New TDHF Studies of Heavy-Ion Dynamics

Sait A. Umar and Volker E. Oberacker

Sait
Umar

Volker
Oberacker

Research supported by:
US Department of Energy, Division of Nuclear Physics
NERSC IBM-SP supercomputer time

TDHF – Basic Facts

Advantages:

- Fully microscopic, parameter-free description of nuclear collisions
- Use same microscopic interaction used in static calculations
- Successful in describing low-energy fusion, deep-inelastic collisions, nuclear molecules, and collective phenomena
- Provides a method for linear response calculations

Shortcomings:

- Only one-body dissipation (includes dynamical dissipation)
- Inclusive information
- Semiclassical (cannot correctly describe widths)
- Does not include pairing
- Cross-channel coupling of final states

A New Generation TDHF Code

- Unrestricted 3-D Cartesian geometry
  - No rotating frame approximation (2D codes)
  - No reflection symmetry (+z/-z)
  - F77/BKN *version: Umar et al, Phys. Rev. C44, 2512 (1991)*

- Basis-Spline discretization for high accuracy
  - *Umar et al, J. Comp. Phys., 93, 426 (1991)*

- Coded in Fortran-95

- Use of modern Skyrme forces with spin-orbit

- No time-reversal symmetry assumed
  - In process of adding the spin-current tensor

Basic TDHF Equations

- Equations of motion obtained from variation of the action

$$\delta \int_{t_1}^{t_2} dt \langle \Phi(t) | H - i\hbar\partial_t | \Phi(t) \rangle = 0 \quad \text{with} \quad H = \sum_{i}^{A} t_i + \sum_{i<j}^{A} v_{ij} + \sum_{i<j<k}^{A} v_{ijk}$$

- Many-body state is a Slater determinant at all times

$$\Phi(r_1 \cdots r_A; t) = \frac{1}{\sqrt{A!}} det|\phi_\lambda(r_i, t)|$$

- Time-dependence of the single-particle states are governed by

$$i\hbar \frac{\partial \phi_\lambda}{\partial t} = h(\{\phi_\mu\})\phi_\lambda$$

- Static HF equations can be obtained by substituting

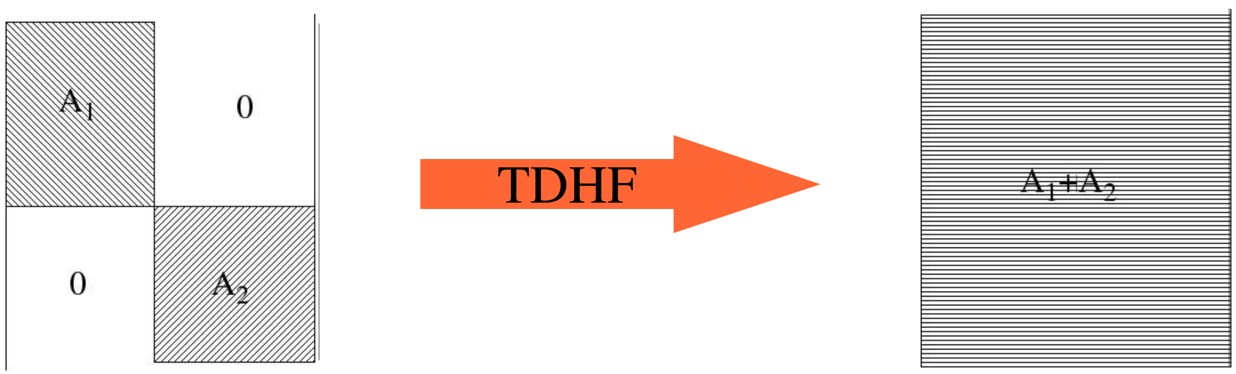
$$\phi_\lambda(\vec{r}, t) = e^{-i\epsilon_\lambda t/\hbar} \chi_\lambda(\vec{r}) \quad \text{as} \quad h(\{\chi_\mu\})\chi_\lambda = \epsilon_\lambda \chi_\lambda$$

Initial TDHF Setup

- Generate HF Slater determinants for each nucleus
- Multiply each determinant by a boost, determined from Coulomb trajectory and the asymptotic E_{cm}, at the initial nuclear separation (above the Coulomb barrier)

for nucleus j $\quad X_j \rightarrow \exp(i\boldsymbol{k}_j \cdot \boldsymbol{R}) X_j$ $\quad$ and $\quad \boldsymbol{R} = \frac{1}{A_j} \sum_{i=1}^{A_j} r_i$

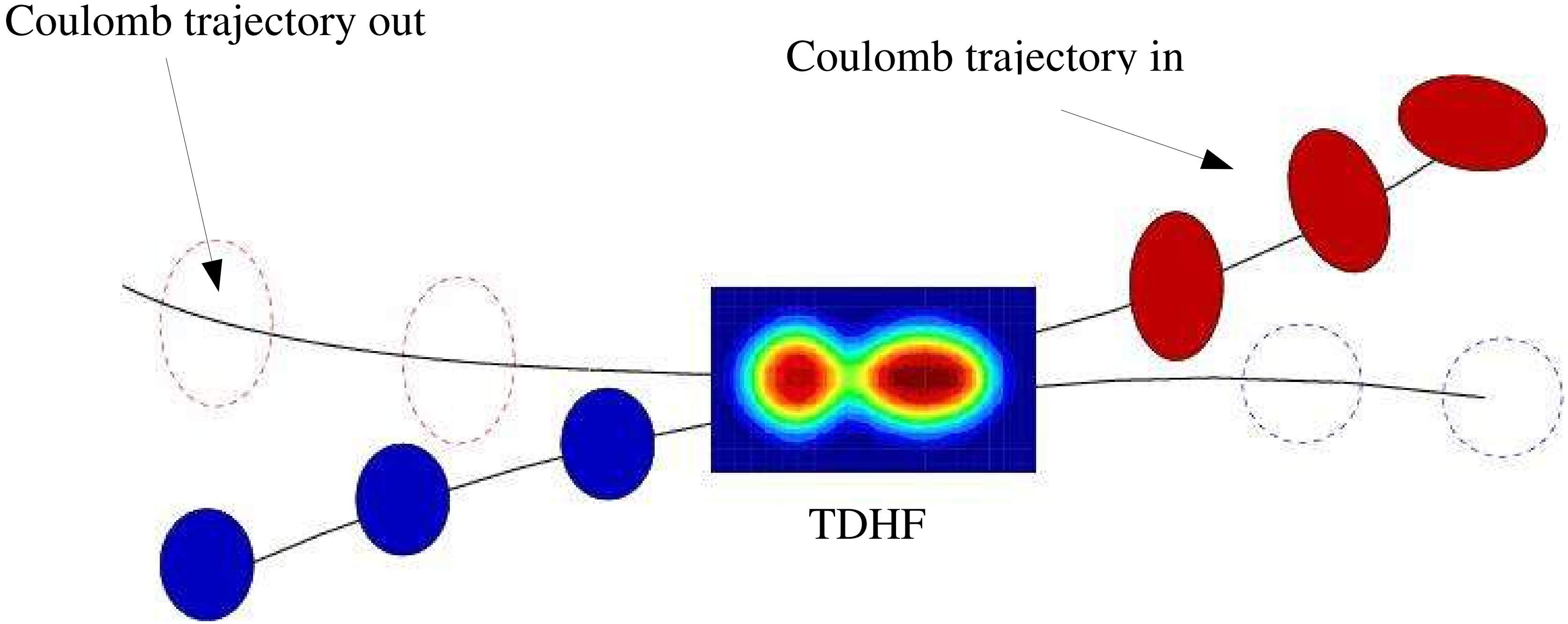
- Combine two determinants into a single one



