Two-centre HO basis for Skyrme HF: α clustering in ^{8}Be and ^{24}Mg $\rightarrow$ ^{12}C+^{12}C as a proof of principles calculations

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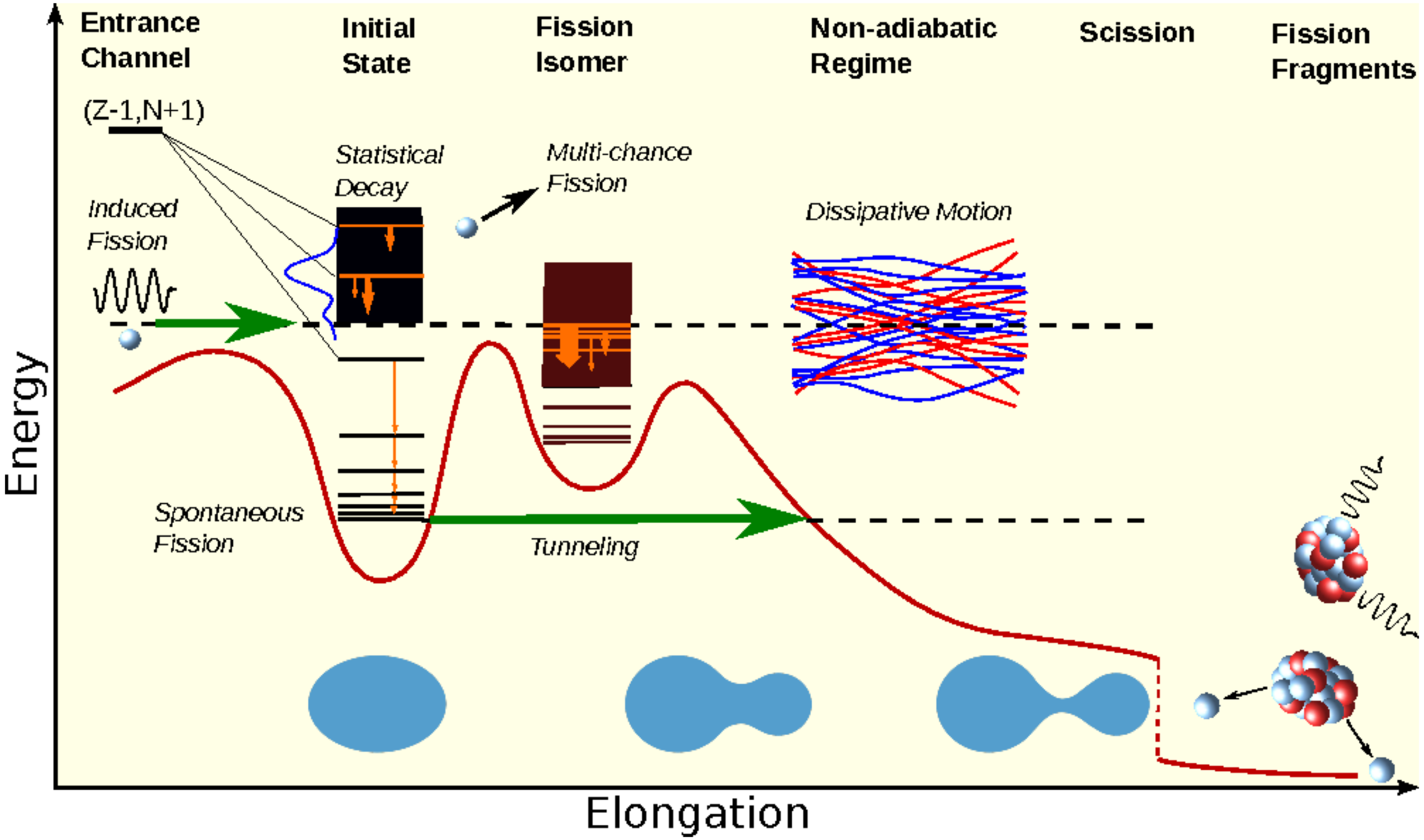
Joint APP, HEPP and NP Conference, Liverpool (April, 2024)

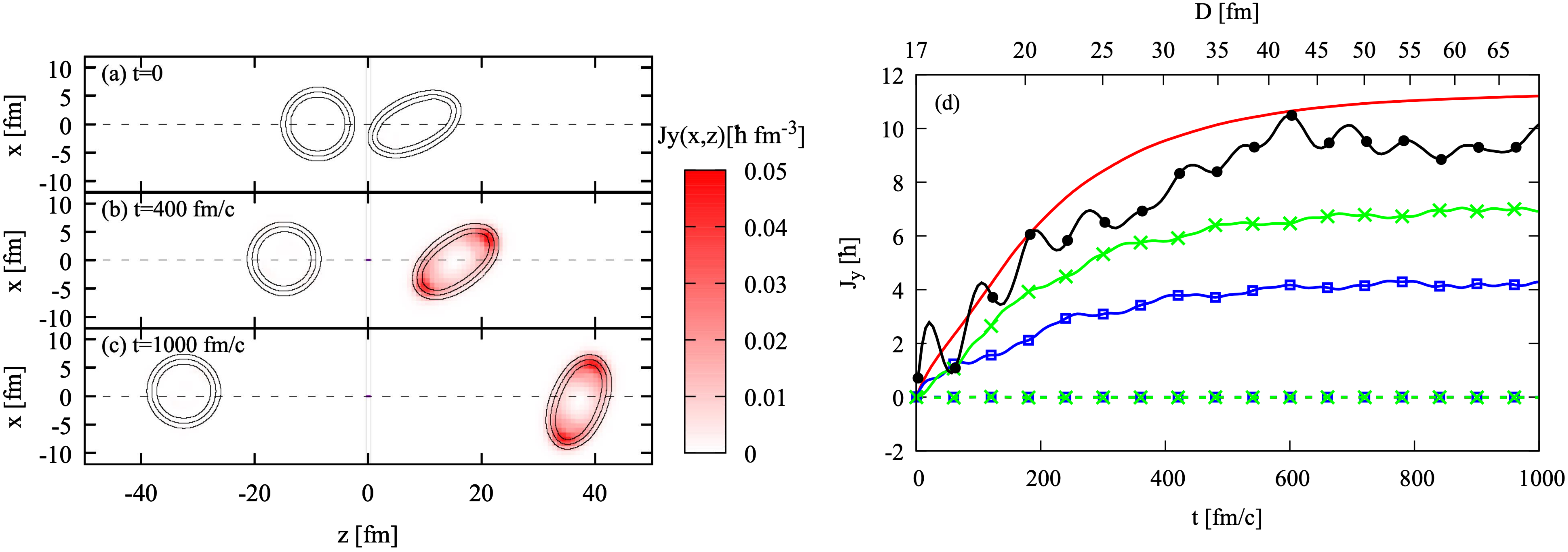
Fission is complex

1. Time-dependent process
2. All particles involved
3. Sensitive to the state of compound nucleus
4. Large deformations
5. Different ways to go through the fission path
6. Description of separated fragments

M. Bender et al 2020, J. Phys. G: Nucl. Part. Phys. 47 113002



And theory and experiment are still fighting (angular momentum generation problem)



