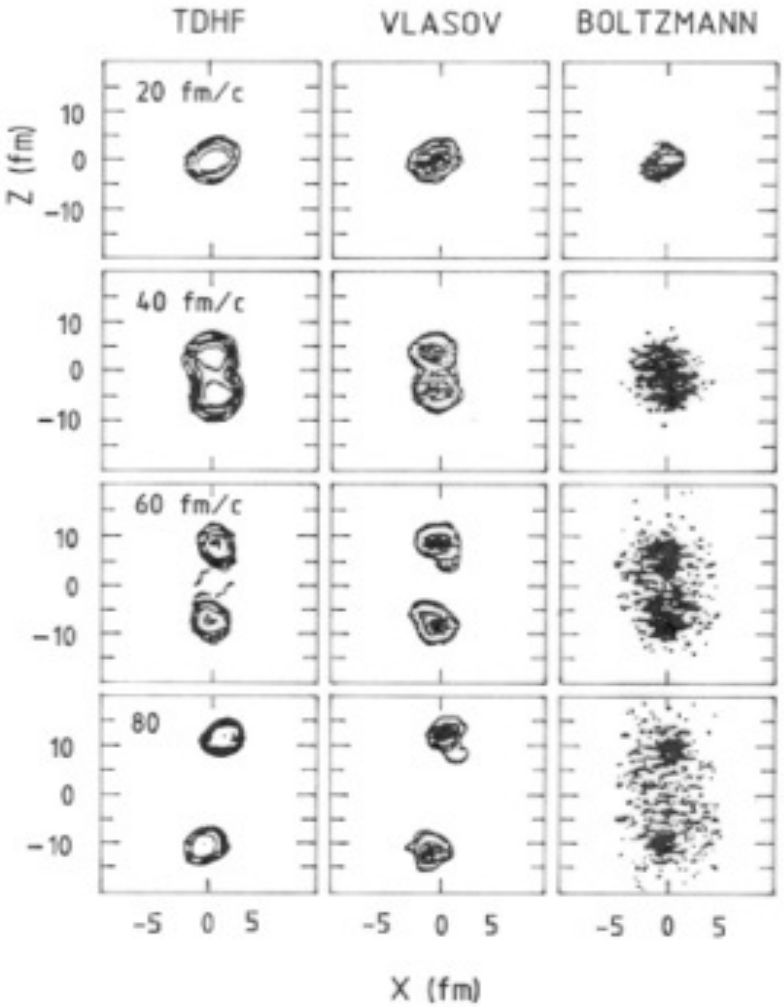
In medium cross section/
Screened Coulomb

Pauli blocking

Fusion in nuclear collisions

Fusion in nuclear collisions

$^{12}C + ^{12}C$ b = 0 E = 85 MeV/A



Fusion in nuclear collisions

Quadrupole moment

in momentum space

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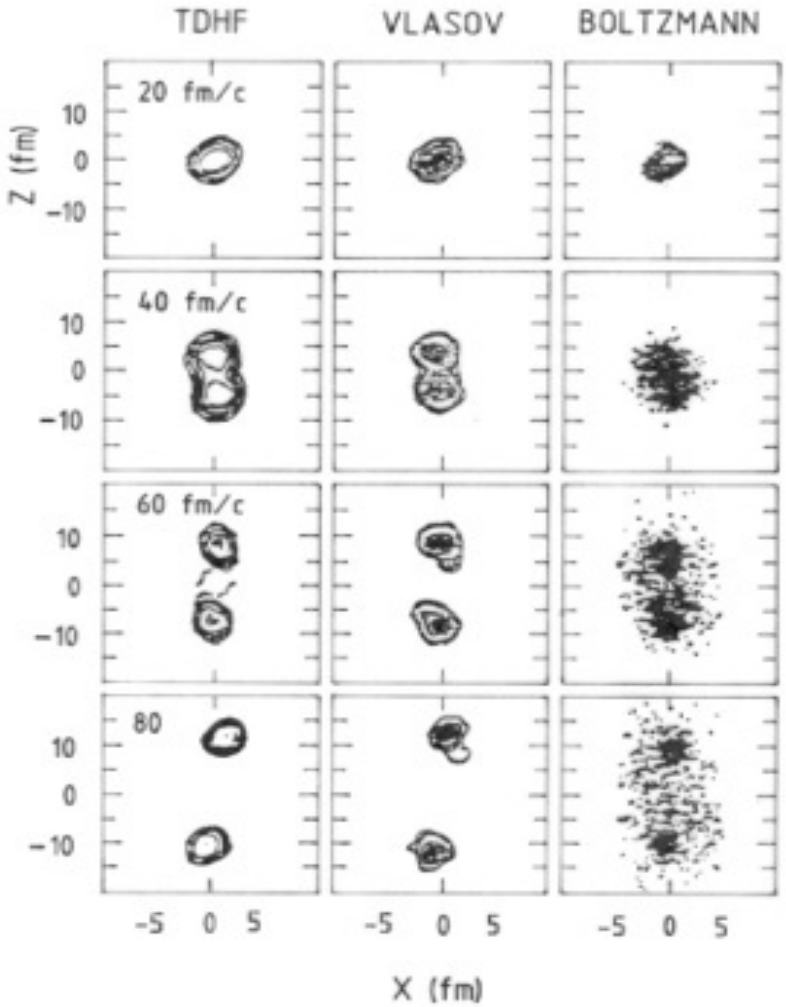

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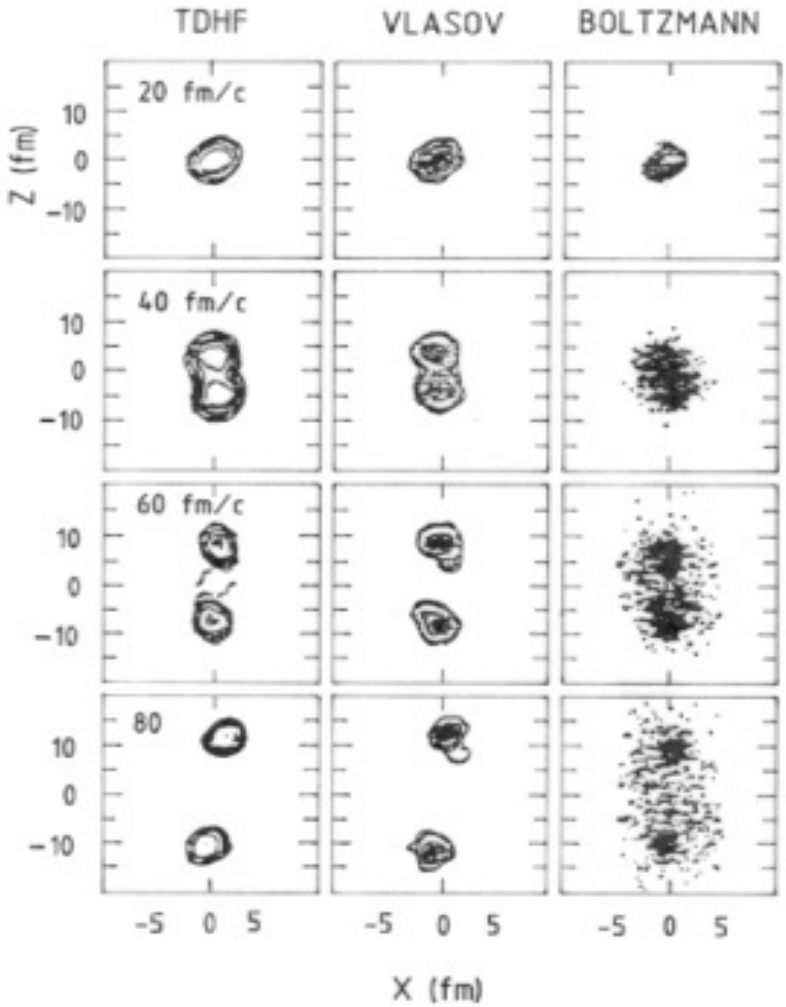

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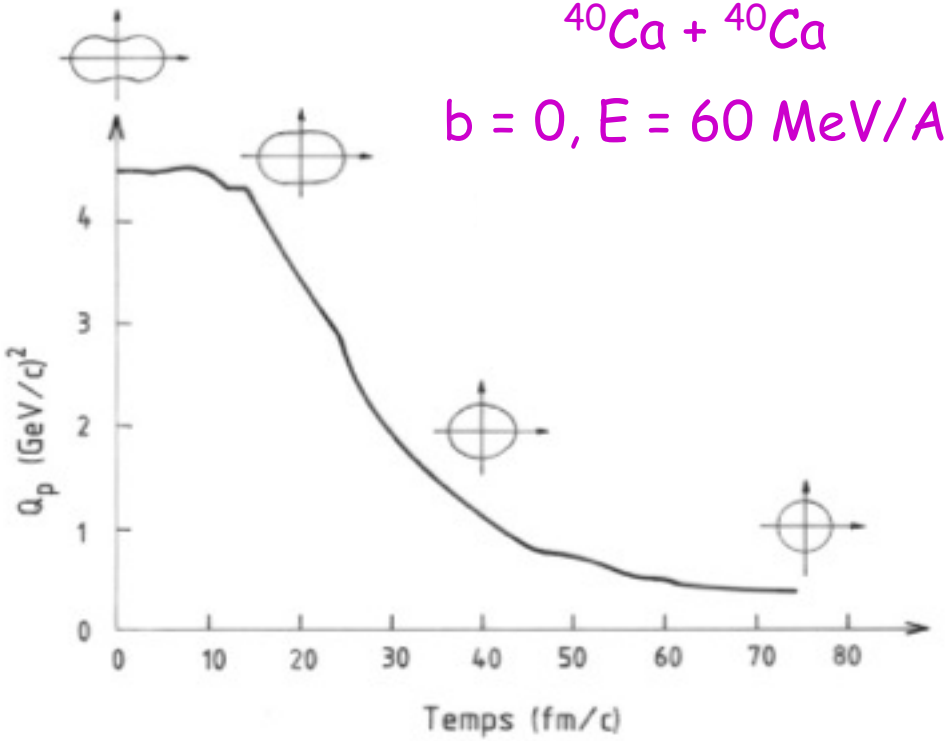
Relaxation in momentum space

$^{40}Ca + {}^{40}Ca$

b = 0, E = 60 MeV/A



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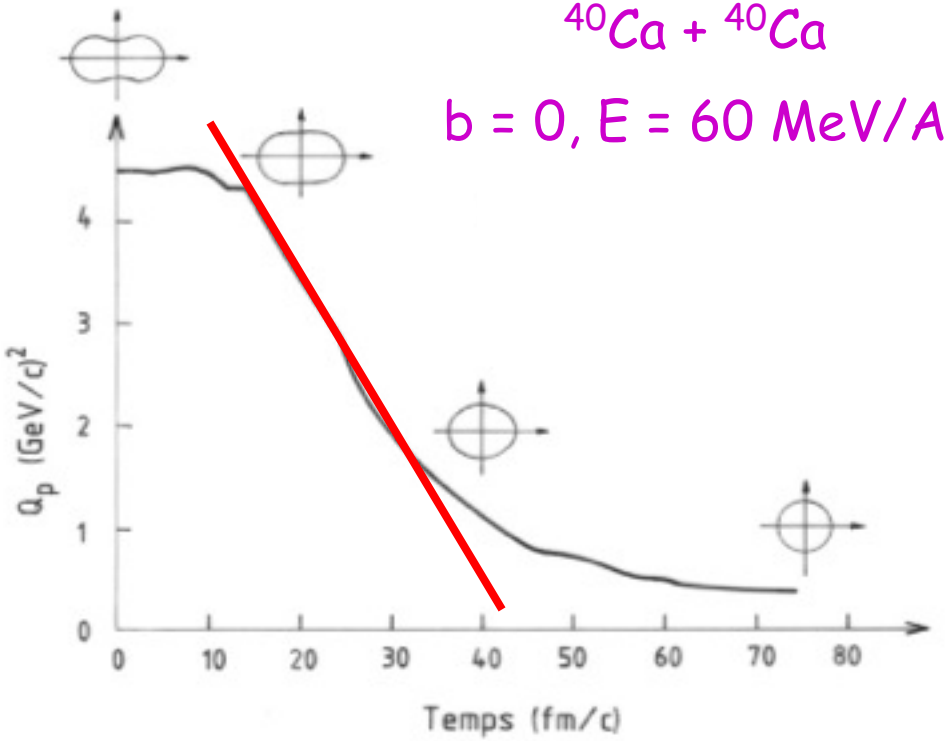