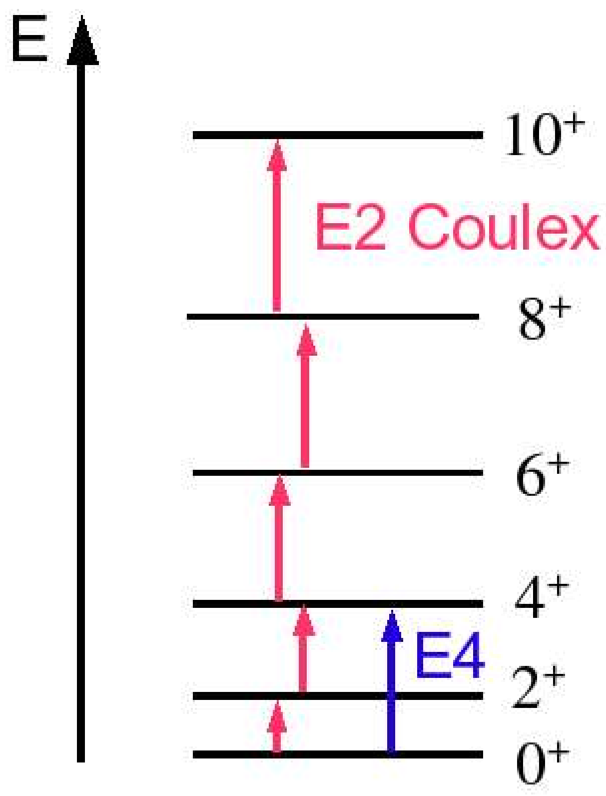
initial state $\qquad$ final state

TDHF Collision Process

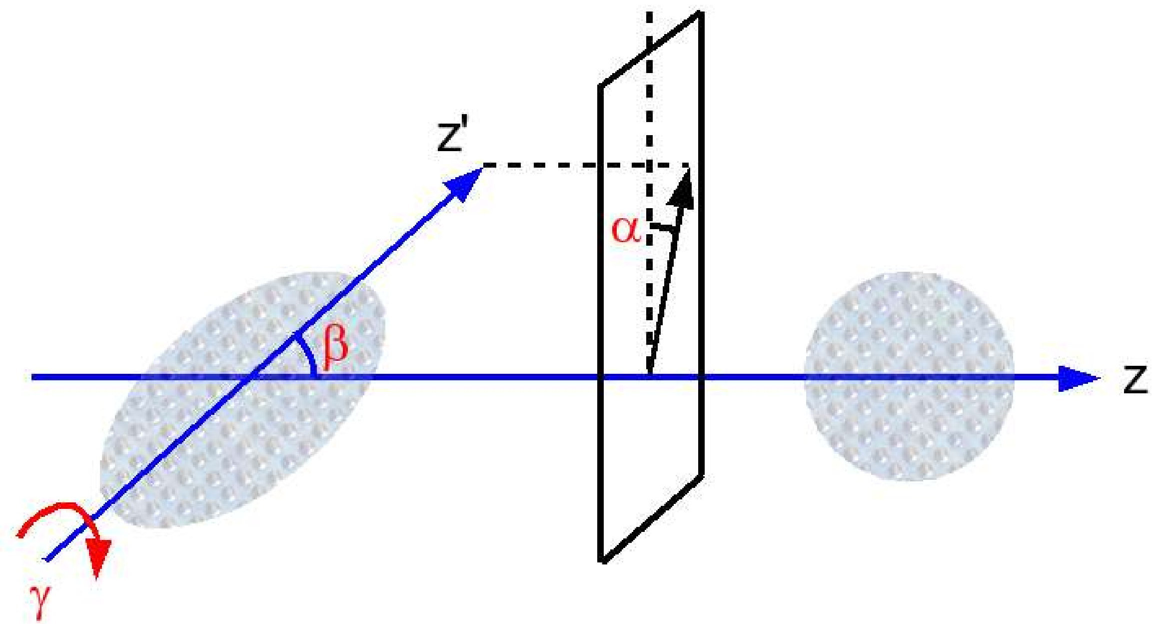
- If final stage contains a single fragment – FUSION
- If final stage contains two fragments – DEEP INELASTIC SCATTERING
- Initial approach is determined by Coulomb interaction only



Dynamic Alignment of Deformed Nucleus Due to Coulomb Excitation



K=0 rotational band



V.E. Oberacker, Phys. Rev. C32, 1793 (1985)

Dynamic Alignment of Deformed Nucleus Due to Coulomb Excitation

$$\left[H_0(X)+V_C(X,\vec{r}(t))\right]\psi(X,t)=i\hbar\frac{\partial}{\partial t}\psi(X,t)$$ ← semi-classical Coul

$$H_0(X)\phi_r(X)=E_r\phi_r(X)$$ ← eigenstates of deformed nucleus

$$\psi(X,t)=\sum_r a_r(t)\phi_r(X)e^{-iE_rt/\hbar}$$ ← expand time-dep. wavefunction

$$i\hbar\dot{a}_r(t)=\sum_s a_s(t)\langle\phi_r(X)|V_C(X,\vec{r}(t))|\phi_s(X)\rangle e^{i(E_r-E_s)t/\hbar}$$ ← coupled diff. eqns