Guillaume Scamps
Phys. Rev. C 106 (2022) 054614

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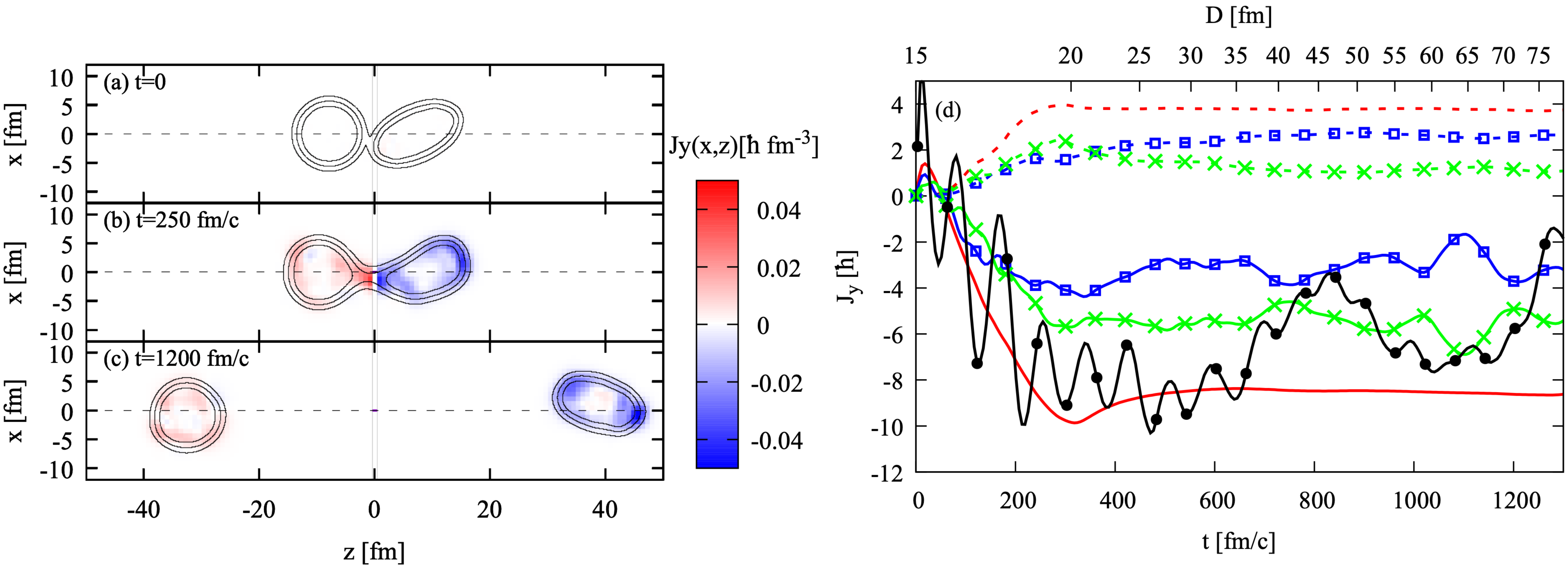

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The main goal of the project is to develop a DFT solver to control fission fragment's…

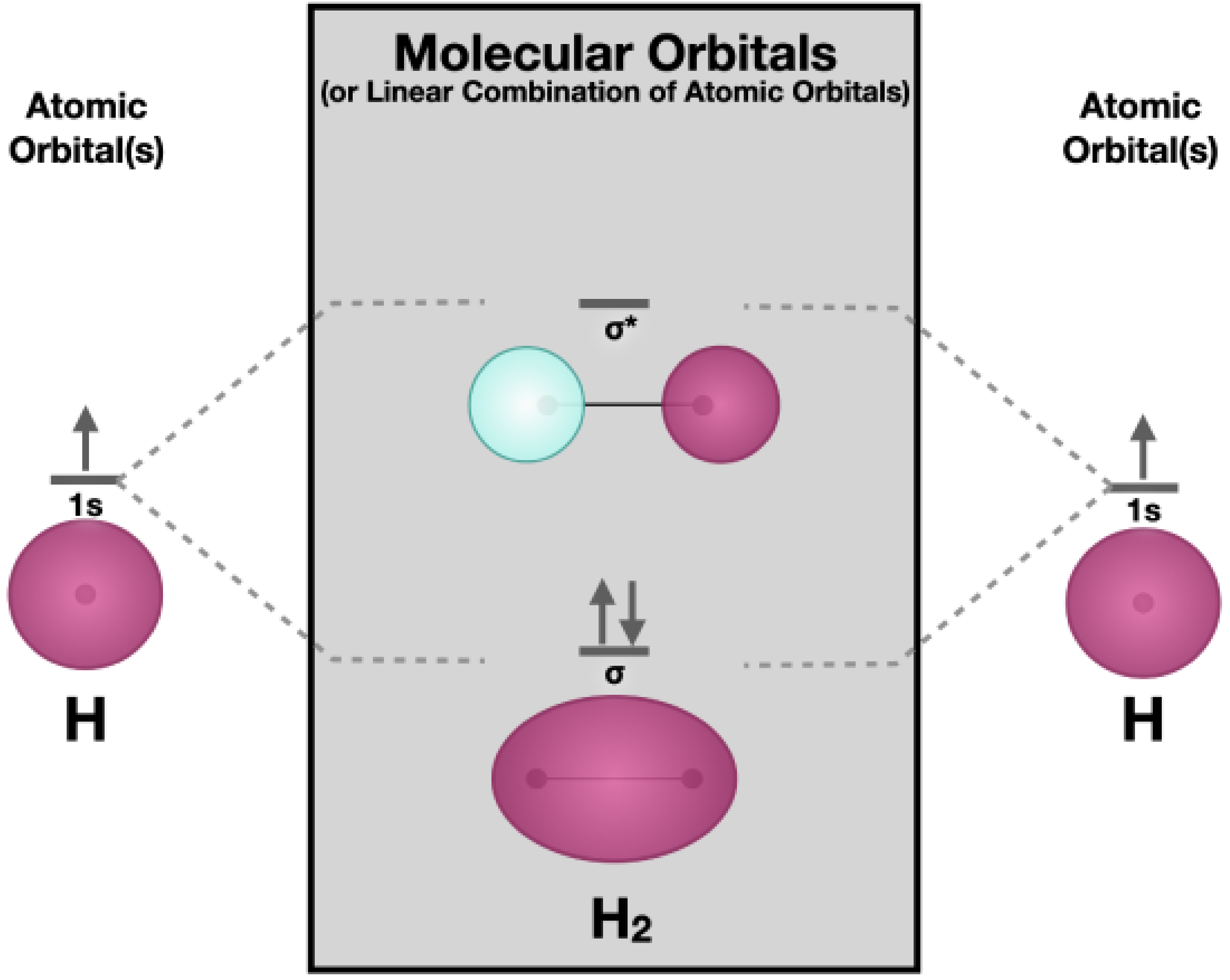
1. Separation
2. Deformation
3. Orientation

In the style of LCAO, the s.p. wave function reads as:

$$\Psi_\alpha(\mathbf{r}\sigma) = \sum_{i=A}^{B}\sum_{\mathbf{n}=0}^{N_0}\sum_{s_z=-1/2}^{1/2} \mathbb{C}_\alpha^{\mathbf{n},i,s_z}\varphi_{n_x,i}(x)\varphi_{n_y,i}(y)\varphi_{n_z,i}(z)\delta_{s_z\sigma}$$

where the (shifted) HO basis states:

$$\varphi_{n_\mu,i}(r_\mu) = \sqrt{\frac{b_{\mu,i}}{\sqrt{\pi}2^{n_\mu}n_\mu!}}H_{n_\mu}\left[b_{\mu,i}(r_\mu - r_{\mu 0,i})\right]e^{-\frac{1}{2}b^2_{\mu,i}(r_\mu-r_{\mu 0,i})^2}$$