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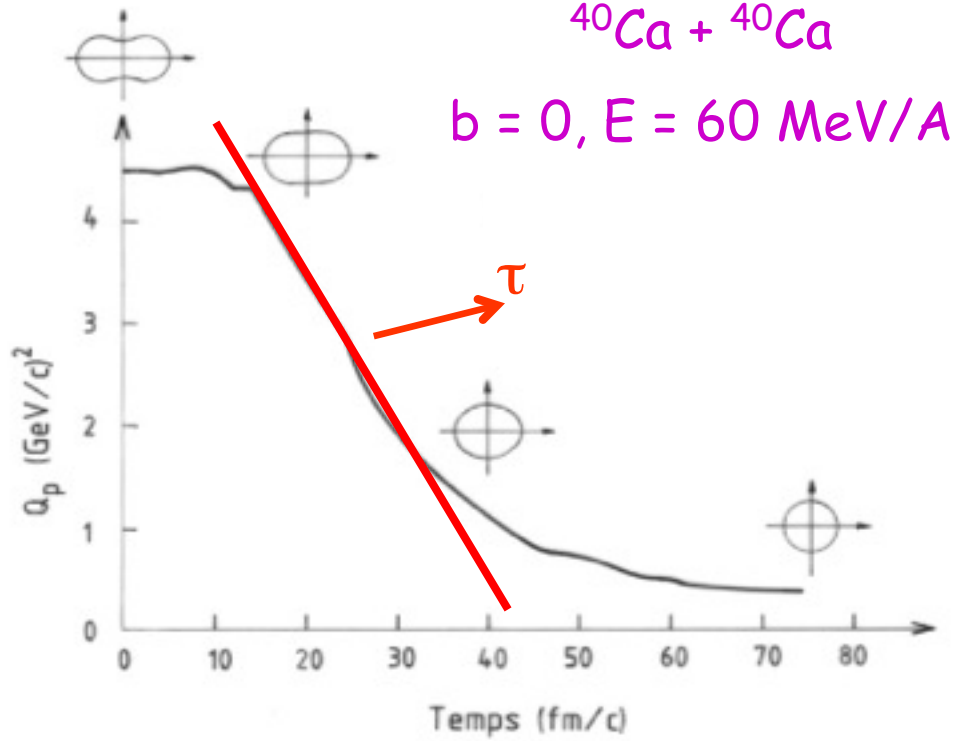

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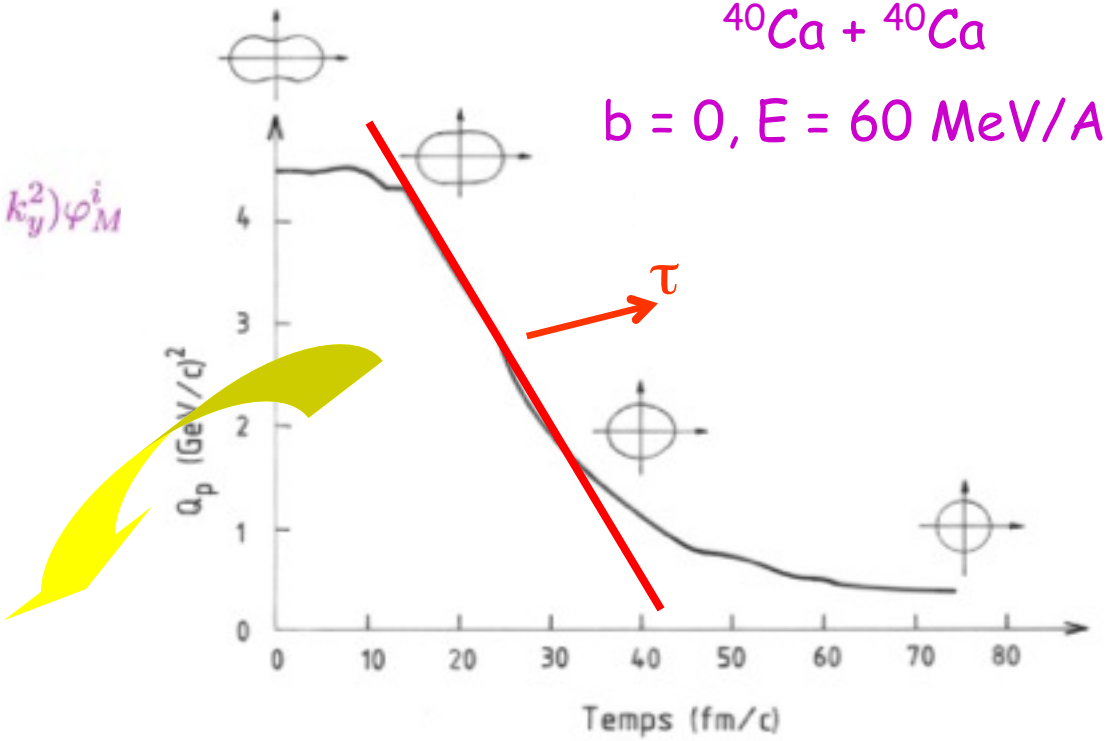

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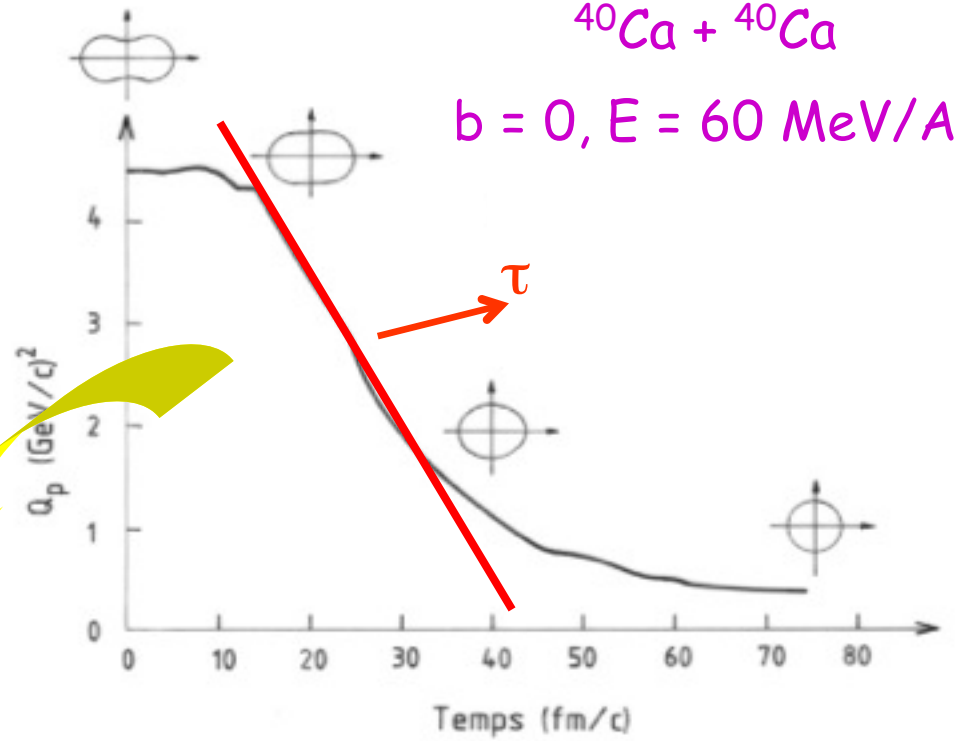

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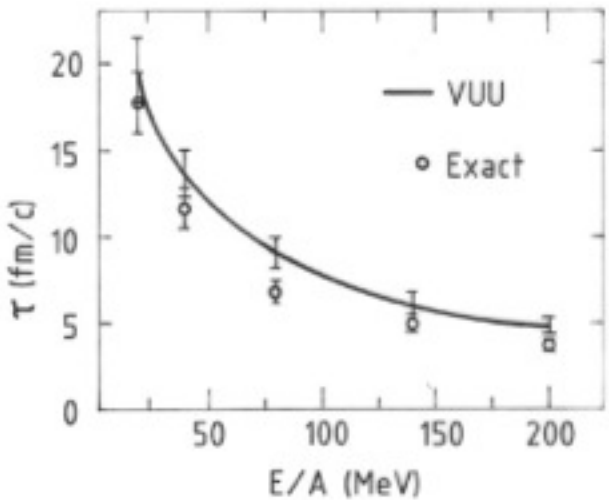

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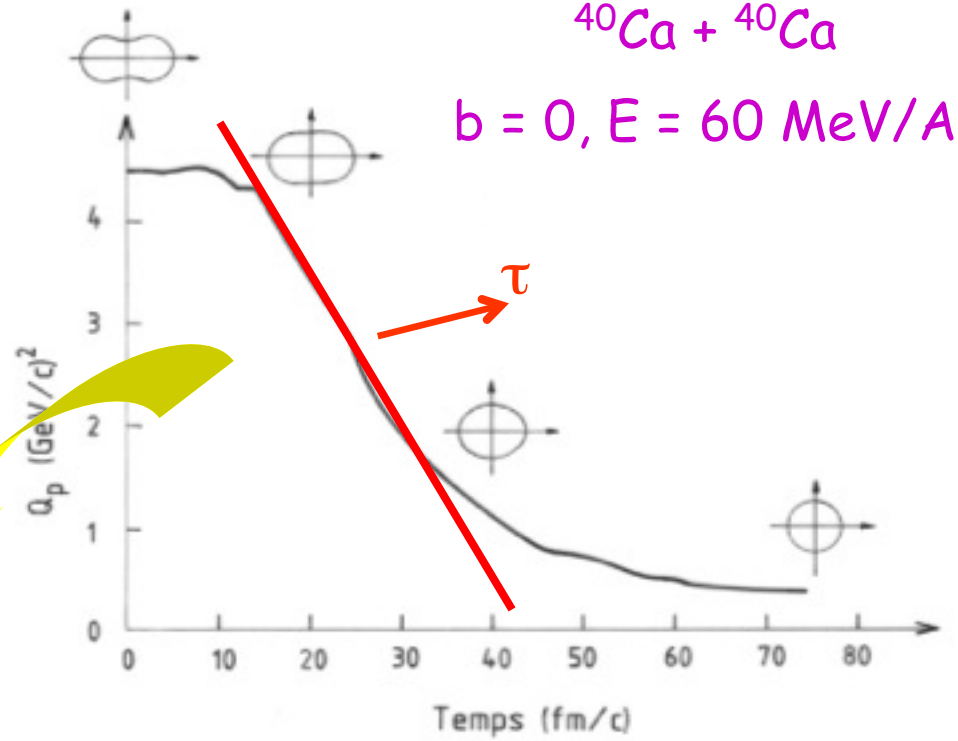