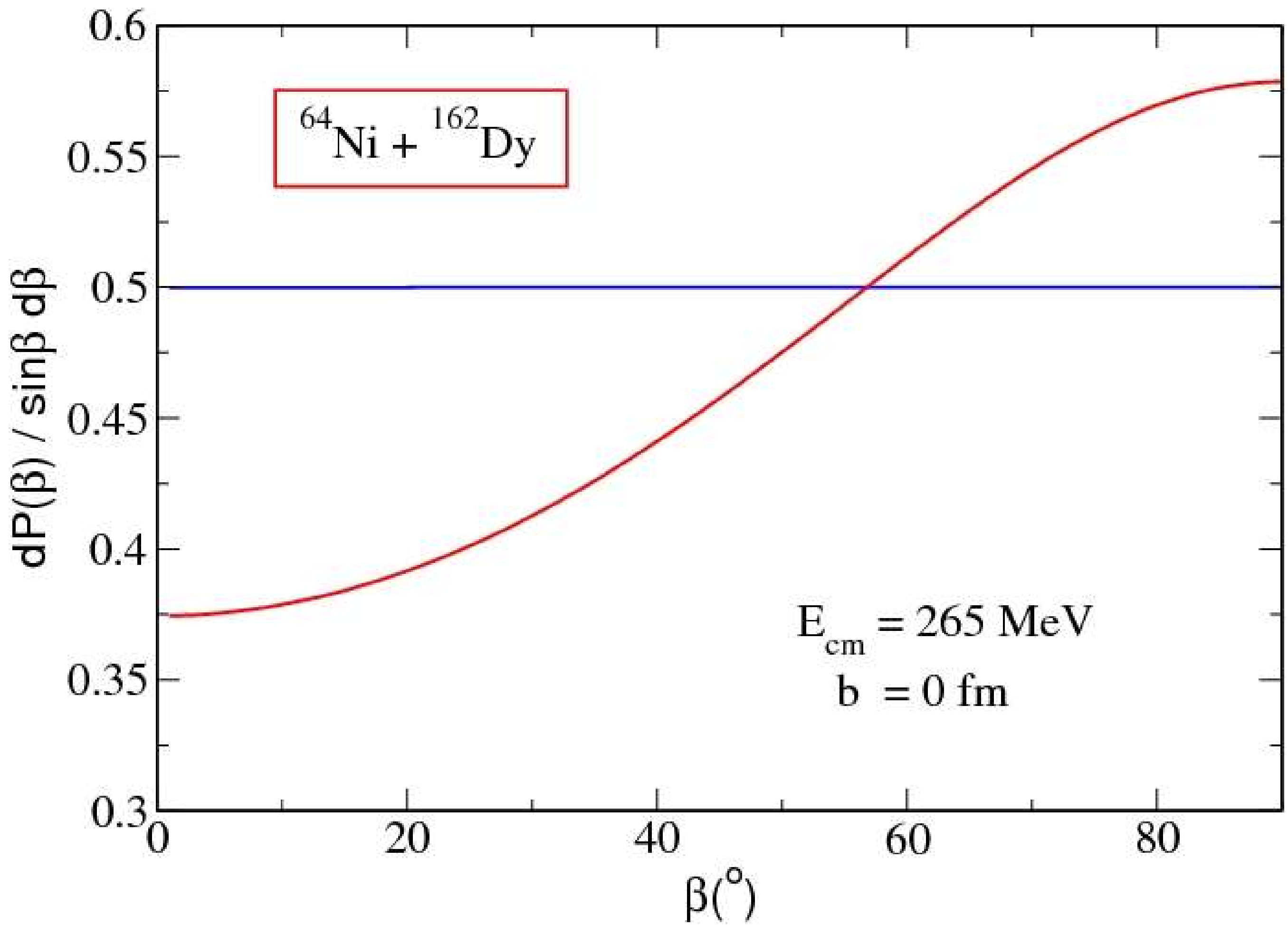
---

$$H_0(X)=T_{rot}(X) \qquad X=(\alpha,\beta,\gamma)$$ ← collective rotor model: Euler angles

$$\phi_r(X)=\left(\frac{2J+1}{8\pi^2}\right)^{1/2}D^{J*}_{M,K=0}(\alpha,\beta,\gamma)=(2\pi)^{-1/2}Y_{JM}(\beta,\alpha)$$ ← g.s. rotational band (K=0)

$$\frac{dP(\alpha,\beta;t)}{\sin(\beta)\,d\beta\,d\alpha}=\int_0^{2\pi}d\gamma|\psi(\alpha,\beta,\gamma;t)|^2\rightarrow\left|\sum_{JM}a_{JM}(t)Y_{JM}(\beta,\alpha)e^{-iE_Jt/\hbar}\right|^2$$ orientation probability

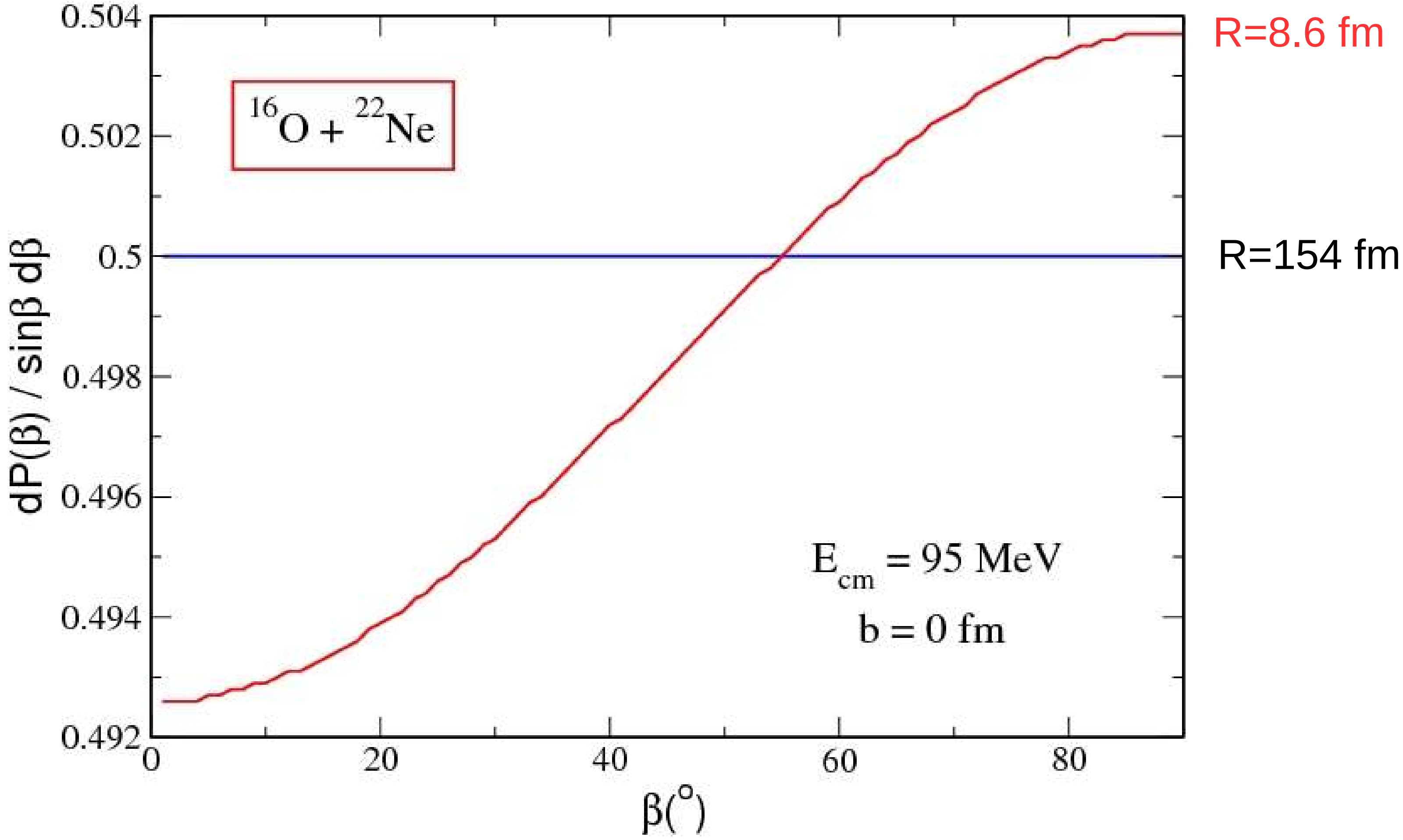
Dynamic Alignment Due to Coulomb Excitation of ^{162}Dy