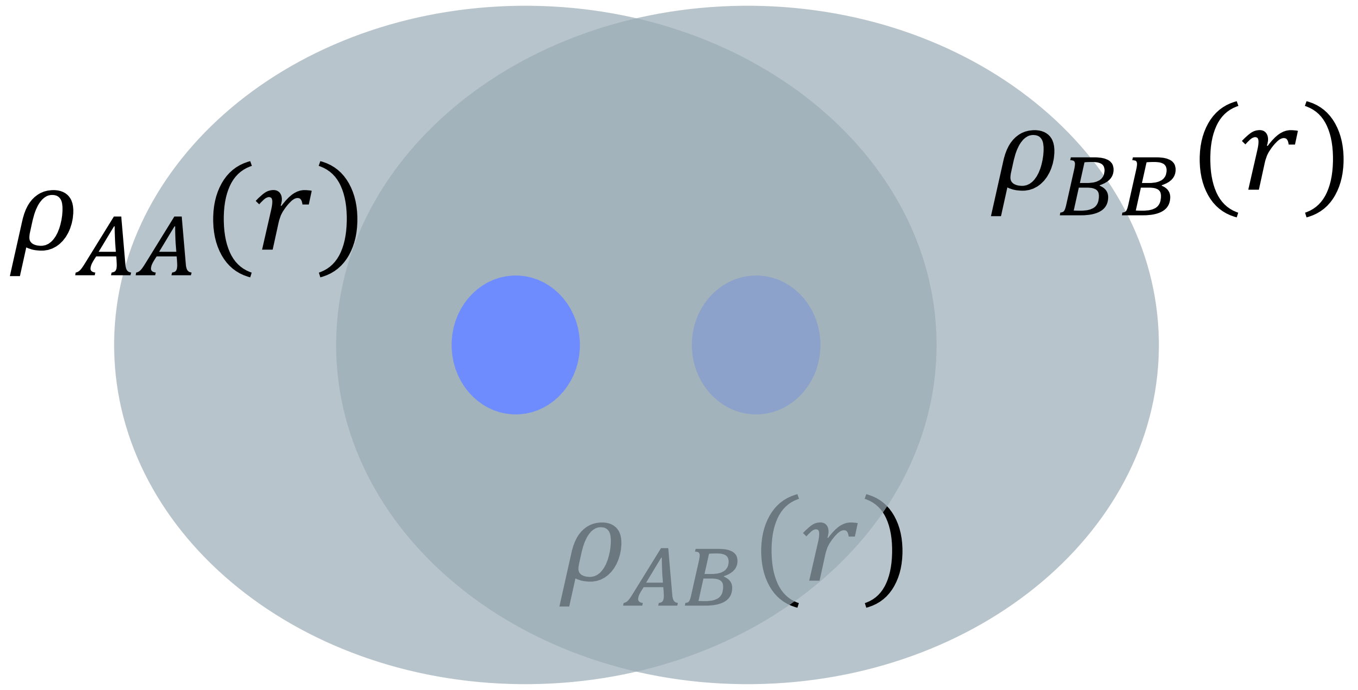
Hass et al., Inorganic Chemistry from Libretexts Chemistry

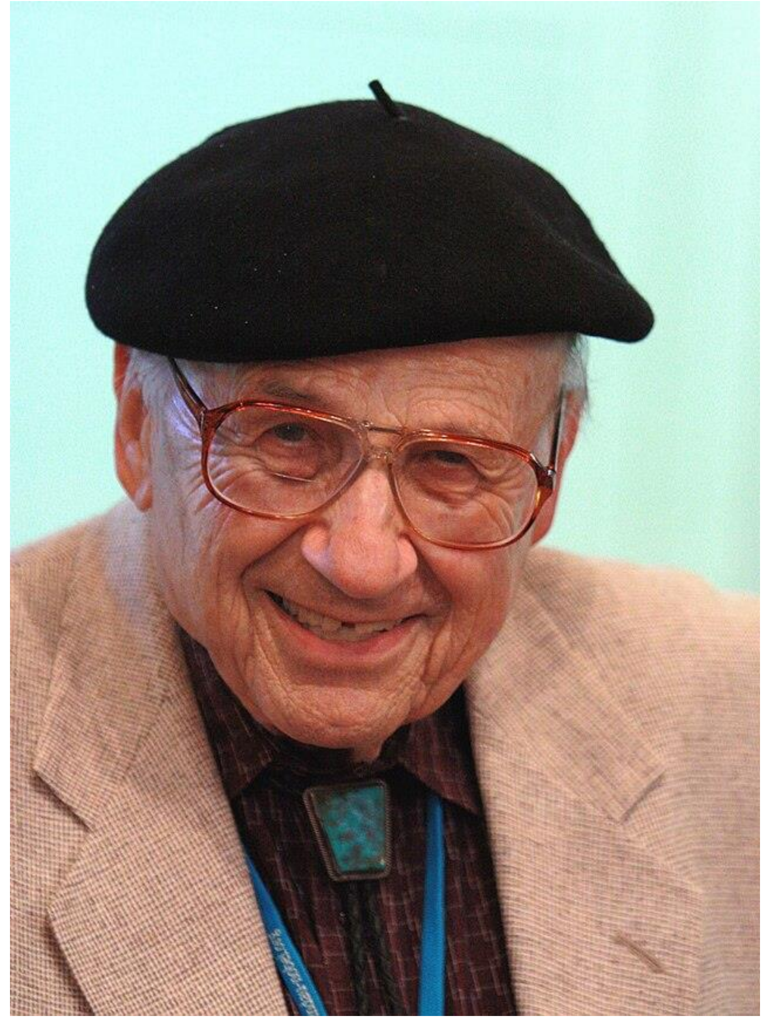
The key ingredient is to build the local density

$$\rho(\mathbf{r}\sigma) = \sum_{\alpha} v_{\alpha}^{2} \Psi_{\alpha}^{*}(\mathbf{r}\sigma)\Psi_{\alpha}(\mathbf{r}\sigma)$$

which now can be expanded as

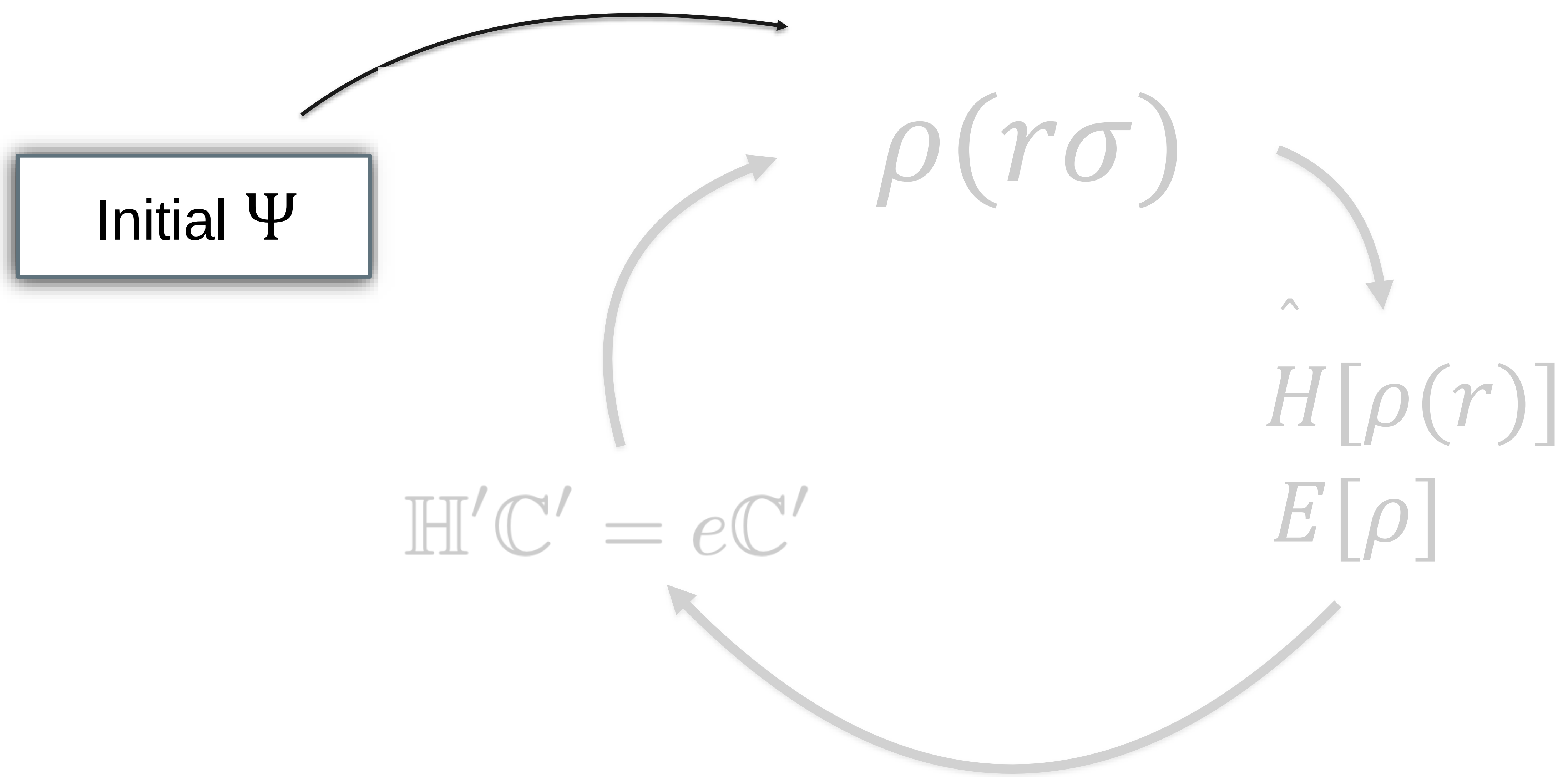
$$\rho(\mathbf{r}\sigma) = \rho(\mathbf{r}\sigma)_{AA} + \rho(\mathbf{r}\sigma)_{BB} + 2\mathrm{Re}\left[\rho(\mathbf{r}\sigma)_{AB}\right]$$