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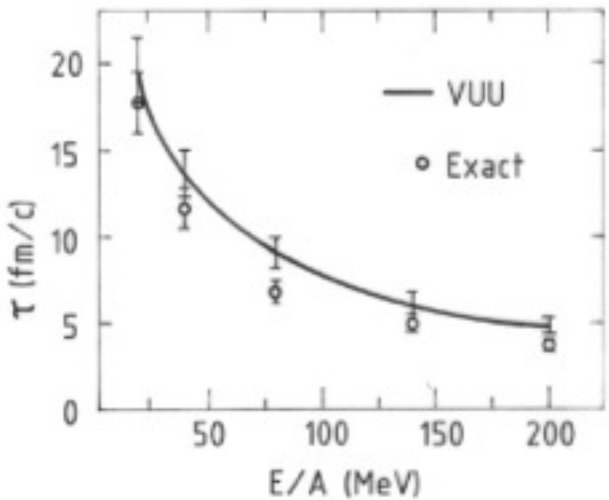

Fusion dynamics

Time scales

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Difficulties with VUU/BUU

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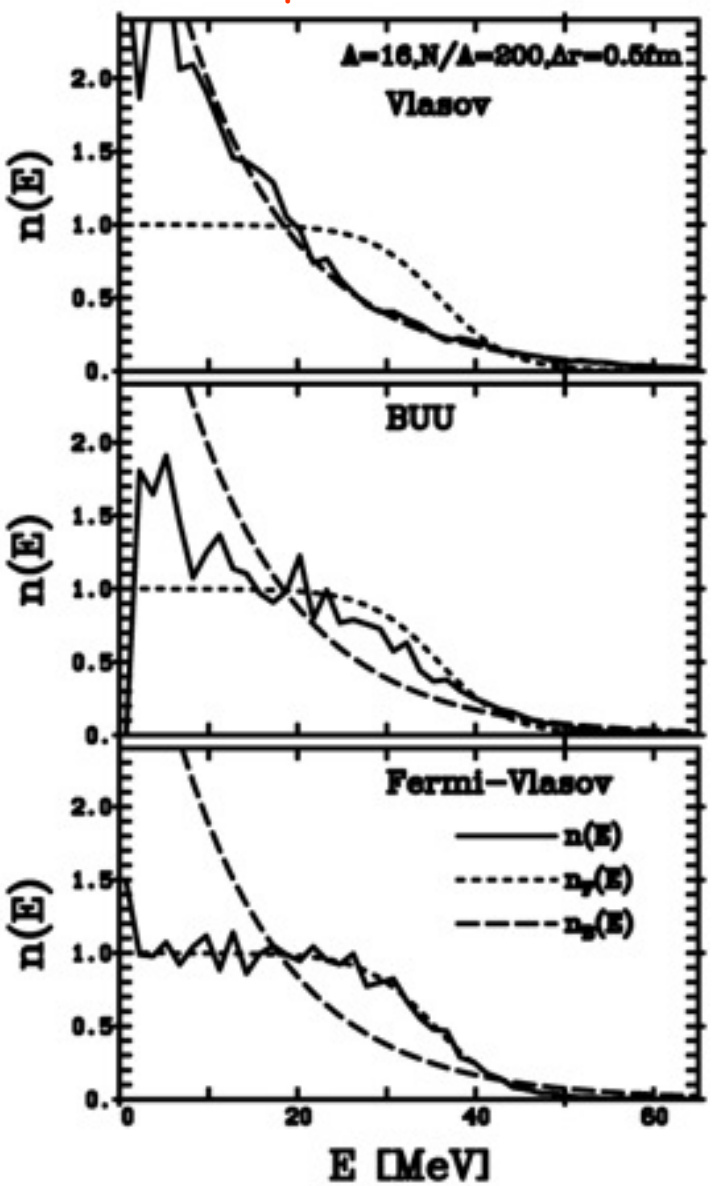
Occupation numbers



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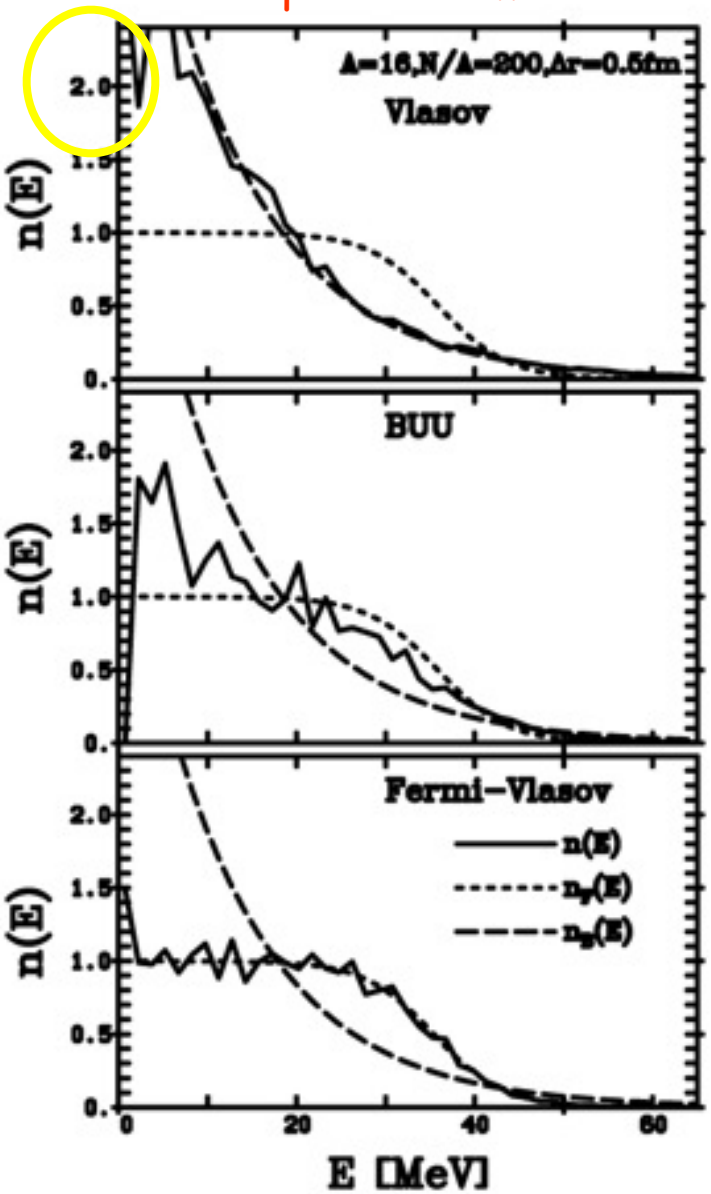

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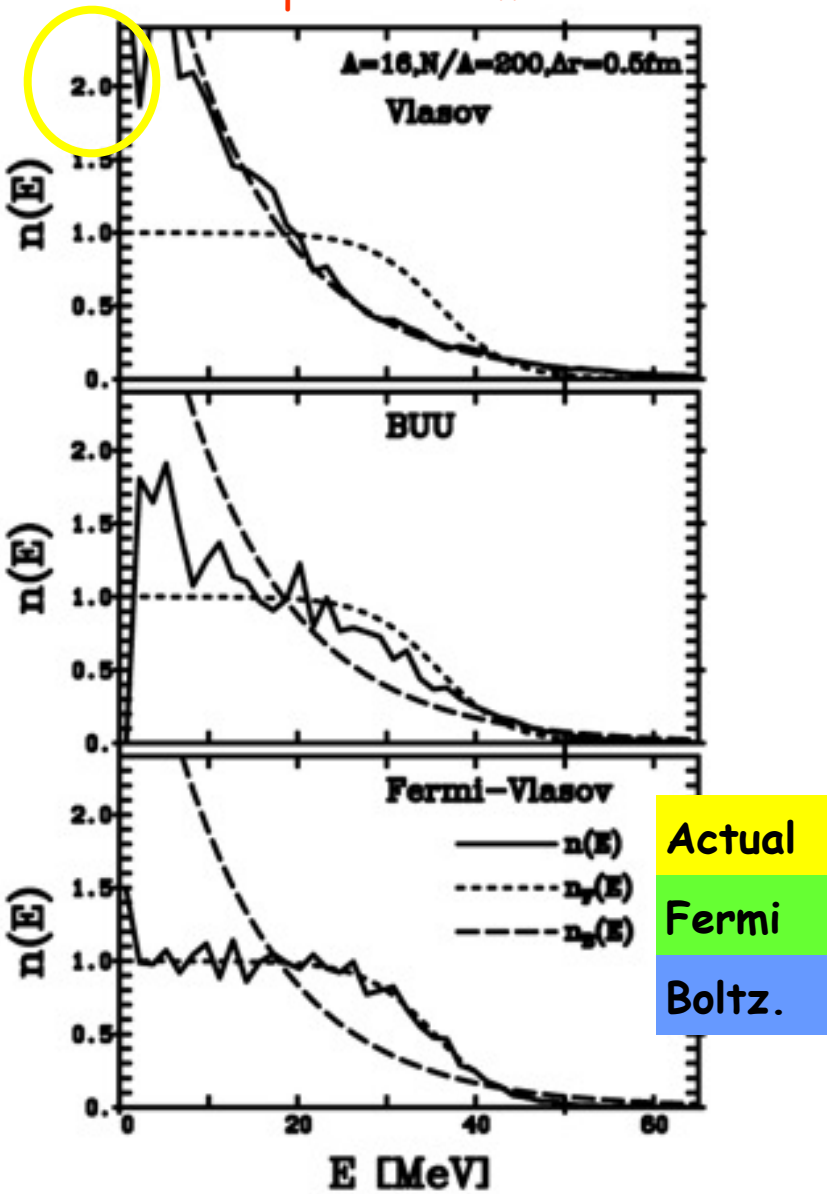