R=13.2 fm

R=1363 fm

Dynamic Alignment Due to Coulomb Excitation of ^{22}Ne



Expression for Fusion Cross-Section

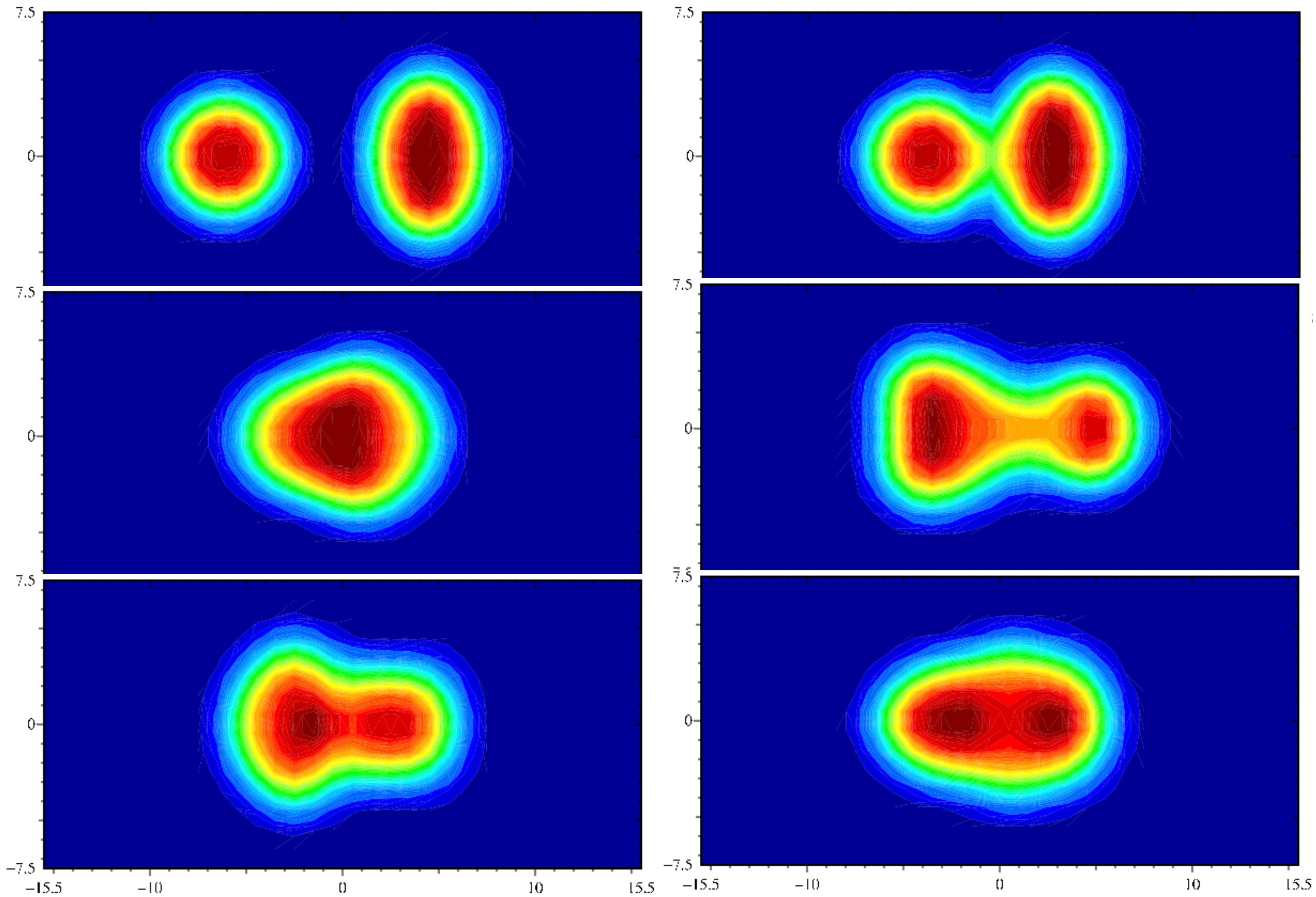
$$\sigma_{fusion}(E_{cm}) = \int_0^{b_{max}} b\,db\,P_{fusion}(b, E_{cm})$$ ← total cross-section

$$P_{fusion}(b, E_{cm}) = \int d\Omega \frac{dP_{fusion}(b, E_{cm}; \beta, \alpha)}{d\Omega}$$ ← fusion probability