W. Kohn
(1923-2016)


P. Hohenberg
(1934-2017)

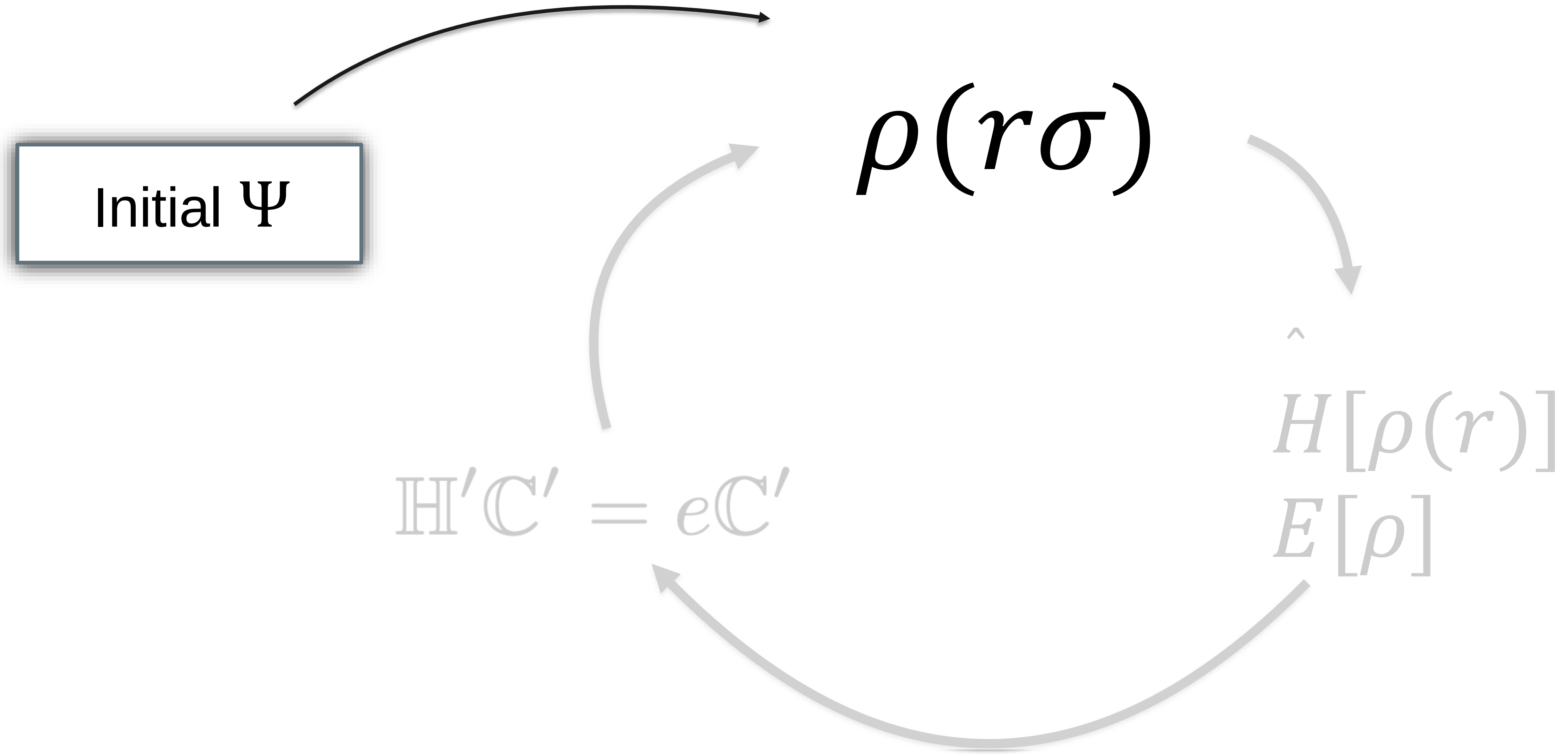
Apart from that, the self-consistent loop stays the same



Step 0:

1. To diagonalise the Nilsson Hamiltonian
2. Densities in space from OCHO calculation

Apart from that, the self-consistent loop stays the same



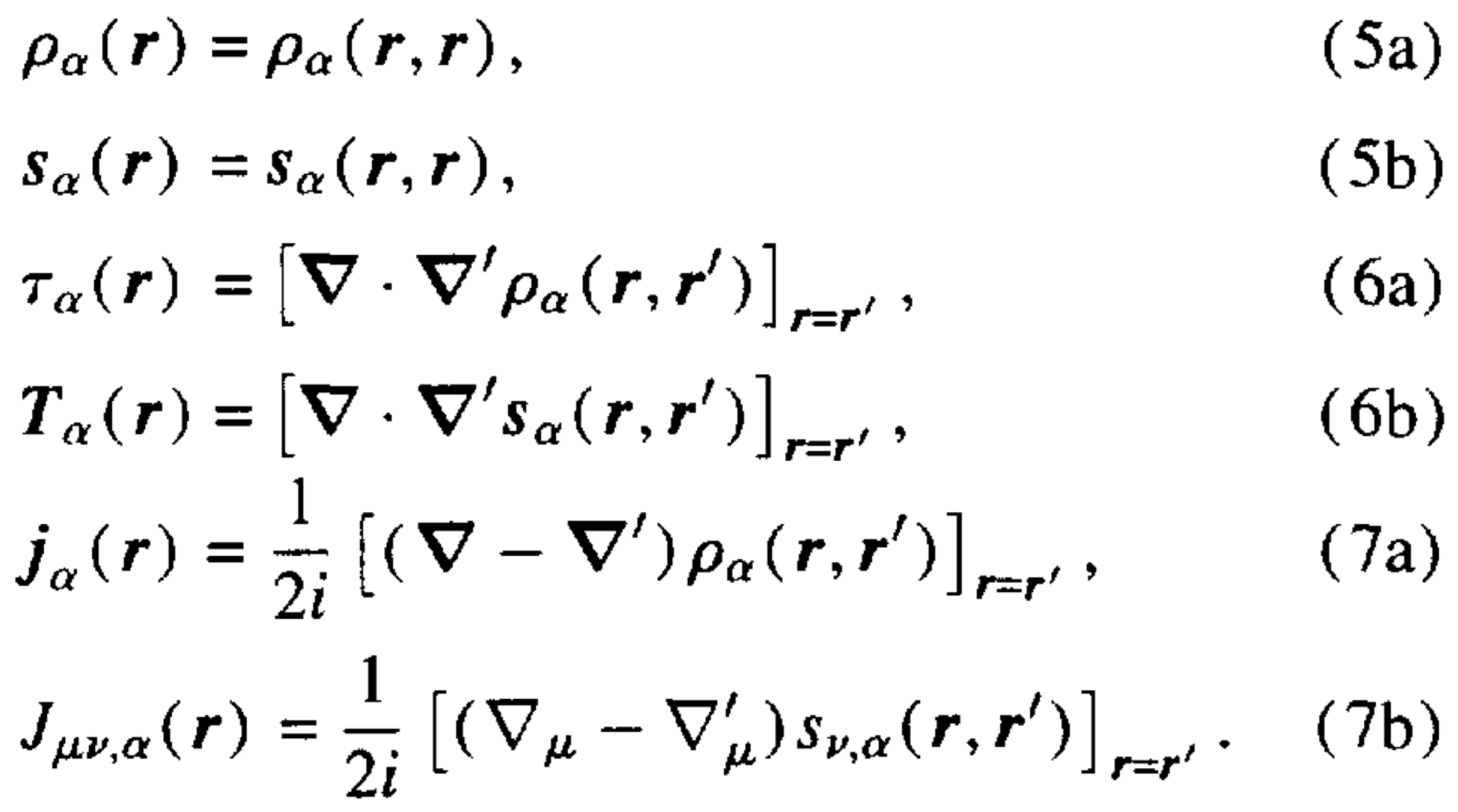
Initial Ψ

$\rho(r\sigma)$

$\hat{H}[\rho(r)]$
$E[\rho]$

$\mathbb{H}'\mathbb{C}' = e\mathbb{C}'$

Step 1:



$$\rho_\alpha(\boldsymbol{r}) = \rho_\alpha(\boldsymbol{r},\boldsymbol{r}), \tag{5a}$$

$$s_\alpha(\boldsymbol{r}) = s_\alpha(\boldsymbol{r},\boldsymbol{r}), \tag{5b}$$

$$\tau_\alpha(\boldsymbol{r}) = \left[\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\rho_\alpha(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}, \tag{6a}$$

$$\boldsymbol{T}_\alpha(\boldsymbol{r}) = \left[\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}'\boldsymbol{s}_\alpha(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}, \tag{6b}$$

$$\boldsymbol{j}_\alpha(\boldsymbol{r}) = \frac{1}{2i}\left[(\boldsymbol{\nabla}-\boldsymbol{\nabla}')\rho_\alpha(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}, \tag{7a}$$

$$J_{\mu\nu,\alpha}(\boldsymbol{r}) = \frac{1}{2i}\left[(\nabla_\mu-\nabla'_\mu)s_{\nu,\alpha}(\boldsymbol{r},\boldsymbol{r}')\right]_{\boldsymbol{r}=\boldsymbol{r}'}. \tag{7b}$$

J. Dobaczewski and J. Dudek 1997 Computer Physics Communications 102 166–182

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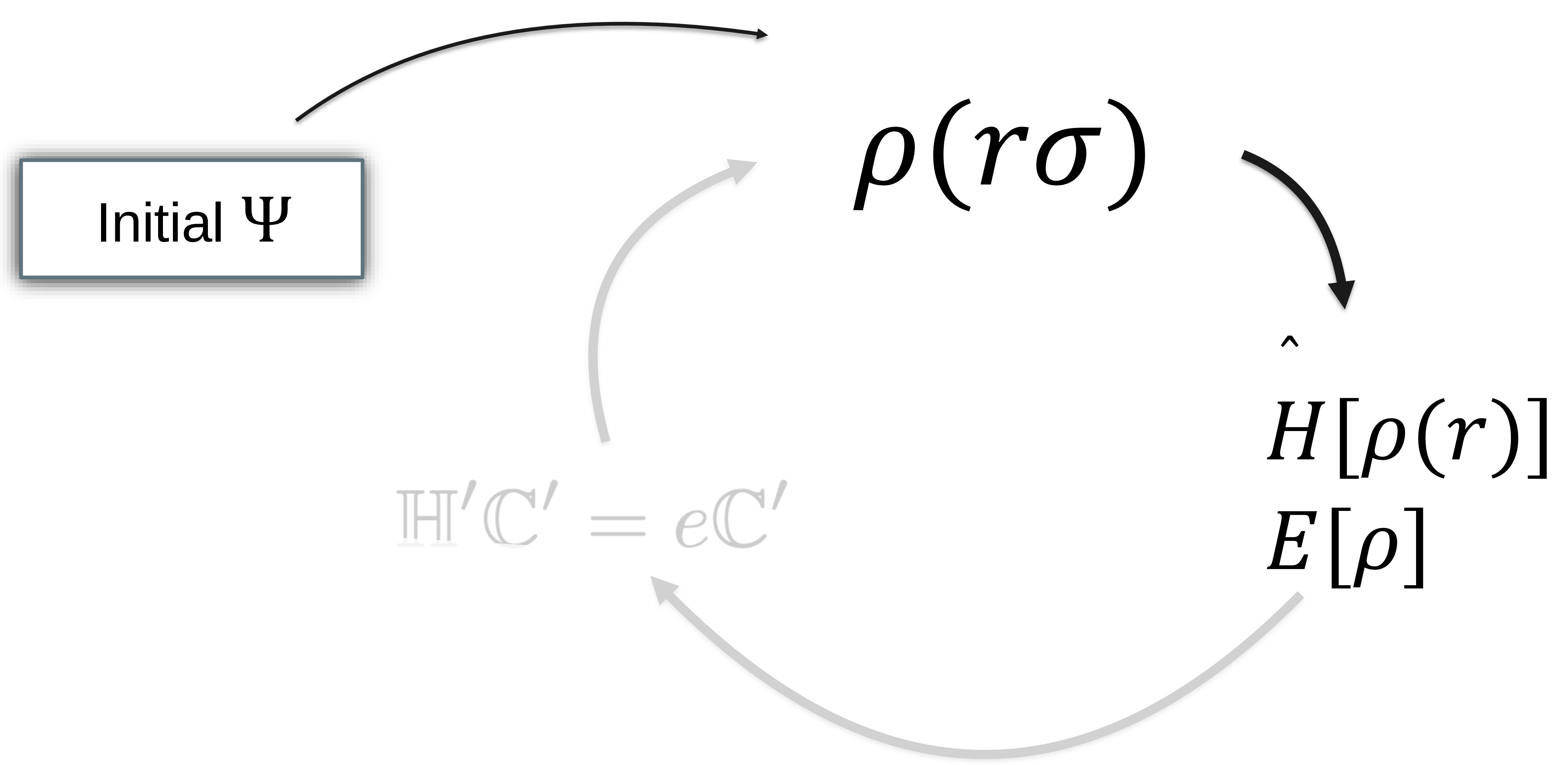


Initial Ψ

$\rho(r\sigma)$

$\hat{H}[\rho(r)]$

$E[\rho]$

$\mathbb{H}'\mathbb{C}' = e\mathbb{C}'$

Step 2:

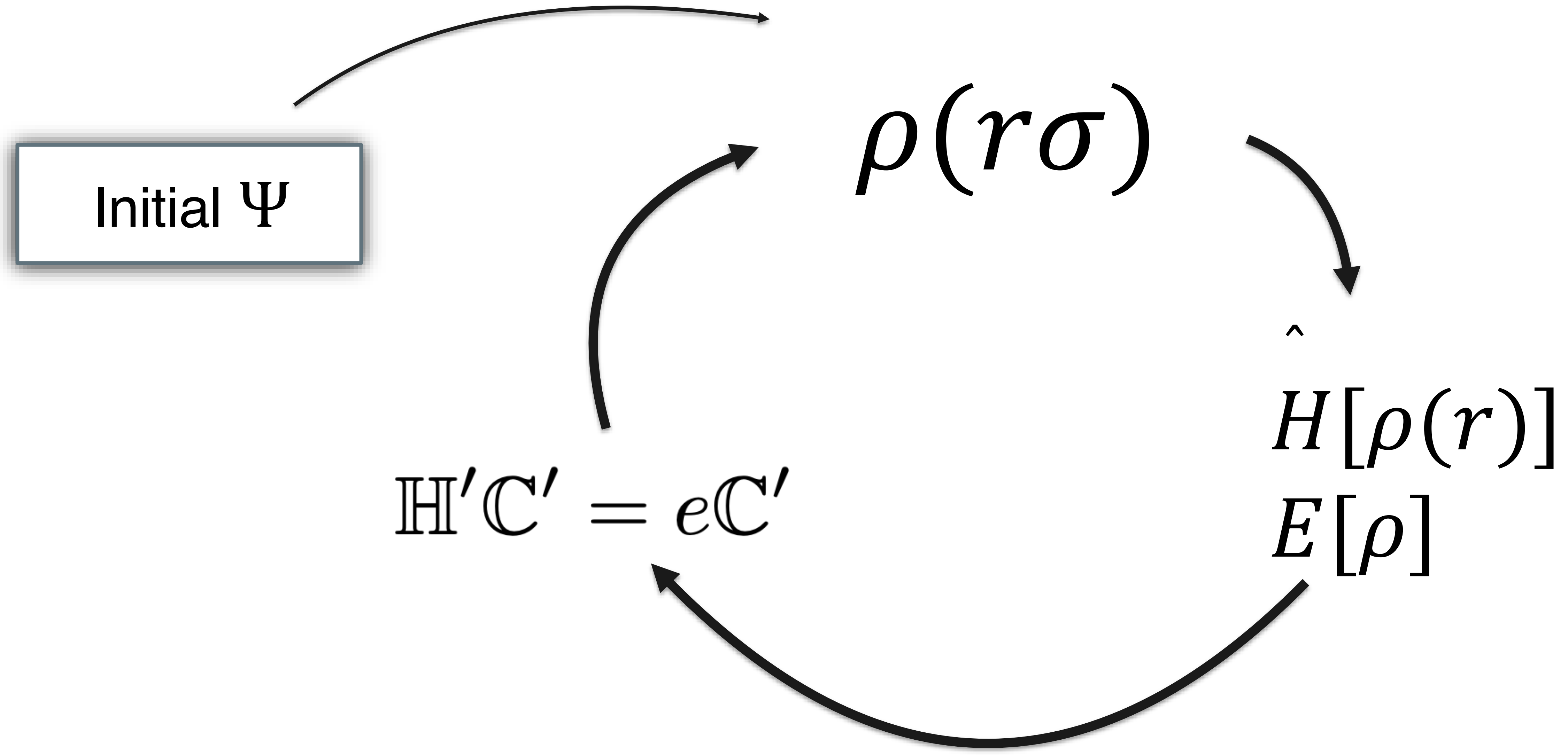
$$\mathcal{E}^{\text{Skyrme}} = \sum_{t=0,1} \int d^3\boldsymbol{r}\,\left(\mathcal{H}_t^{\text{even}}(\boldsymbol{r}) + \mathcal{H}_t^{\text{odd}}(\boldsymbol{r})\right), \qquad (11)$$

