# *Mean field* and *nucleonic degrees of freedoms* in **Orthogonal Wave Function Dynamics** for *heavy-ion collisions*

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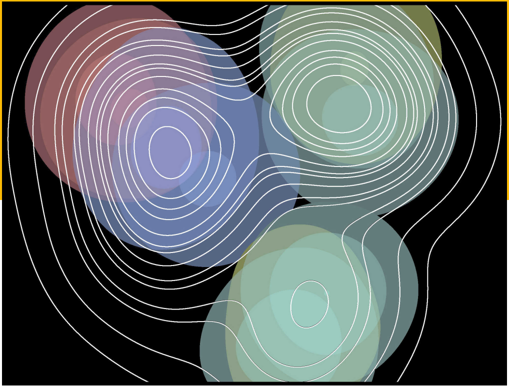
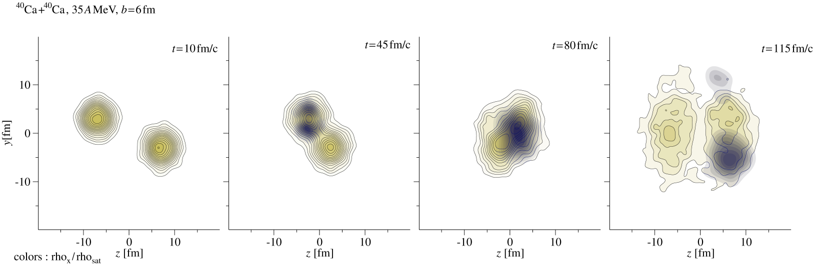


*Nusym, Caen 12 / 9 / 2024*

# The purpose first

A scheme to overcome some usual semi-classical approximations in transport approaches to HIC.

- Tracking wave-function evolution (widening, shape...).
- Preserving nucleonic correlations (avoiding splitting of a WF among two nuclei).
- Describing a large range of energy regimes, starting from low energy.
- Improving stability.




e.g. : tracking one external neutron (blue) in Ca40+Ca40 at 35AMeV

# Microscopic models for nuclear dynamics

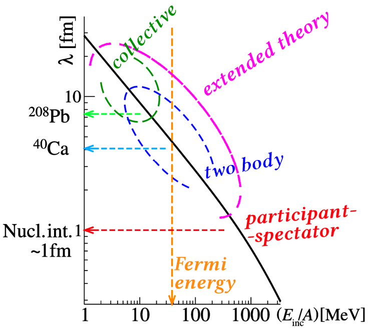
- Rich variety of microscopic models at low energy [Simenel PPNP 2018, Maruhn-Reinhard-Suraud Simple Models of Many-Fermion Systems 2010]

→ Not easy extension to HIC conditions [Sorensen PPNP 2024] :
two-body dissipation incompatible with low-energy requirements, (non-locality, orthogonality, single-Slater evolution...)

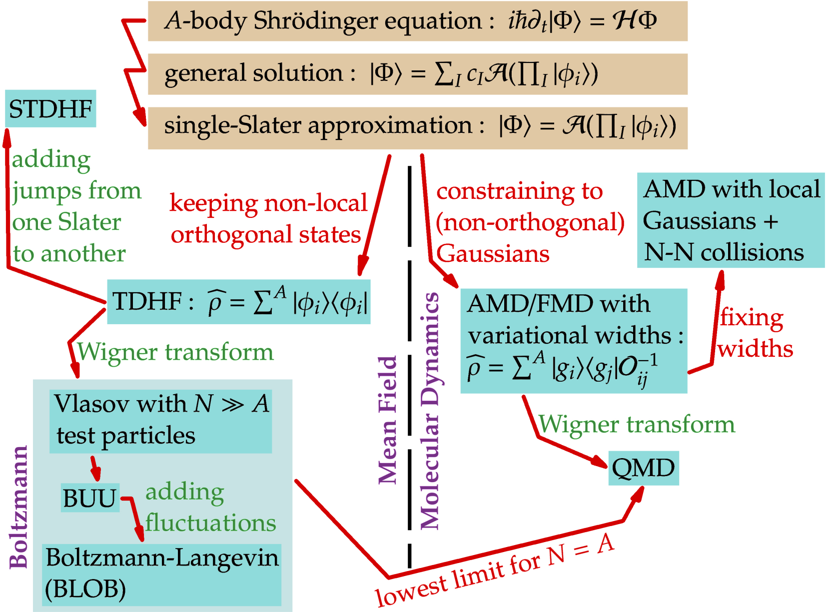
→ Computational requirements differ

- Widely recurrent scheme for HIC applications : Mean field (MF) vs Molecular dynamics (MD) [Ono Randrup EPJA30 2006, Wolter PPNP 2022]