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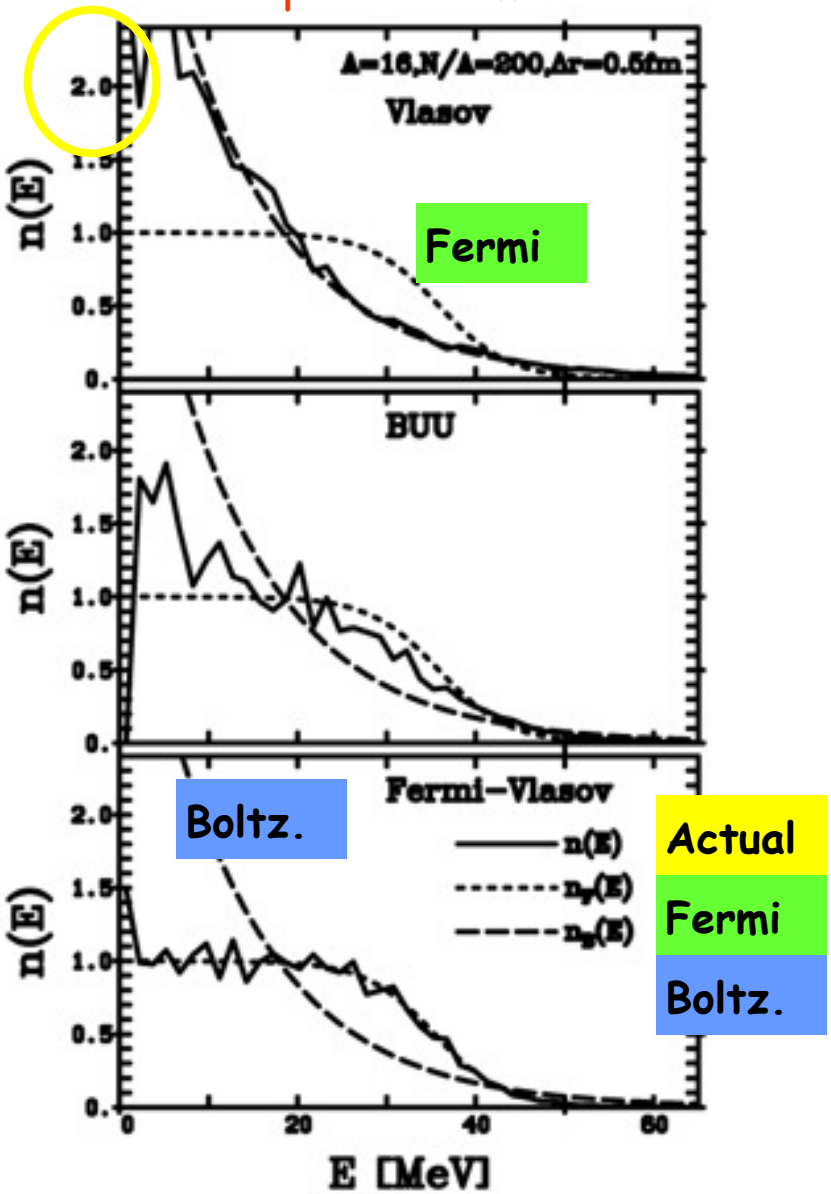

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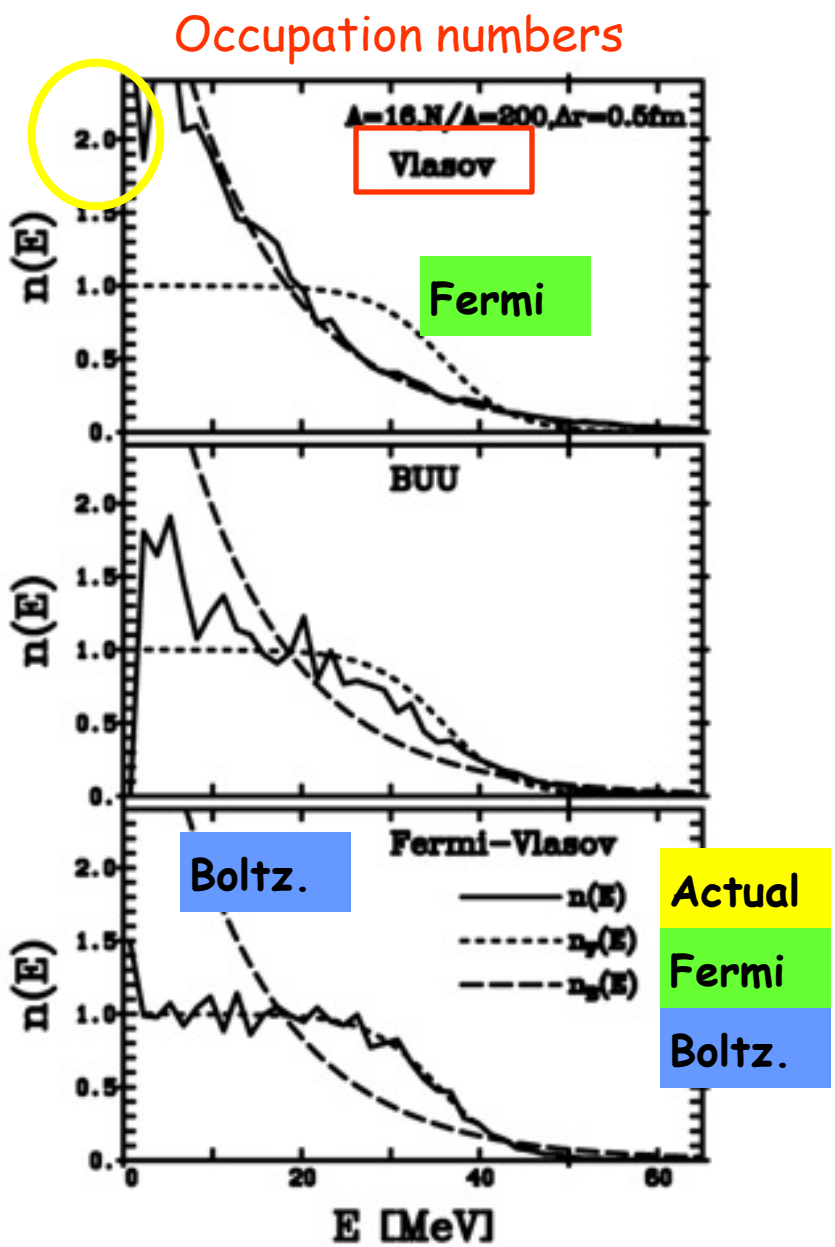

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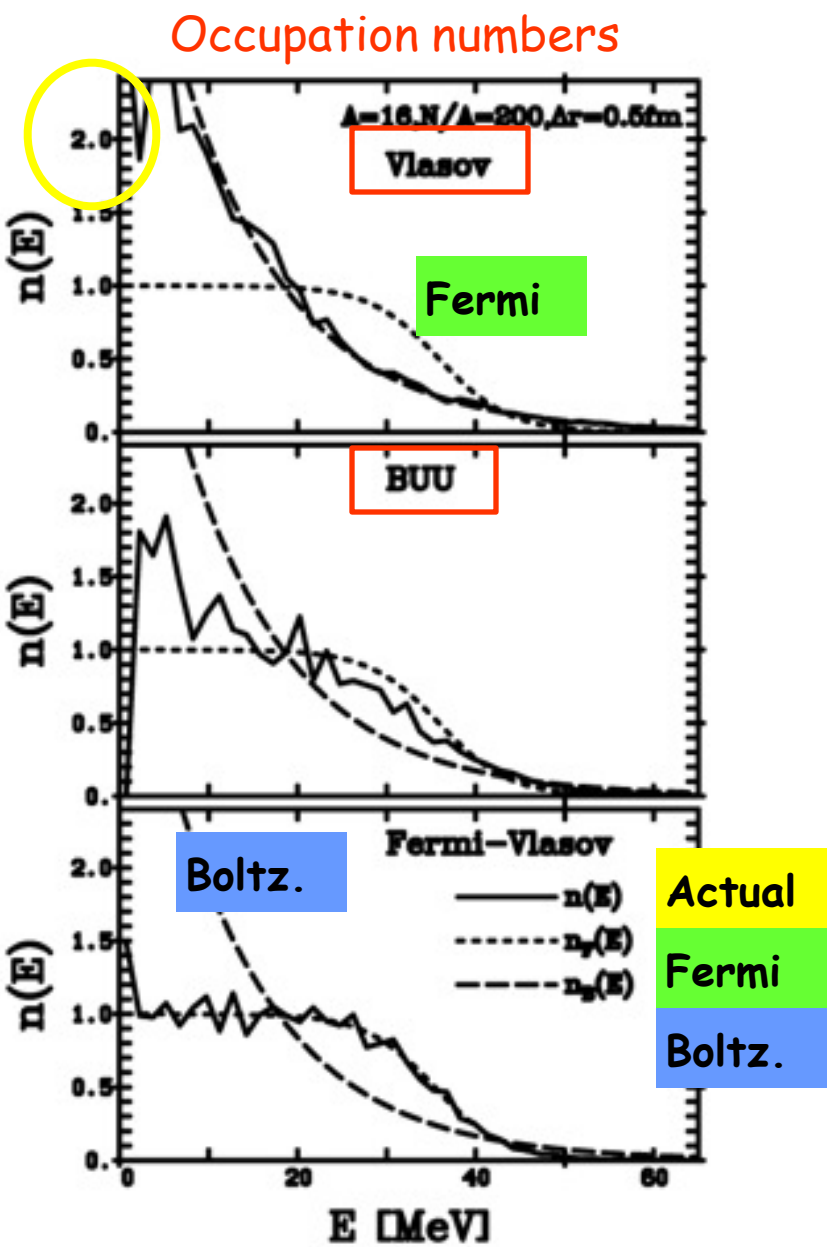

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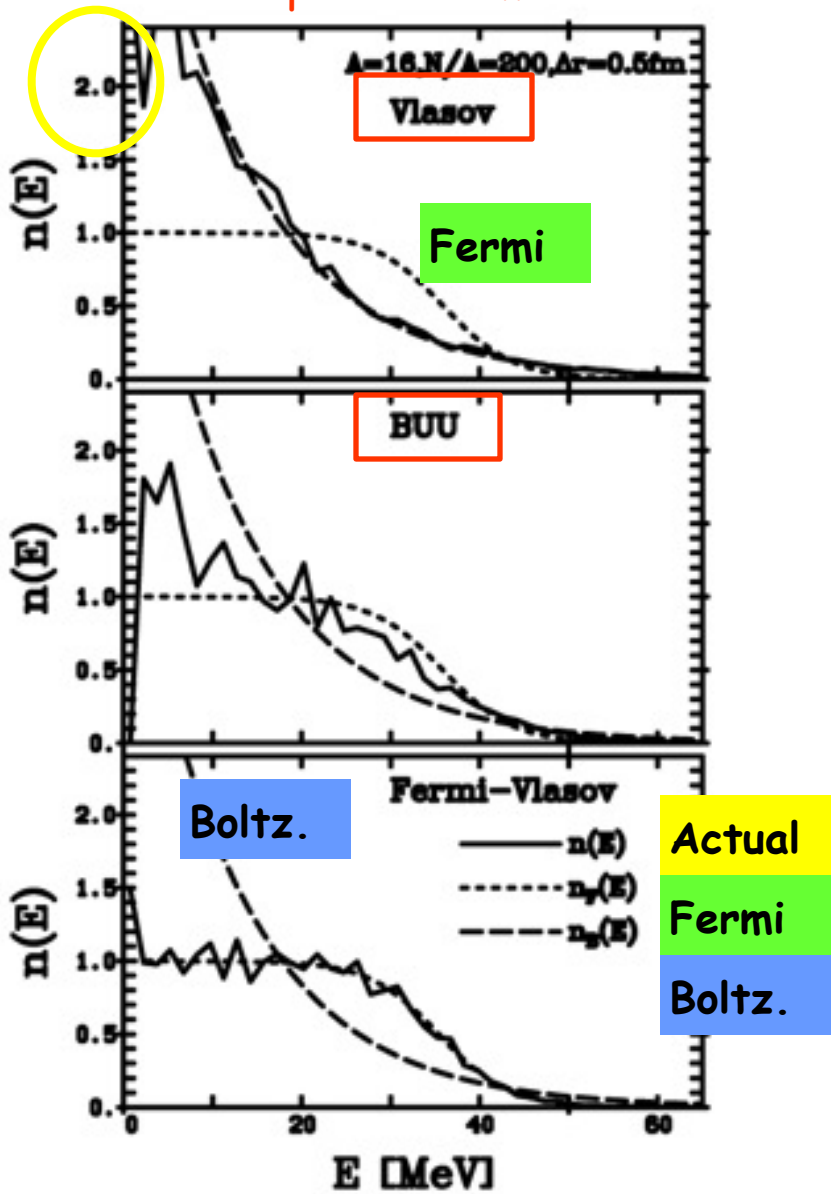