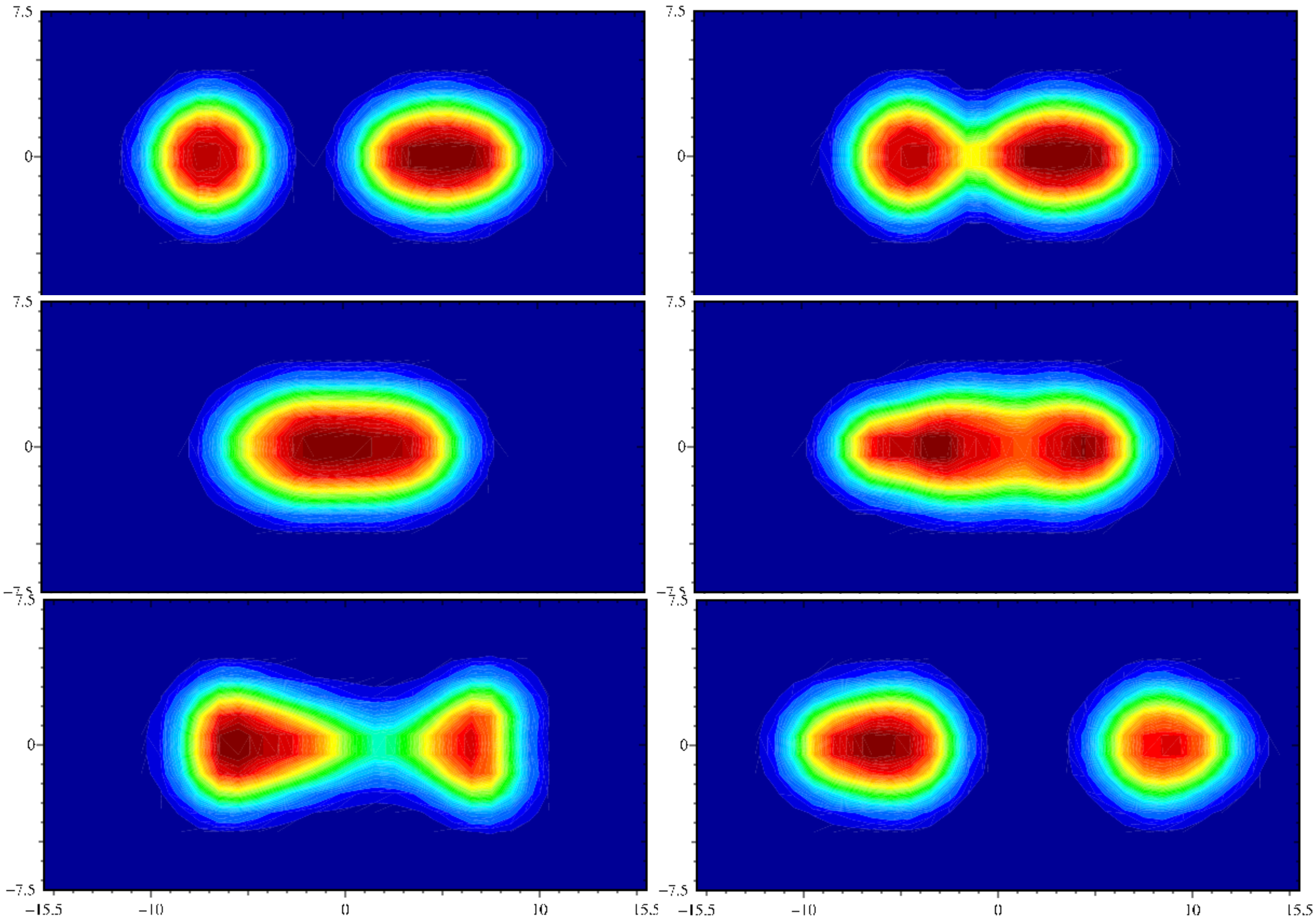
$$\frac{dP_{fusion}(b, E_{cm}; \beta, \alpha)}{d\Omega} = \frac{dP_{orientation}(b, E_{cm}; \beta, \alpha)}{d\Omega} \cdot P_{TDHF}(b, E_{cm}; \beta, \alpha)$$

$$P_{TDHF}(b, E_{cm}; \beta, \alpha) = \begin{cases} 1 & \text{TDHF fuse} \\ 0 & \text{TDHF does not fuse} \end{cases}$$

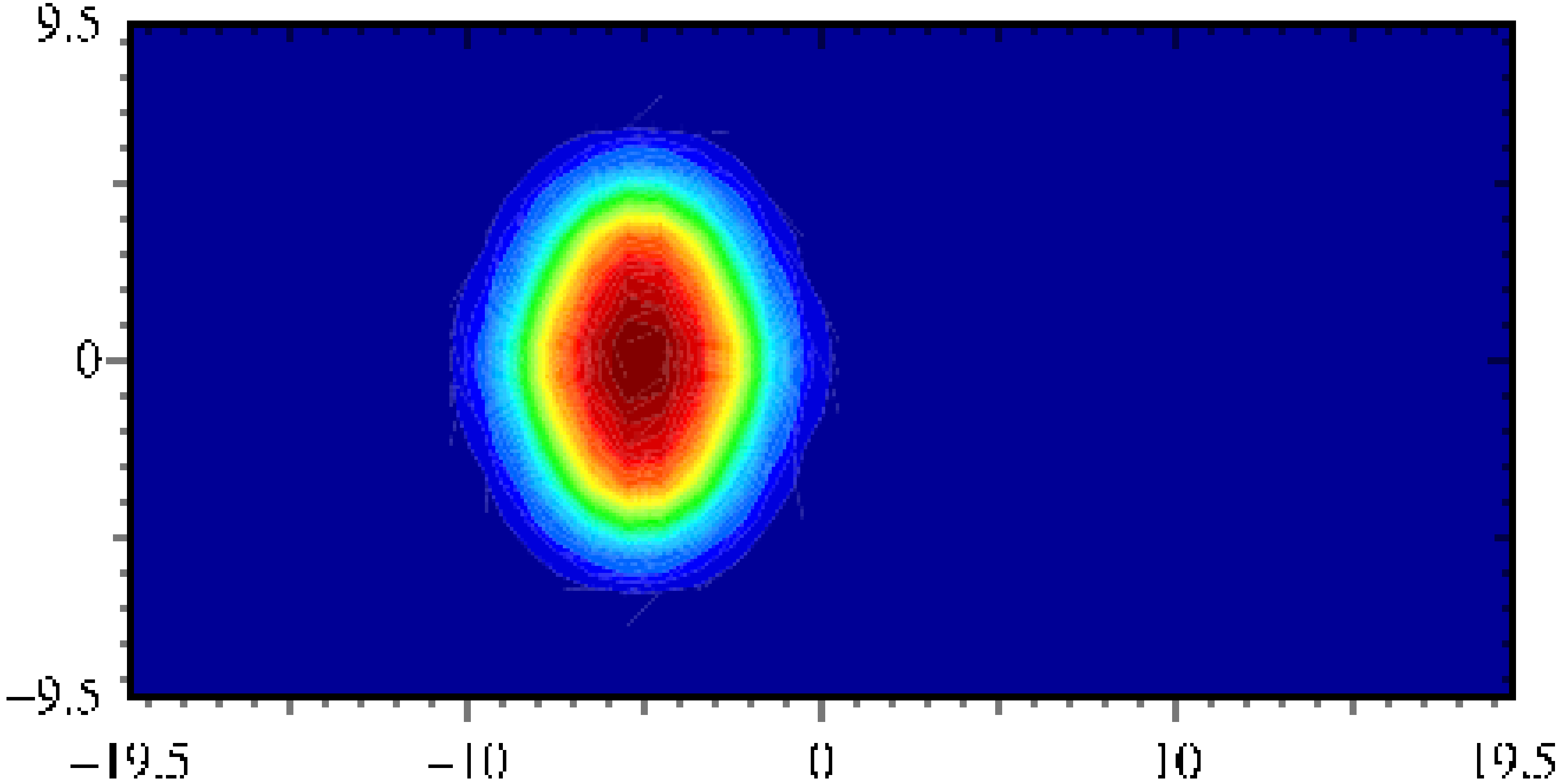
$^{16}O+^{22}Ne$ (alignment 1) E/A=2.5 MeV