- Hereafter : familiar to unusual context in transport models, flash review



# Usual scheme and approximations



# Usual scheme and approximations

*Usual approximations* :

- Single Slater $\Rightarrow$ deterministic
- Decoherence $\rightarrow$ locality
- Wigner transform $\Rightarrow$ quantum operators $\rightarrow$ phase-space
- simple-basis decomposition (Gaussians)
- non-orthogonal system $\Rightarrow$ overlaps
- freezing packet variances $\Rightarrow$ dismissing non-local effects
- Quasiparticle lowest limit $\Rightarrow$ e.g. BUU $\rightarrow$ QMD

# Less conventional approaches

$A$-body Shrödinger equation : $i\hbar\partial_t|\Phi\rangle = \mathcal{H}\Phi$

general solution : $|\Phi\rangle = \sum_I c_I \mathcal{A}(\prod_I |\phi_i\rangle)$

single-Slater approximation : $|\Phi\rangle = \mathcal{A}(\prod_I |\phi_i\rangle)$

keeping non-local orthogonal states

TDHF : $\widehat{\rho} = \sum^A |\phi_i\rangle\langle\phi_i|$

decomposition into wavelets, splines, h.o., Gaussians,... : $|\phi_i\rangle = \sum^N c_{ij}|g_j\rangle$

Gaussians with interference terms

decoherence approximation : $\rho = \sum^N |c_{ij}|^2|g_i\rangle\langle g_j|$

constraining to (non-orthogonal) Gaussians

AMD/FMD with variational widths : $\widehat{\rho} = \sum^A |g_i\rangle\langle g_j|O^{-1}_{ij}$

fixing widths

AMD with local Gaussians + N-N collisions

lowest limit for $N = A$

Wigner transform

semi-classical approximation : $f(x,k) = \sum^N w_i\tilde{g}_i(x,k)$

# Less conventional approaches

• *DYWAN* → decomposition into a dynamical orthogonal basis of wavelets [Jouault Sebille, de la Mota NPA 1996]

→ But actually : wavelets refitted into Gaussians + decoherence + Wigner tr. → weighted semiclassical quasipart. with variational width [Besse PRC 2022, Dinh Nuovo Cim 2022]

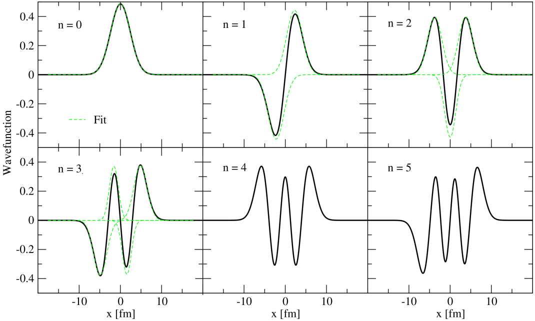
• back to delocalized wave functions without decoherence and Wigner tr. [Dinh PhD tel-04072941 2022]
→ recalls early AMD / FMD (with variational widths) for $N \rightarrow A$ [Feldmeier NPA 1990, NPA 1995]

# Gaussian decomposition

- HO routine applied to neutron/proton Skyrme potentials → HF states

→ each level is decomposed in as many Gaussians as the number of extrema

→ positive/negative amplitude → constructive/destructive interference




$$\varphi_{(n_x,n_y,n_z)}(\vec{x}) = \sum_i^{\tilde{N}} g_i(\vec{x}) = \sum_i^{N_x} \sum_j^{N_y} \sum_k^{N_z} g_{n_x,i}(x)\ g_{n_y,j}(y)\ g_{n_z,k}(z)$$

| $N_{\max}$ | $g_{N_{\max}}$ | $\sum_N^{N_{\max}} g_N$ | $2\sum_N^{N_{\max}} g_N$ |
|---|---|---|---|
| 0 | 1 | 1 | 2 |
| 1 | 3 | 4 | 8 |
| 2 | 6 | 10 | 20 |
| 3 | 10 | 20 | 40 |
| 4 | 15 | 35 | 70 |
| 5 | 21 | 56 | 112 |