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- Genuine effects in fragment production

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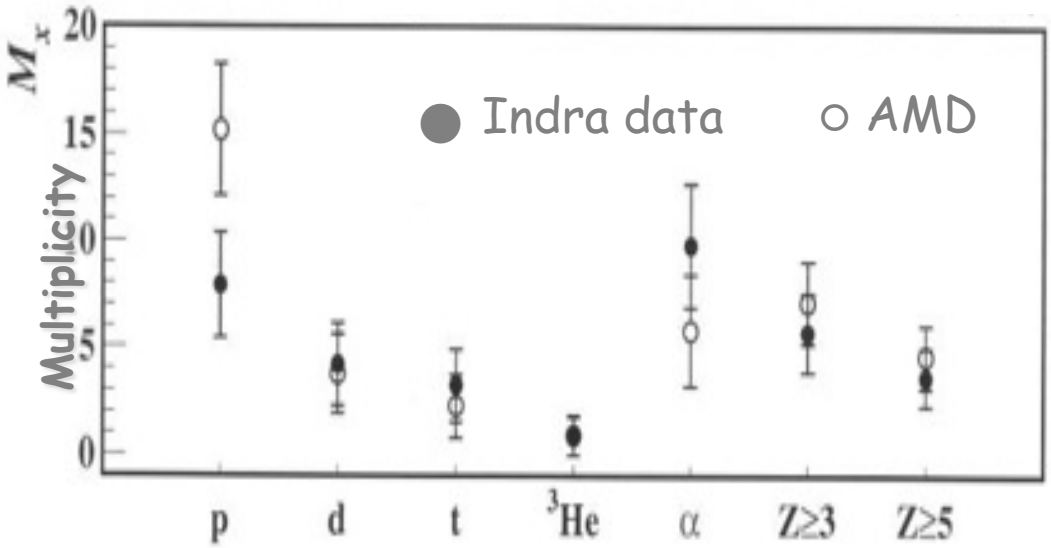

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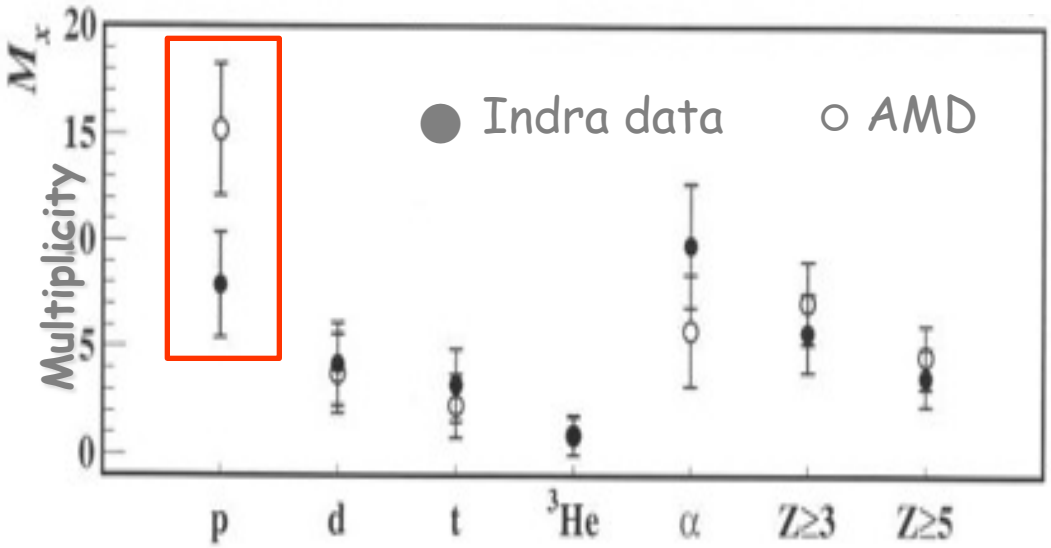

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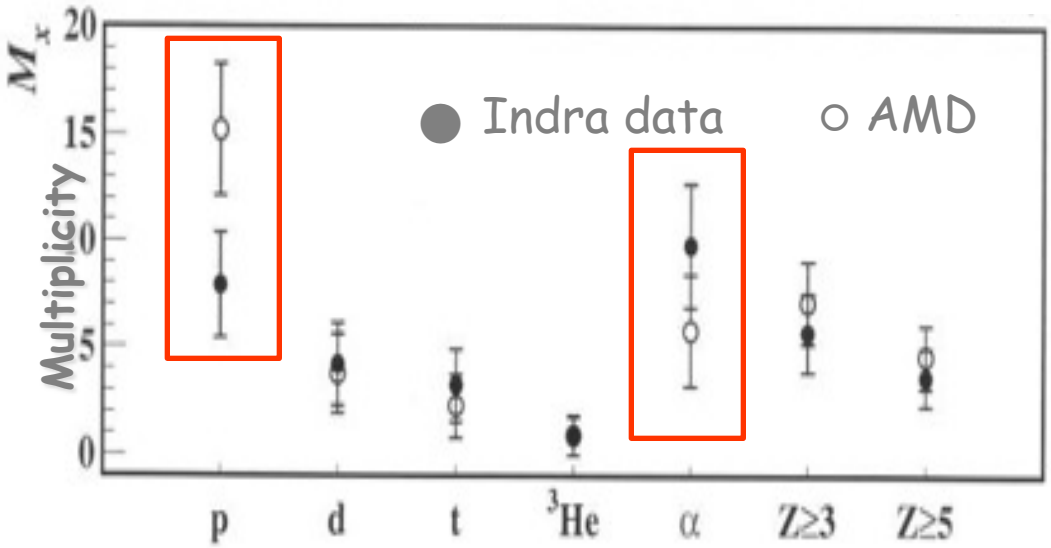

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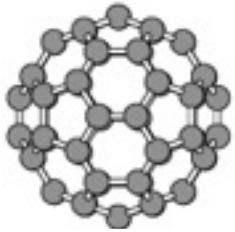

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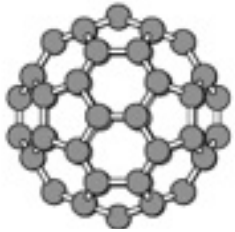

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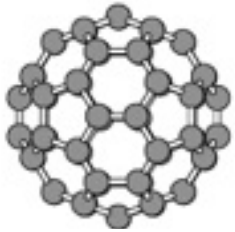

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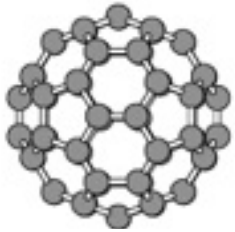

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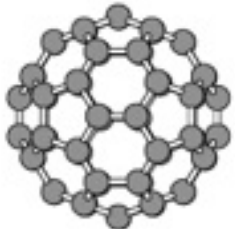

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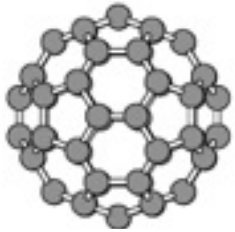

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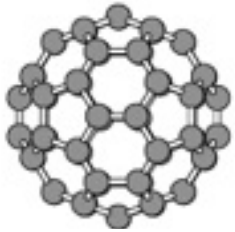

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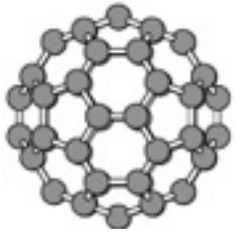

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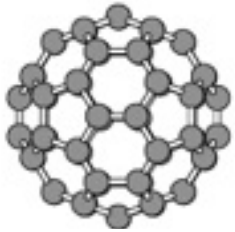

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$$i\partial_t \hat{\rho} = [\hat{h}[\hat{\rho}], \hat{\rho}] + \hat{I}_{coll}[\hat{\rho}]$$

Quantum kinetic equation

Caution : $\hat{\rho}(\mathbf{r}, \mathbf{r}', t)$ is the body density **MATRIX** , not the standard TDDFT matter density $\varrho(\mathbf{r}, t)$ ($\hat{\rho} \neq \varrho$)

Involved object... Need of **simplifications** for realistic finite systems

A quantum relaxation time ansatz

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starting point: $\hat{\rho}(t) = \sum_\alpha |\phi_\alpha(t)\rangle W_\alpha(t) \langle\phi_\alpha(t)|$

(1) mean-field propagation: $|\phi_\alpha^{(\mathrm{mf})}\rangle = \hat{U}(t+\Delta t, t)|\phi_\alpha(t)\rangle$

$W_\alpha(t) = W_\alpha^{(mf)} = \text{const.}$

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(3)

density-constrained mean field (DCMF)

1. $\hat{\rho}_{eq} = \hat{\rho}_{eq}[\varrho_{mf}(\mathbf{r})\,, \mathbf{j}_{mf}(\mathbf{r}), E_{mf}]$

$= \sum_\alpha |\phi'_\alpha\rangle W'_\alpha \langle\phi'_\alpha|$

2. intrinsic excitation energy E^*_{intr}

(4)

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$\hat{\rho}(t+\Delta t) = \hat{\rho}_{mf} - \frac{\Delta t}{\tau_{\mathrm{relax}}}[\hat{\rho}_{mf} - \hat{\rho}_{eq}]$

(4)

relaxation time:

$\hbar\tau_{\mathrm{relax}}^{-1} = 0.40\,\sigma_{ee} r_s^{-2}\, E^*_{\mathrm{intr}}/N$

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$\hat{\rho}(t+\Delta t) = \sum_\alpha |\phi_\alpha(t+\Delta t)\rangle \tilde{W}_\alpha \langle\phi_\alpha(t+\Delta t)|$

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Lunch break...