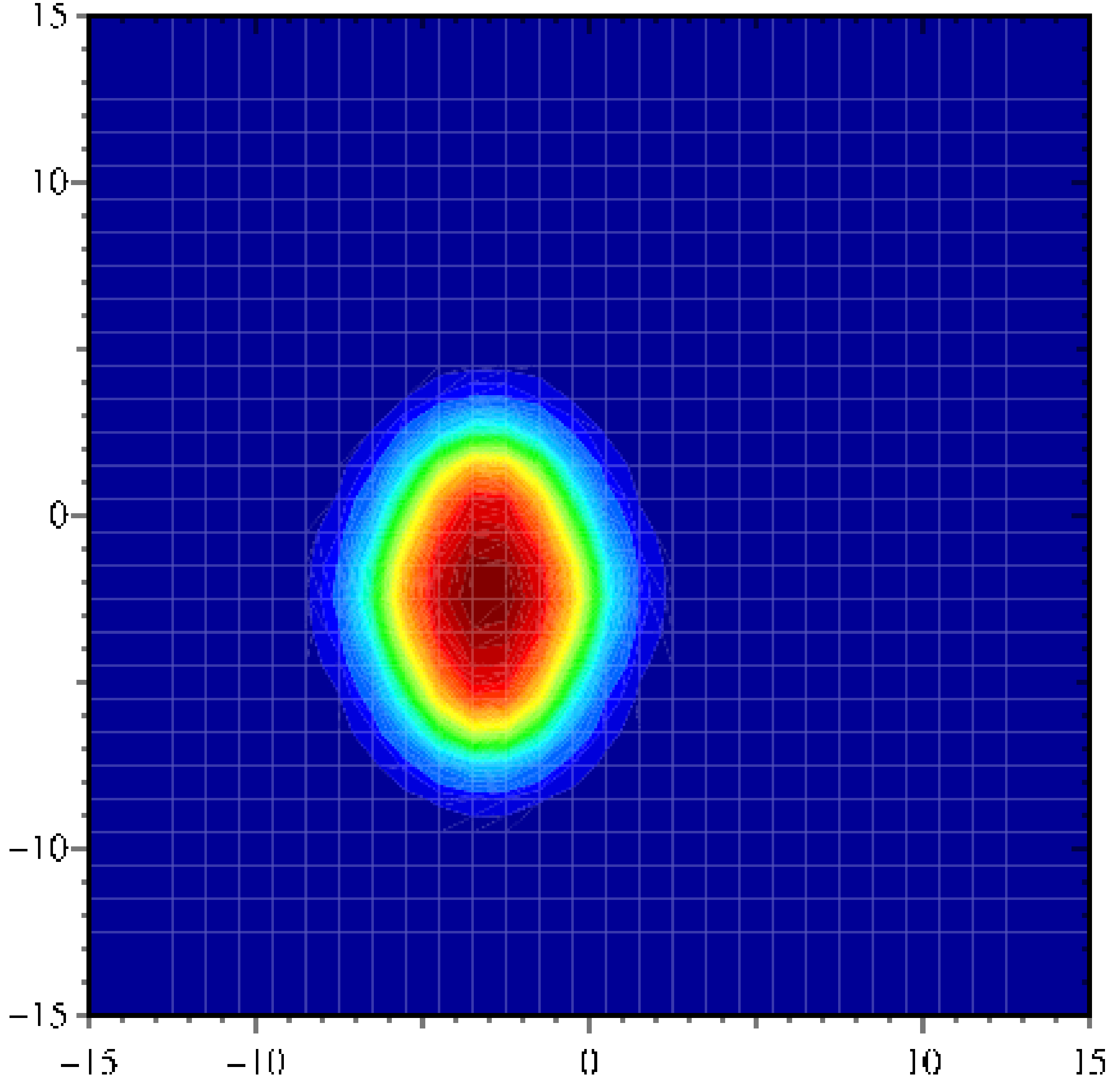
$^{16}O+^{22}Ne$ (alignment 2) E/A=2.5 MeV