# Searching for a new scheme

$A$-body Shrödinger equation : $i\hbar\partial_t|\Phi\rangle = \mathcal{H}\Phi$

general solution : $|\Phi\rangle = \sum_I c_I \mathcal{A}(\prod_I |\phi_i\rangle)$

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fixing widths

decomposition into wavelets, splines, h.o., Gaussians,... : $|\phi_i\rangle = \sum^N c_{ij}|g_j\rangle$

$A$ orthogonal wave functions with $k$ Hermite modes

reducing to weighting functions

Gaussians with interference terms

lowest limit for $N = A$

decoherence approximation : $\rho = \sum^N |c_{ij}|^2|g_i\rangle\langle g_j|$

Wigner transform

semi-classical approximation : $f(x,k) = \sum^N w_i\tilde{g}_i(x,k)$

# Searching for a new scheme

- Problem with delocalized wave functions

→ difficult to treat overlaps in presence of strong perturbations (i.e. collision term)

⇒ new fully orthogonal scheme : one Gaussian per nucleon used as a weighting function to build a hierarchy of Hermite modes
→ no need to fit the initial states

→ obtain AMD / FMD (with variational widths) by restricting to the weighting function

# Hermite parameterization

$$\varphi = g_n(\vec{x}) \cdot \sum_I \frac{C_I}{\text{norm}} H_I\left(\frac{x-x_n}{\sqrt{(2\chi_{n,x})}}, \frac{y-y_n}{\sqrt{(2\chi_{n,y})}}, \frac{z-z_n}{\sqrt{(2\chi_{n,z})}}\right)$$

- $I$ is a level superindex, e.g. $N_{\max} = 6$

$\rightarrow$ number of levels : $\sum_k^{N_{\max}} \frac{(k+1)(k+2)}{2}$

$\rightarrow |I| = 84$

- built on the weighting function

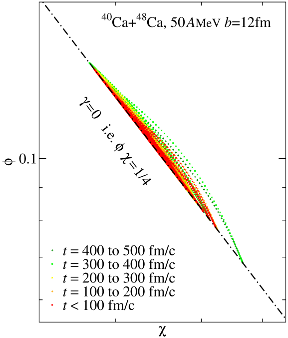
$$g_n(\vec{x}) = g_n^x(x) g_n^y(y) g_n^z(z)$$

$$g_n^x(x) = \left(\frac{1}{2\pi\chi_n}\right)^{1/4} e^{-\xi_n \frac{(x-x_i)^2}{2} + ik_n(x-x_i)}$$

with $\xi_n = \frac{1}{2\chi_n} - 2i\gamma_n$

- $\gamma_n = \frac{\sigma_n}{2\chi_n}$ links the variational widths
- this set is orthogonal
- A collision term would act on the level weights and numbers

very gentle situation (without collisions)



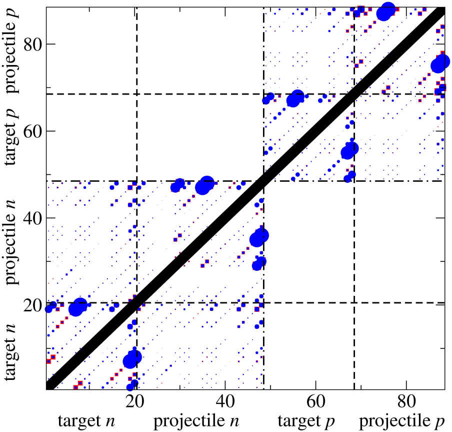
# Re-orthogonalization

- Re-orthogonalization procedure → all scattered states after collisions are re-orthogonalized to the system.
- Example of orthogonality anomalies before treatment :

→ external levels mostly affected

→ satisfactory orthogonality in the overlap terget-projectile

$^{48}$Ca+$^{40}$Ca, 25 $A$ MeV, $b$=9 fm, d$t$=0.2 fm/c




scalar product (N,M) [*Re:blue Im:red*]