$$h'_p = -\frac{\hbar^2}{2m}\Delta + \left(\Gamma_0^{\text{even}} + \Gamma_0^{\text{odd}} - \Gamma_1^{\text{even}} - \Gamma_1^{\text{odd}}\right) + U^{\text{Coul}} + U^{\text{mult}} - \omega_y \hat{J}_y. \qquad (26\text{b})$$

J. Dobaczewski and J. Dudek 1997 Computer Physics Communications 102 166–182

Apart from that, the self-consistent loop stays the same

Step 3: To diagonalise the Hamiltonian and “try again”



Initial Ψ

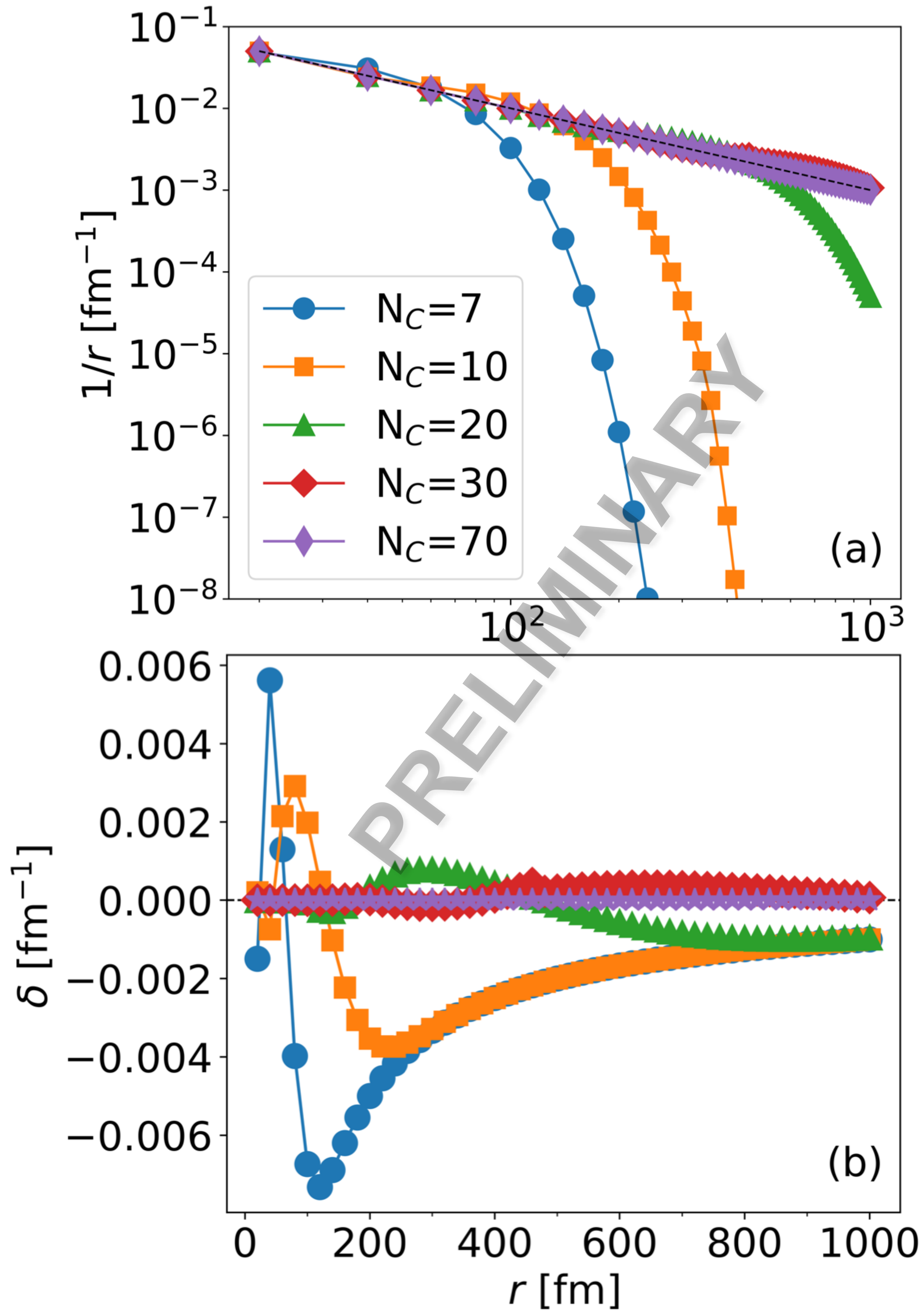
$\rho(r\sigma)$

$\hat{H}[\rho(r)]$
$E[\rho]$

$\mathbb{H}'\mathbb{C}' = e\mathbb{C}'$

Since the basis is not orthogonal we transform $\mathbb{H}\mathbb{C} = e\mathbb{N}\mathbb{C}$

through Löwdin’s canonical orthogonalisation.



We implemented the full Coulomb interaction: direct+exchange*

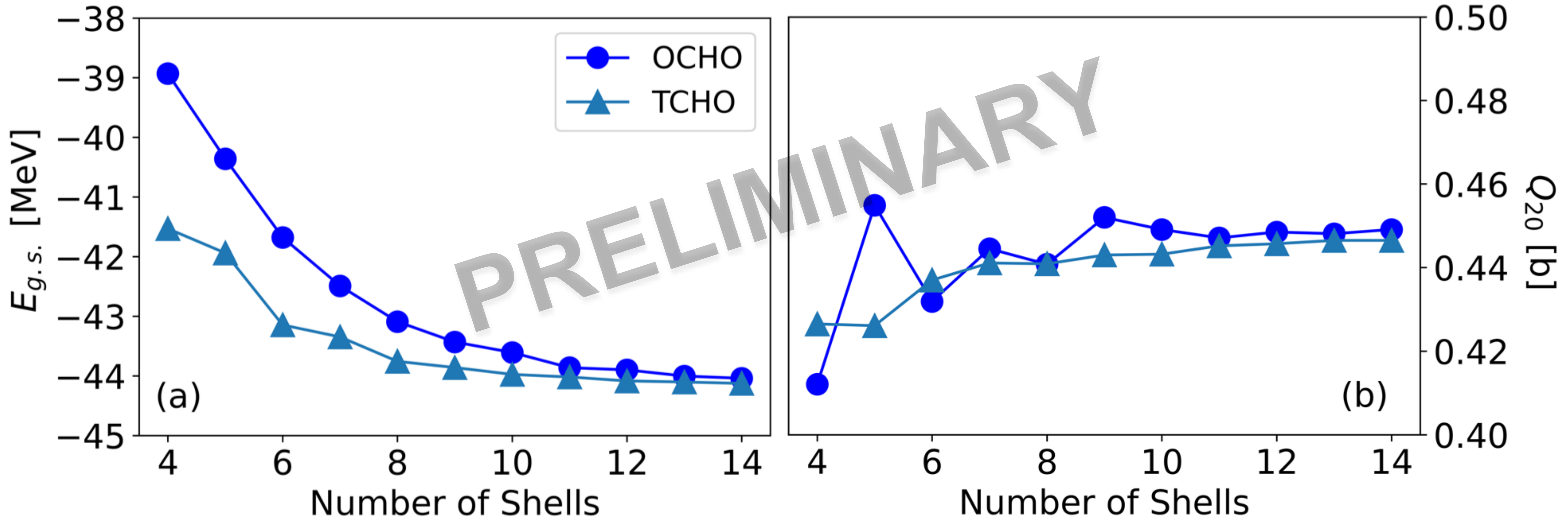
$$\hat{V}(\mathbf{r}_1,\mathbf{r}_2)=\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}\hat{\sigma}_0^{(1)}\hat{\sigma}_0^{(2)}\delta^{(1)}_{\tau,p}\delta^{(2)}_{\tau,p}\left(1-\hat{P}^{\sigma}\hat{P}^{\tau}\hat{P}^{\mathbf{r}}\right)$$

expanding the form factor
as a sum of Gaussians

$$\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}=\sum_{\gamma}^{N_C}A_{\gamma}e^{-a_{\gamma}(\mathbf{r}_1-\mathbf{r}_2)^2}$$