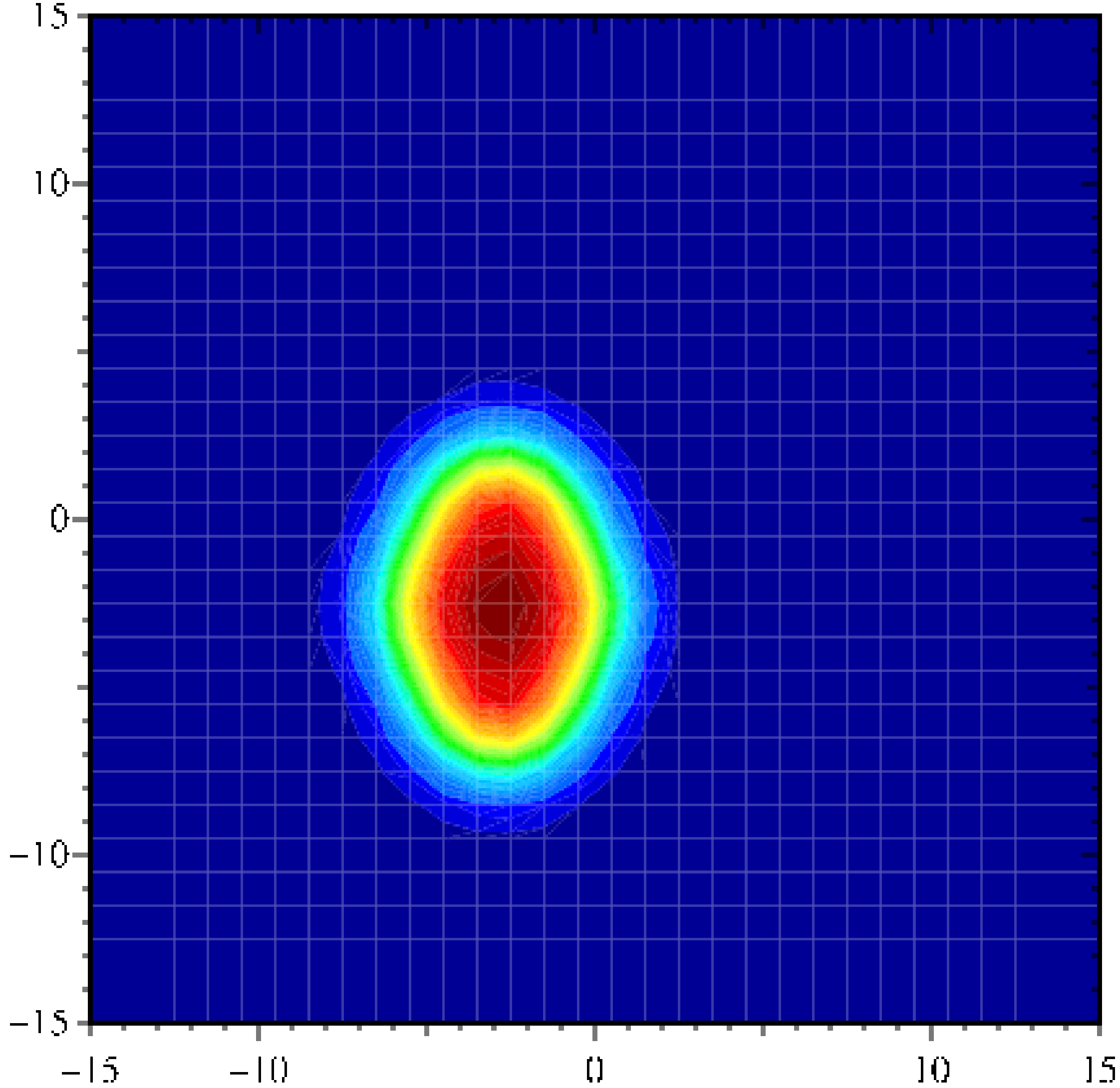
$^{16}O+^{34}Ne$ (alignment 1), E_{cm} = 115 MeV, b = 0 fm



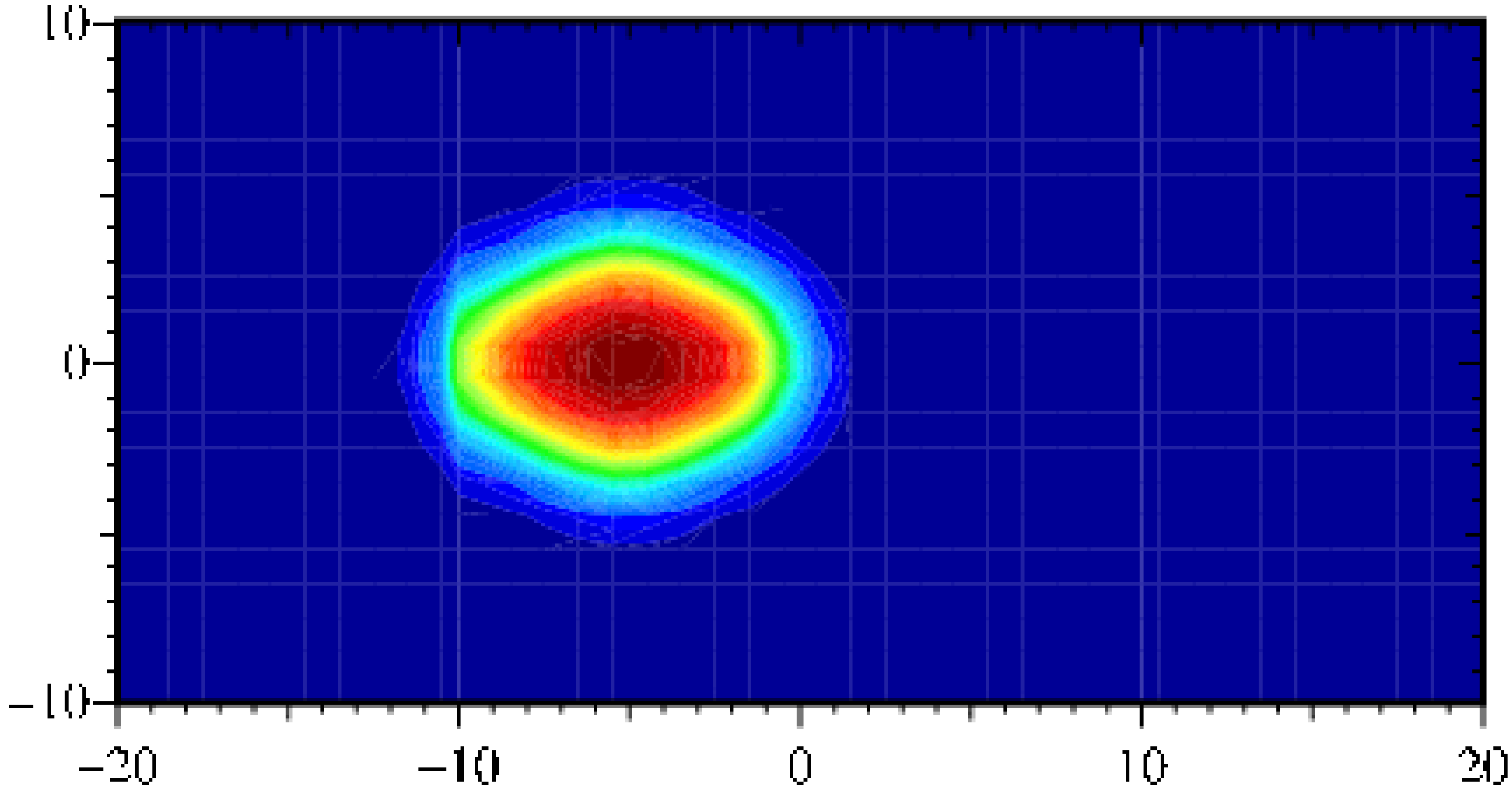
$^{16}O+^{34}Ne$ (alignment 1), E_{cm}= 115 MeV, b = 7 fm