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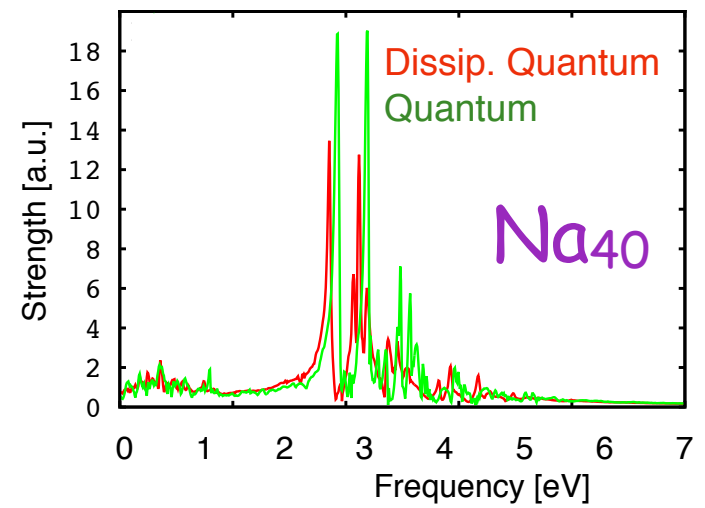

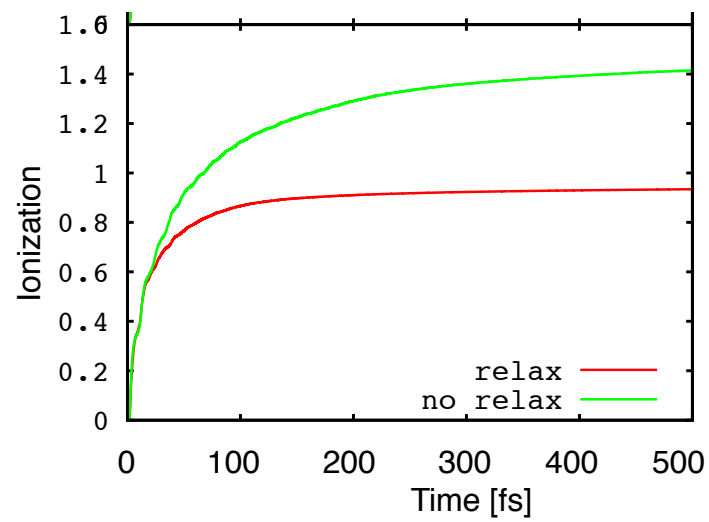

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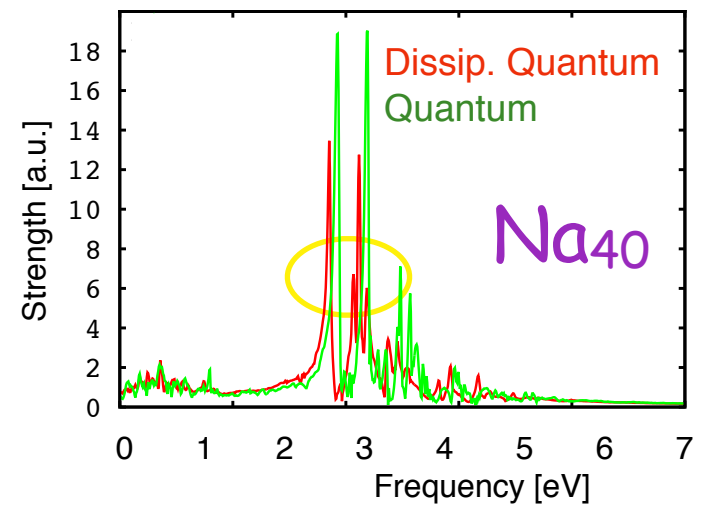

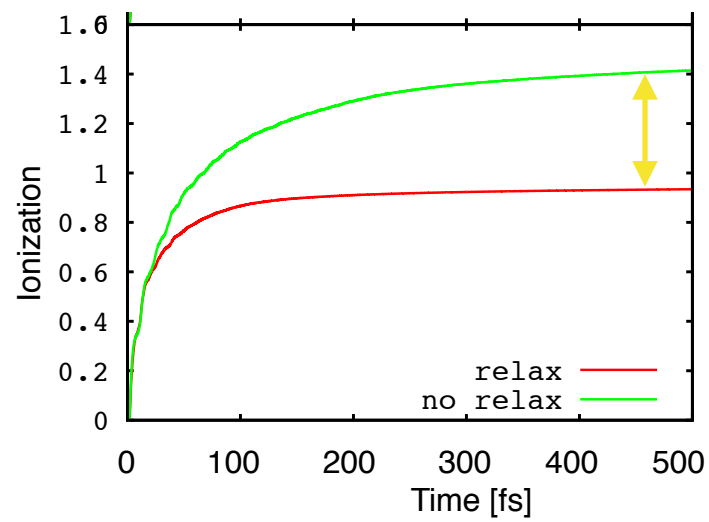

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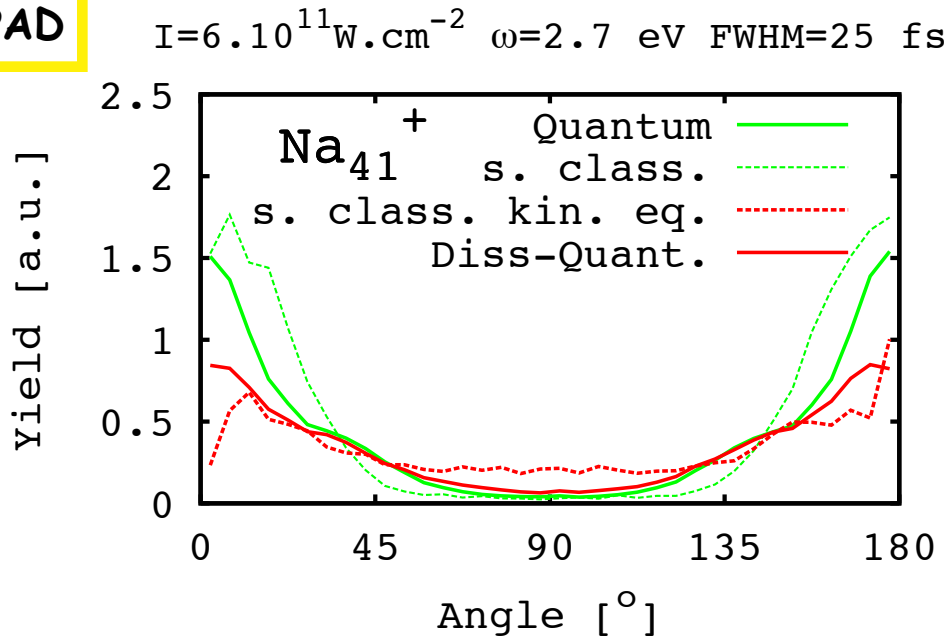

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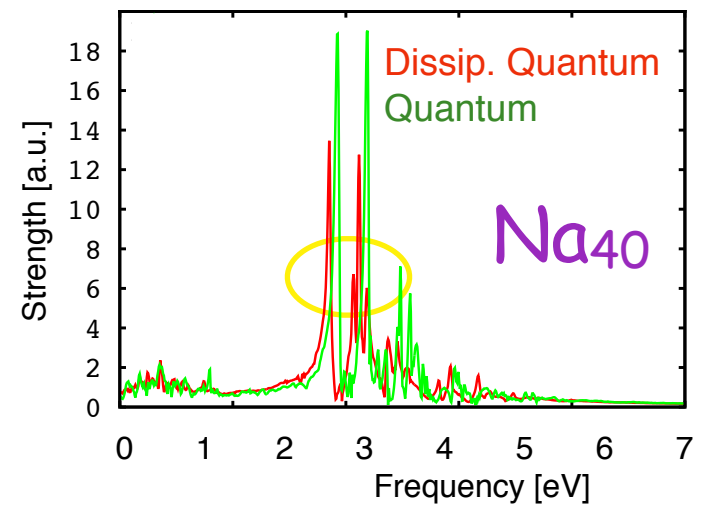

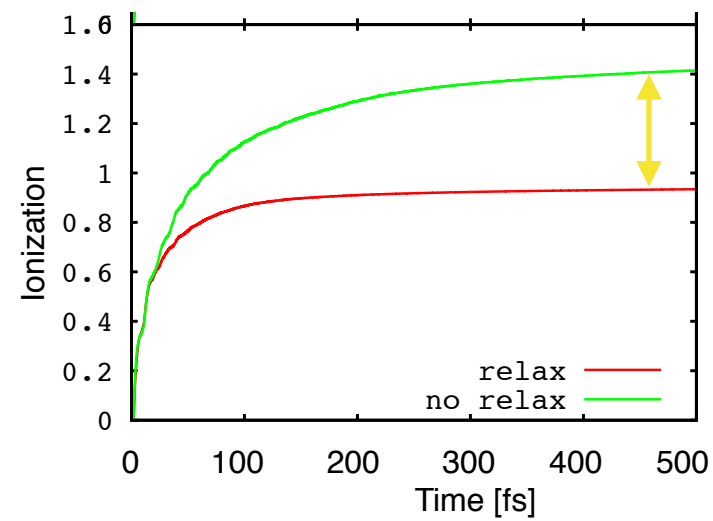

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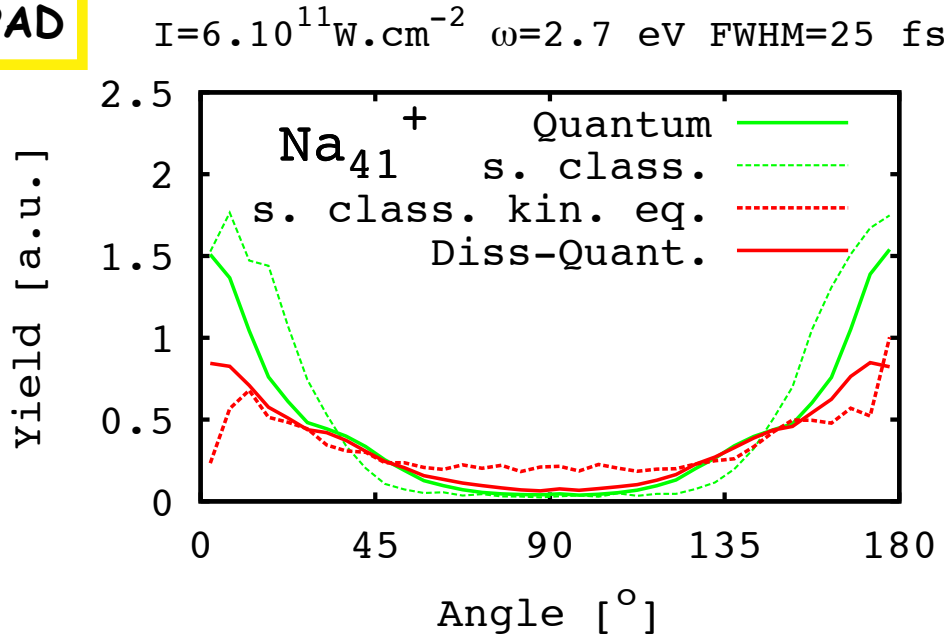

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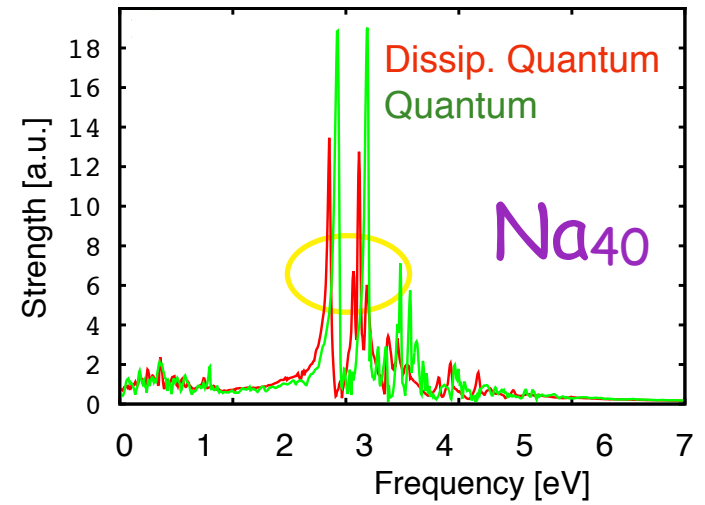

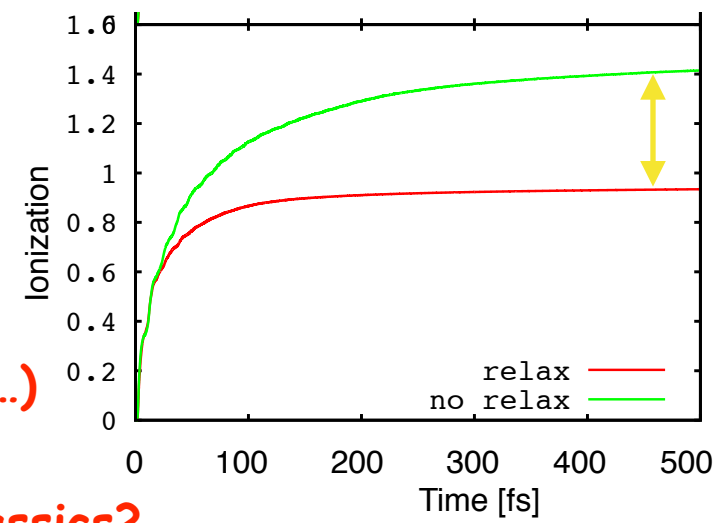

Sizable effects (ionization, response, PAD…)

Large temperature ~1.5 eV

First quantum theory; better than semi classics?