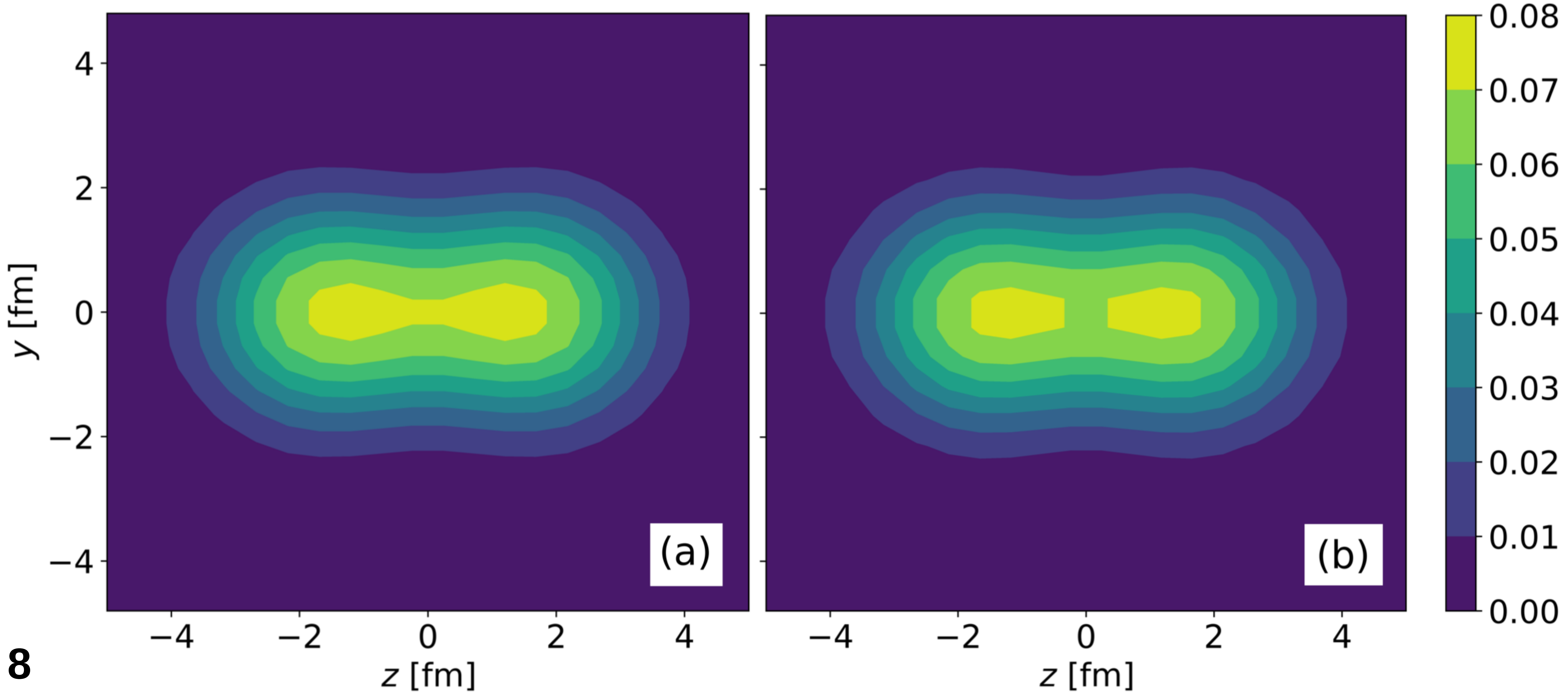
*The impact of the exchange term in the scission configuration has been never explored.

^{8}Be as $\alpha + \alpha$



The TCHO basis seems to capture the structure even for a smaller number of shells

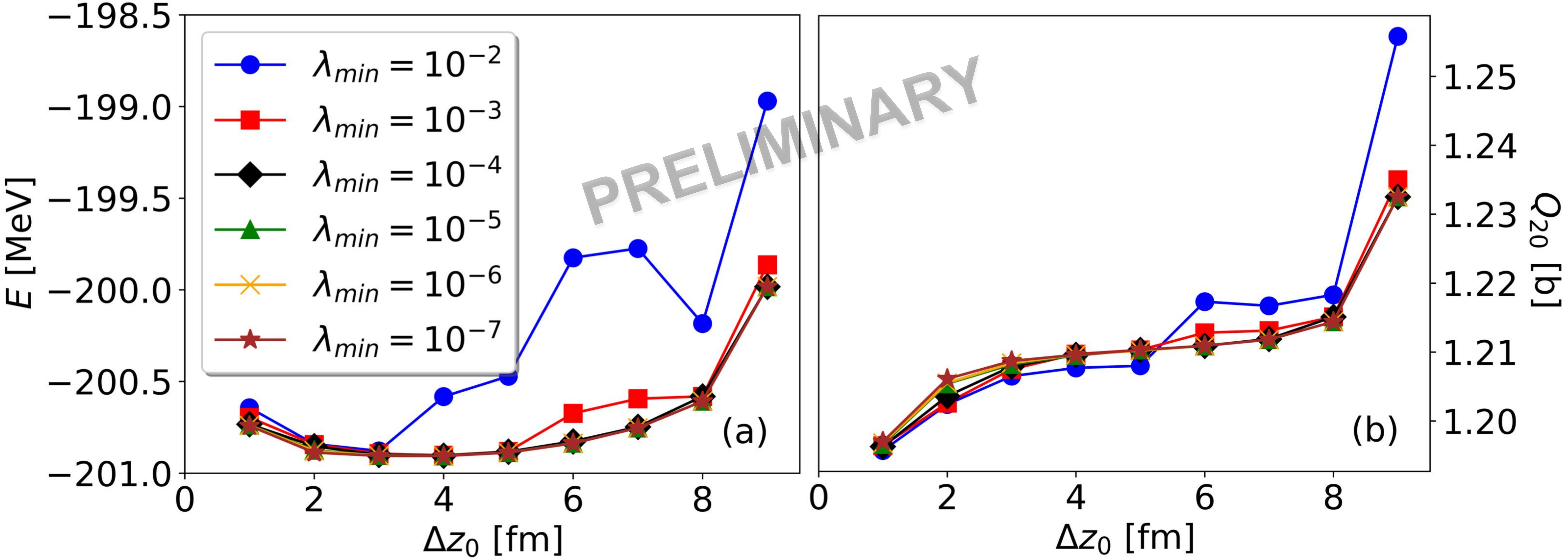
OCHO: deformed basis adapted to g.s. deformation
TCHO: spherical bases adapted to ^{4}He separated 2 fm.



Neutron density for N_0=14 (OCHO) and N_0=10(TCHO).