# Test. Collisional dynamics in Ca40+Ca40

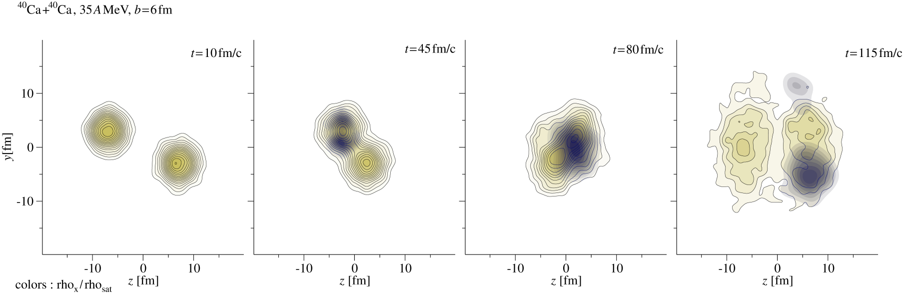
Knowing that,

- One-body density is not sufficient to build up N-N corr.
- No decoherence approximation was done

1) *Mean-free path* from collapsing at random two wave functions on their one-body density distribution → collision probability

2) centroids boosted like in a semiclassical approach, rotated, translated

3) *Pauli* : not from phase space occupancy but from the probability of finding an orthogonal solution for the scattered states ⇒ new variances and new level scheme

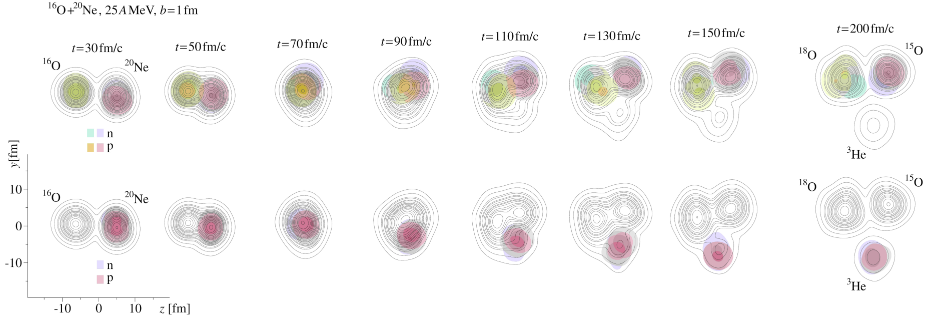


# Test. Collisional dynamics in O16+Ne20

- effect of orthogonality, collisions, and NN-correlations ⇒

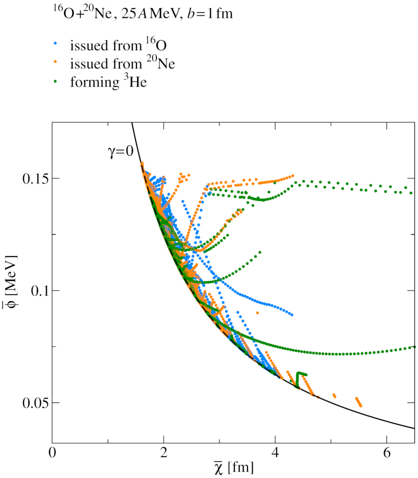
1) exchange of neutrons and protons between projectile and target

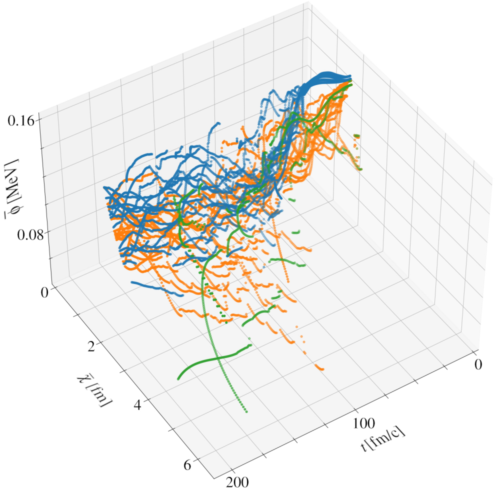
2) three wave functions rearrange into a 3He cluster



# wave-function evolution

- tracking the average widths of the lower mode of each wave function.
- jumps are produced by collisions followed by a level rearrangement.
- trajectories moving away from the bunch : splits and emissions.



# Conclusions

New approach to overcome some common approximations
→ still preliminary but successful in handling mean field and NN correlations

*Future applications in view*

- very peripheral collisions
- low-density neck at Fermi energy in a less classical (hydrodynamic) picture
- tracking particle correlations from an emitting source
- testing nuclear interaction in a wider range of energies within the same model

Part of this work → PhD work of Hung Viet Dinh and post collaboration