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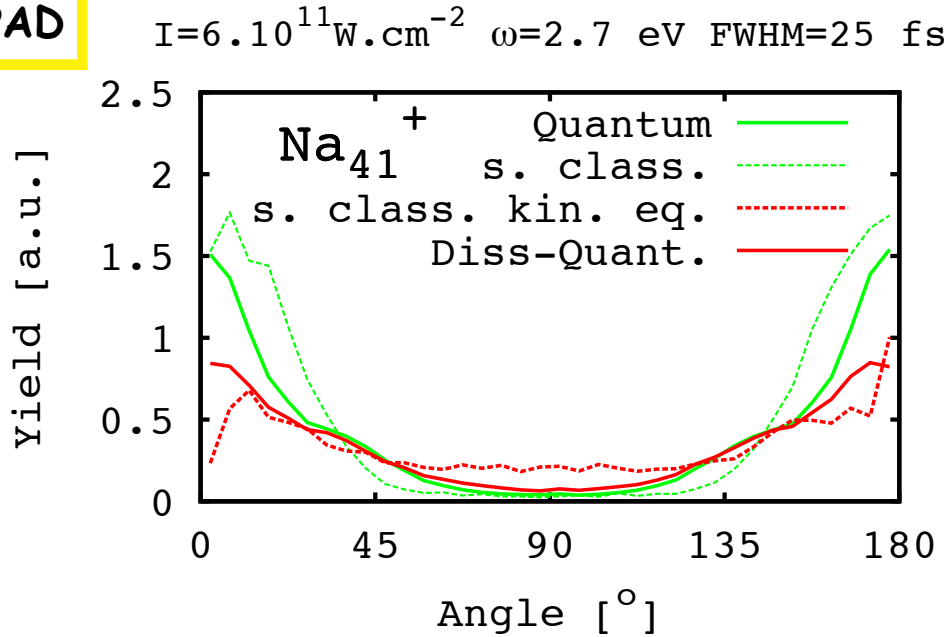

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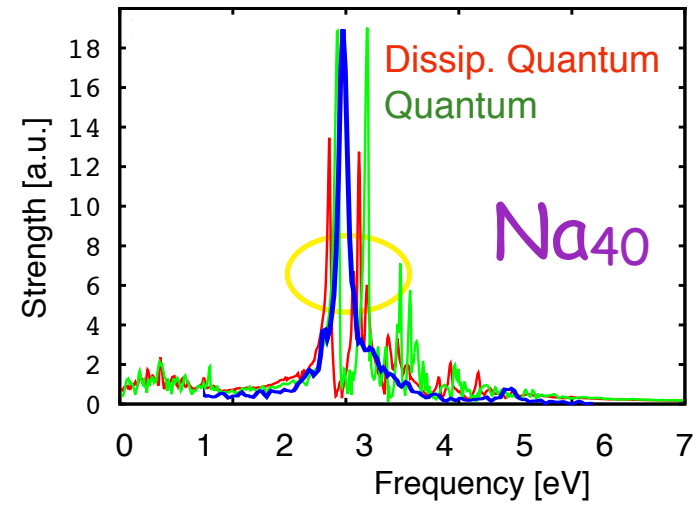

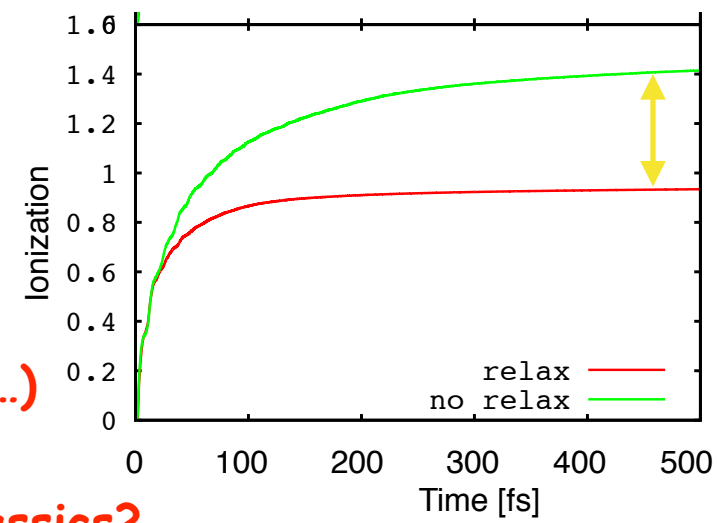

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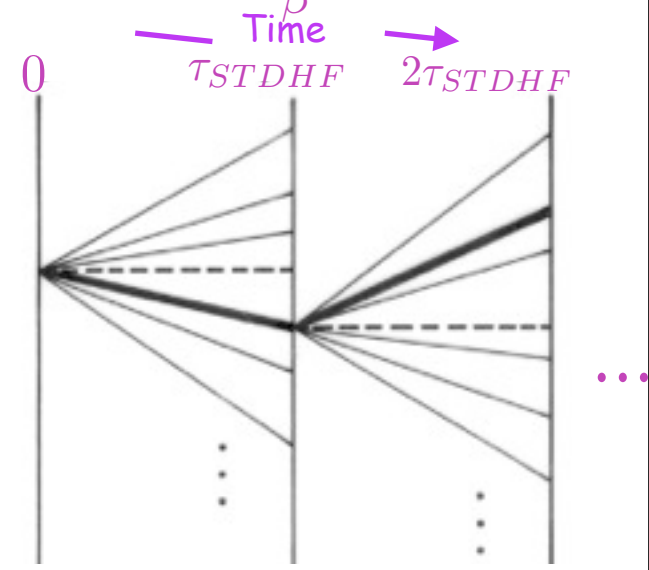

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TDHF
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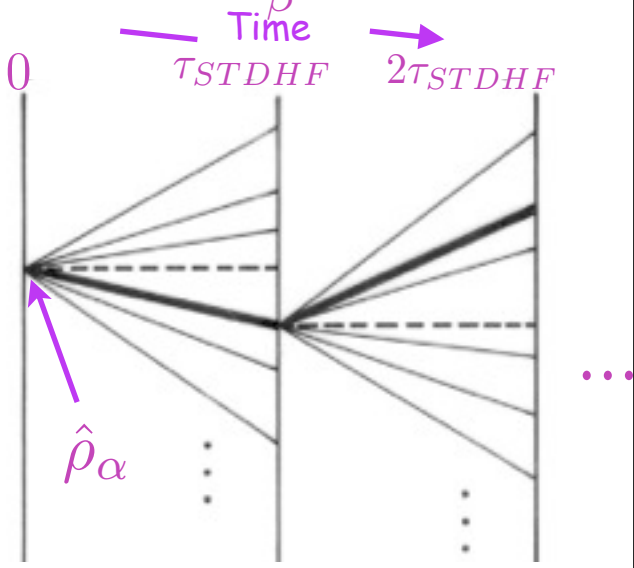

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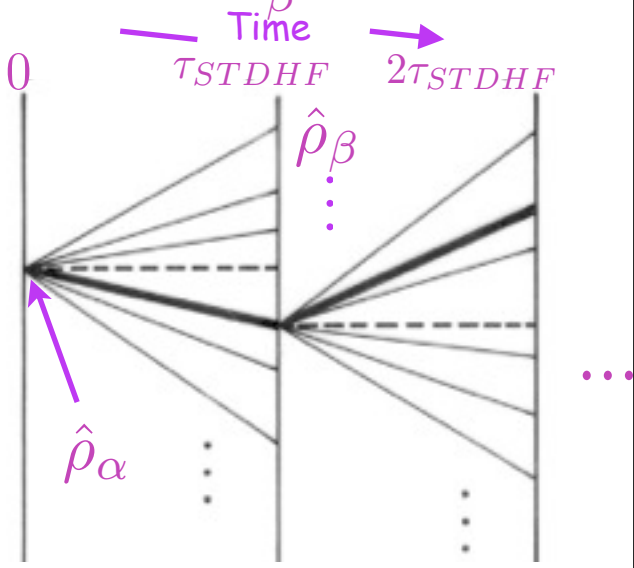

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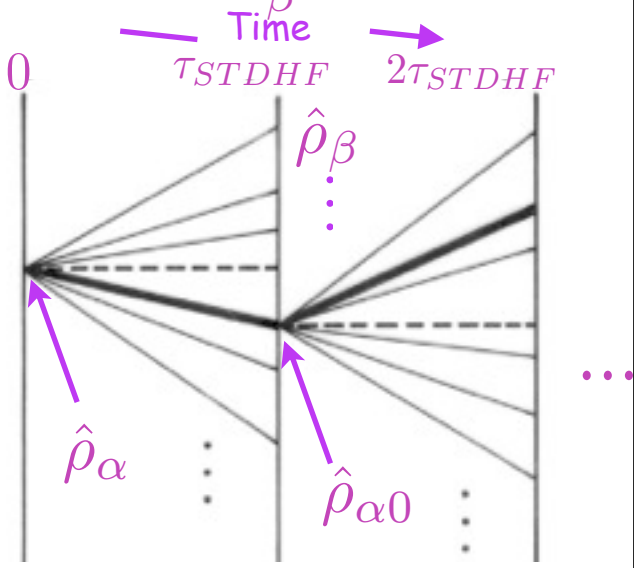

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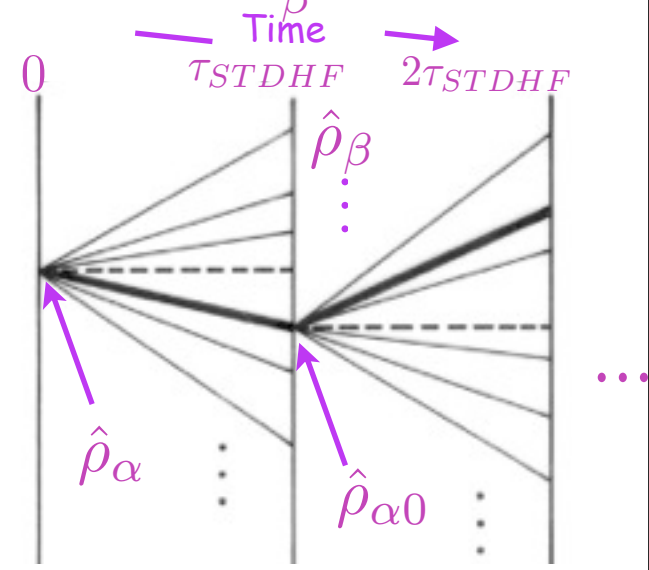