$^{24}Mg \rightarrow {}^{12}C + {}^{12}C$

TCHO method works also for describing compound nuclei



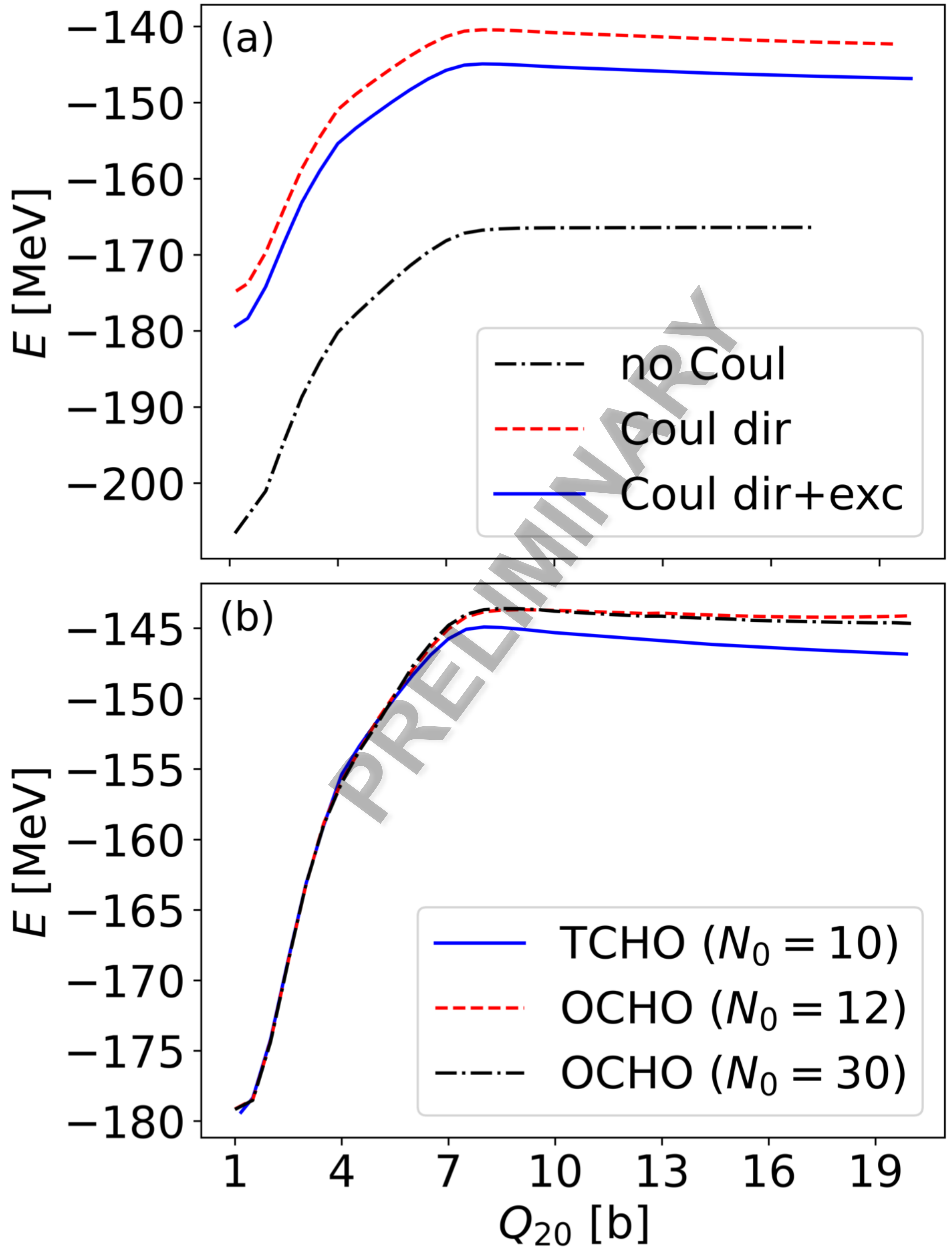
A cut-off of 10^{-4} is enough for a good convergence of results.

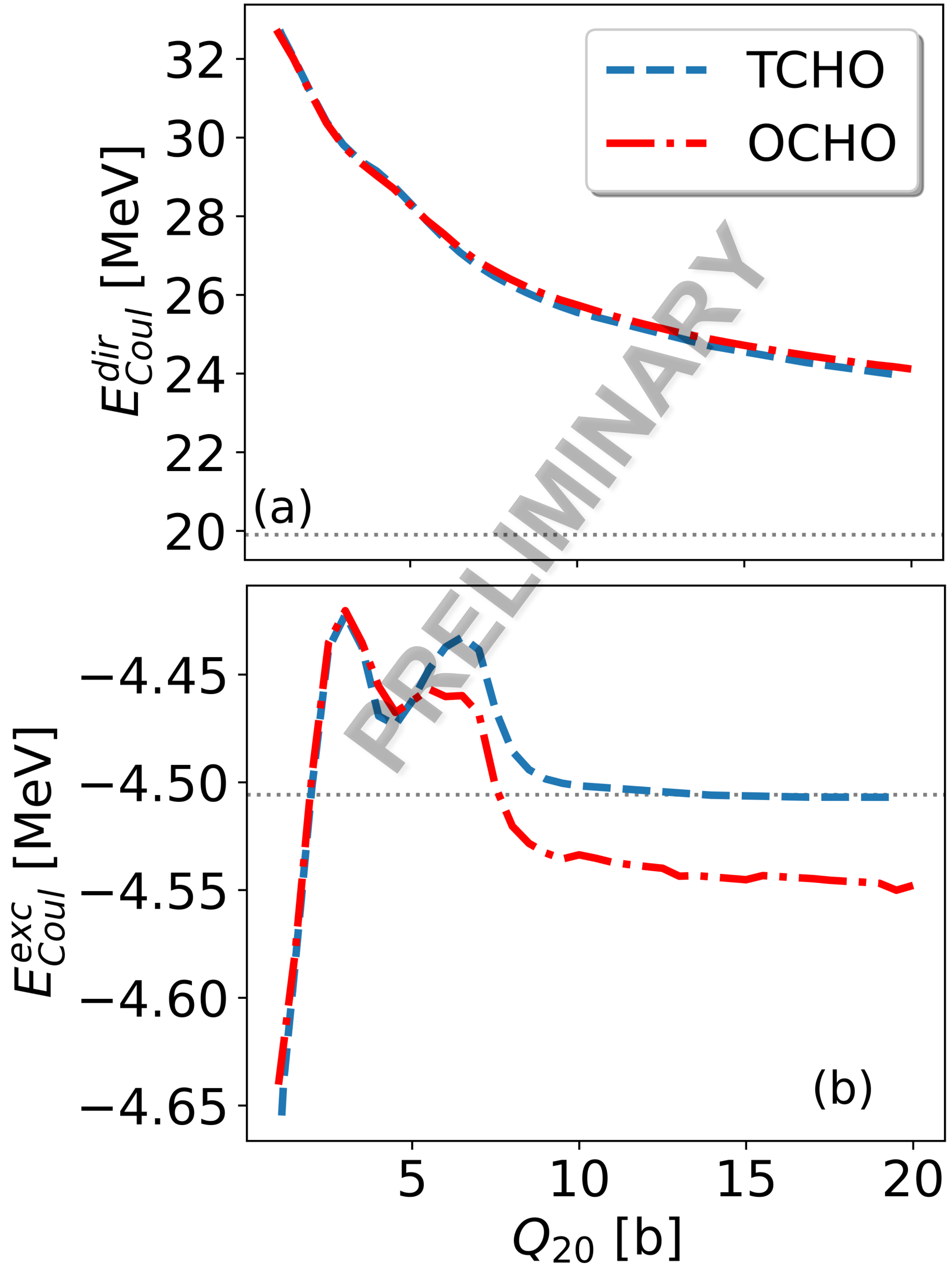
^{24}Mg → ^{12}C + ^{12}C

Even with a small number of shells, the tail after scission is better reproduced

No need of additional constraints in higher-rank multipole deformations

Axiality obtained self-consistently due to co-axial bases.





DFT solver free of assumptions, as much general as possible

J. Dobaczewski (2019), arXiv:1910.03924

Novel functionals in two-centre 3D basis

- Asymmetric fission
- Orientation of fragments
- Fission paths and inertia tensor in adiabatic approx.
- Fragment distributions using Langevin equations

Correlations using QRPA

Two-centre time-dependant HO basis

- Test thermal approximation (QRPA+time evolution)
- Test adiabatic approximation (odd nuclei)

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Constraints in the fragment population (upcoming publication)

- Most favourable paths
- Odd-mass nuclei: where does the loner nucleon go?
- alpha particle emission

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