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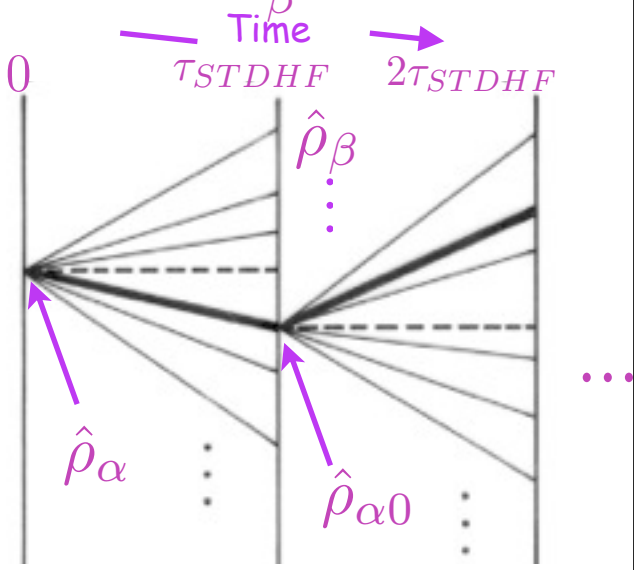

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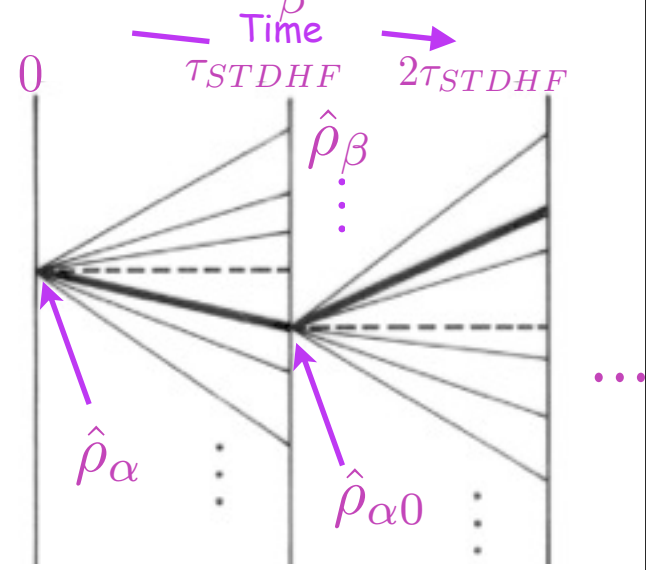

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STDHF in wavefunction form

- STDHF directly in terms of wavefunctions (Slater) $\hat{\rho}_\alpha \longrightarrow |\Phi_\alpha\rangle$
- Ensemble strategy of stochastic jumps : $|\Phi_\alpha\rangle \longrightarrow \{|\Phi_\beta\rangle\,, W_{\alpha\beta}\}$
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- Note the «forgiving» excitations (laser,...) in terms of phase space

Test case

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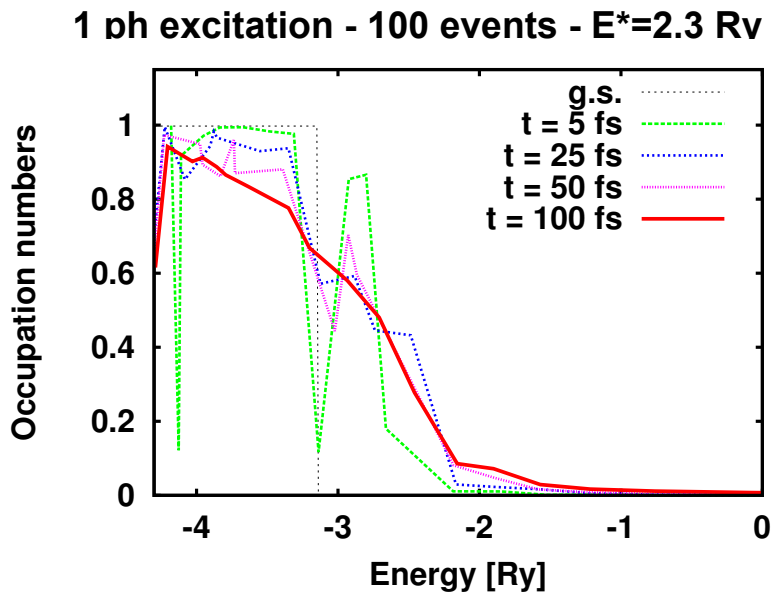

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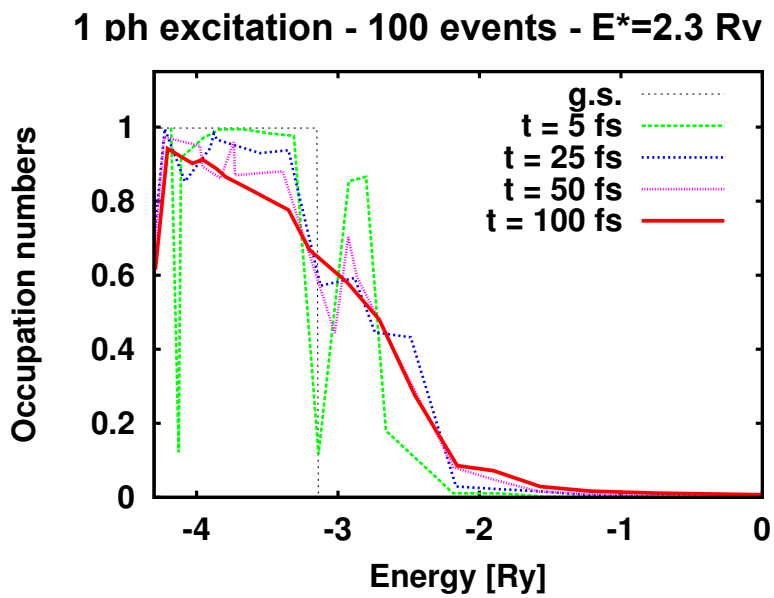
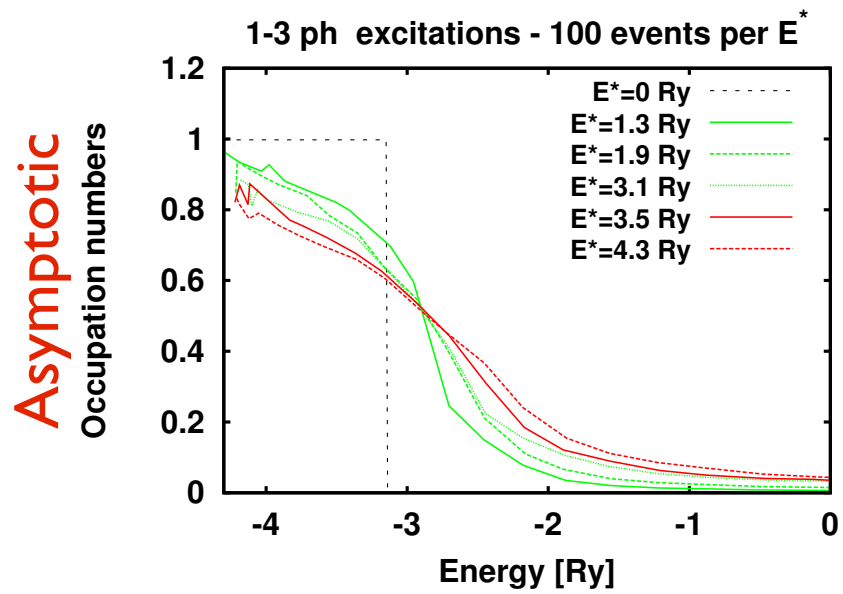
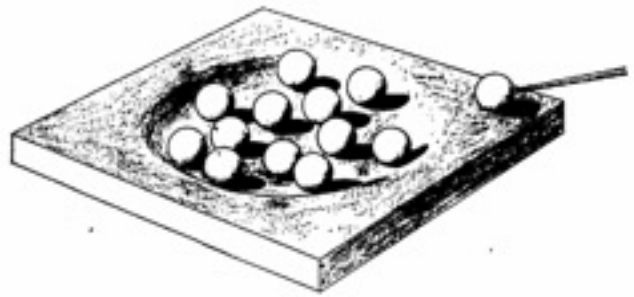




Towards the inclusion of dissipative effects in Quantum Time Dependent Mean-field Theories

neutron on nucleus



Dissipative mechanisms

in finite quantum systems

An old story…

N. Bohr, Science, 1937

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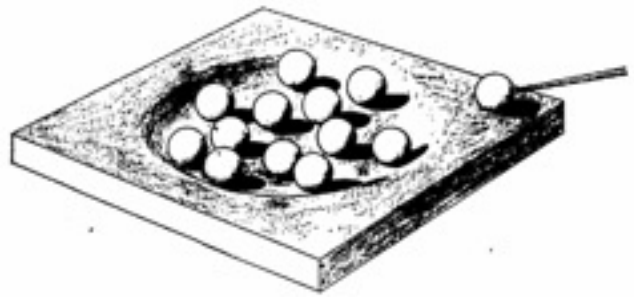

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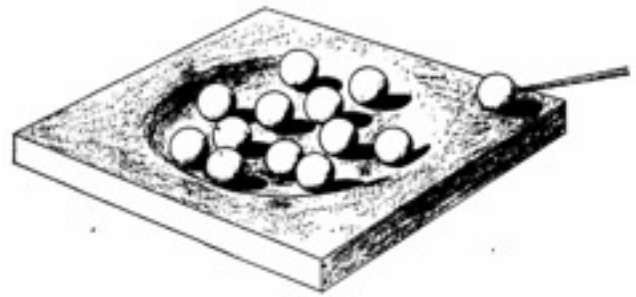

Dissipative mechanisms

in finite quantum systems

Several important results

- Key role of quantum effects
- Semi classical kinetic equations sometimes applicable
- Relaxation time ansatz done/ in the oven
- Stochastic extension of TDLDA done/ in the oven
- Tractable dissipative mean field in the near future

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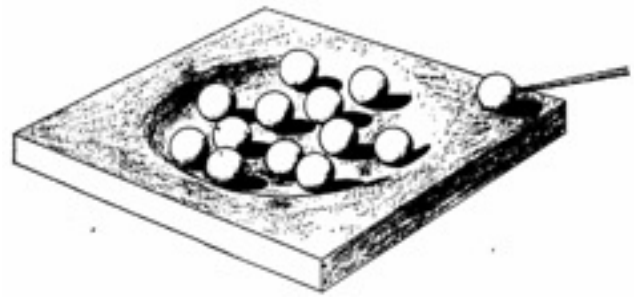

Many directions to be investigated
- Further analysis of relaxation time ansatz (quantum rate, systematics, photoelectron spectra,…)
- (Re)derivation of a kinetic-like theory
- Tests of kinetic-like approaches
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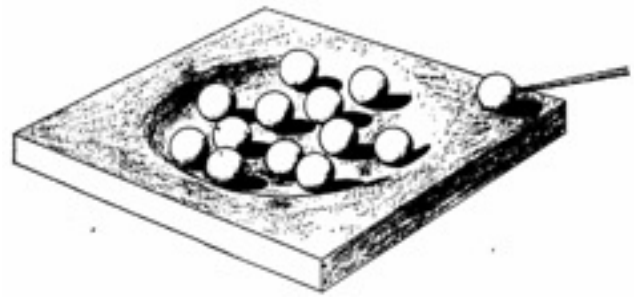

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