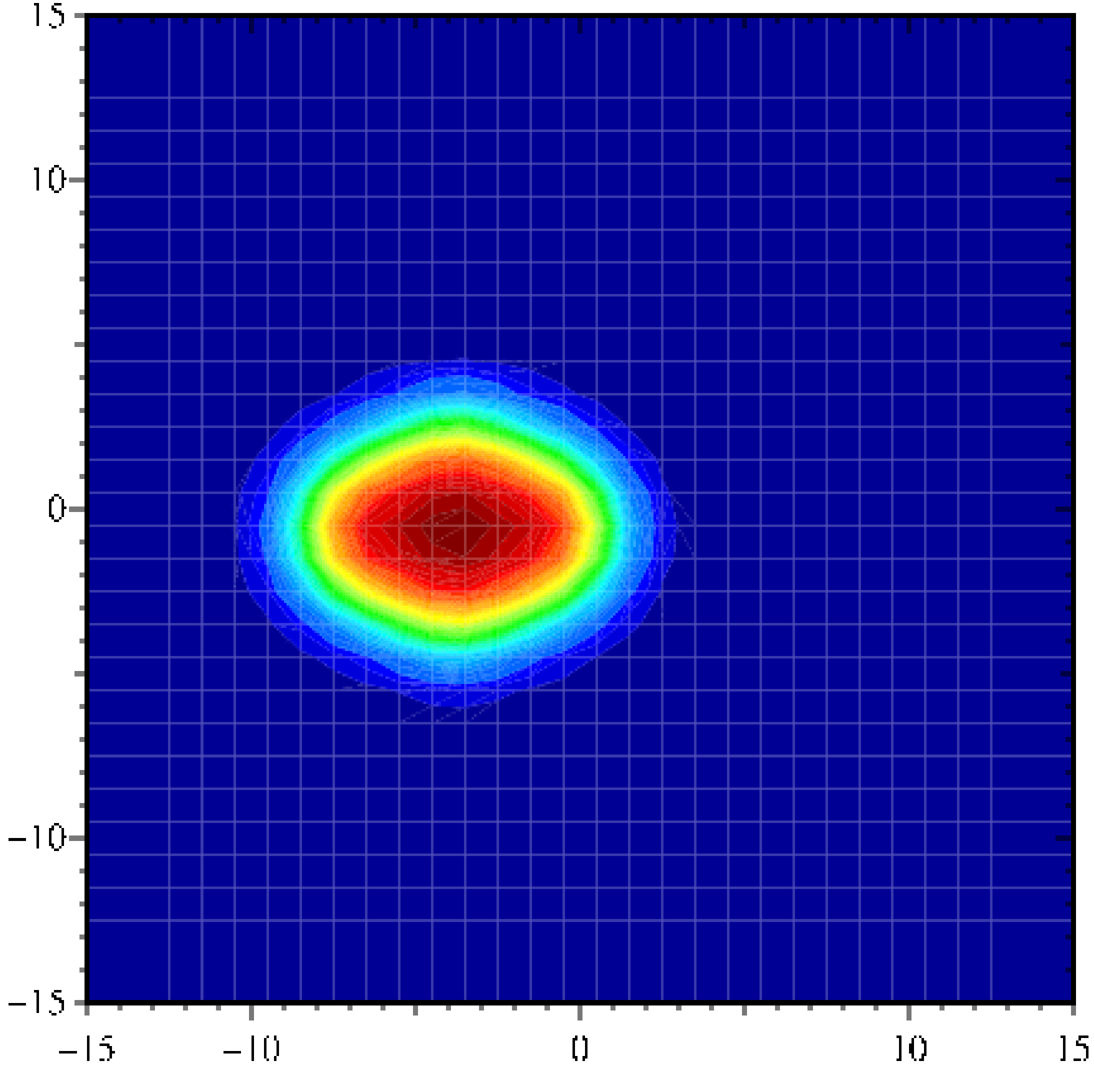
$^{16}O+^{34}Ne$ (alignment 1), E_{cm}= 115 MeV, b = 8 fm



^{16}O+^{34}Ne (alignment 2), E_{cm}= 115 MeV, b = 0 fm

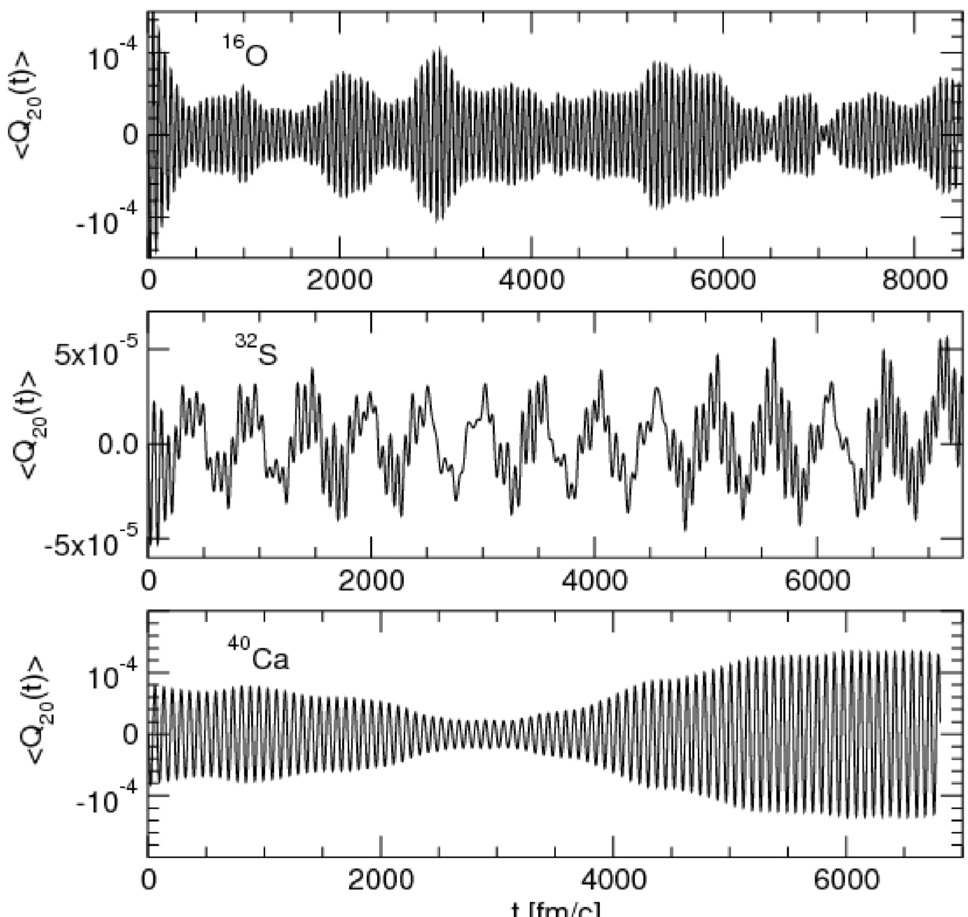


$^{16}O+^{34}Ne$ (alignment 2), E_{cm}= 115 MeV, b = 2 fm



Response via TDHF

- Start with a well converged HF solution
- Hit the nucleus with a small pulse to excite various modes
- Use TDHF to follow time-evolution



$$H_{ex}(t)=\hat{F}\,f(t)$$

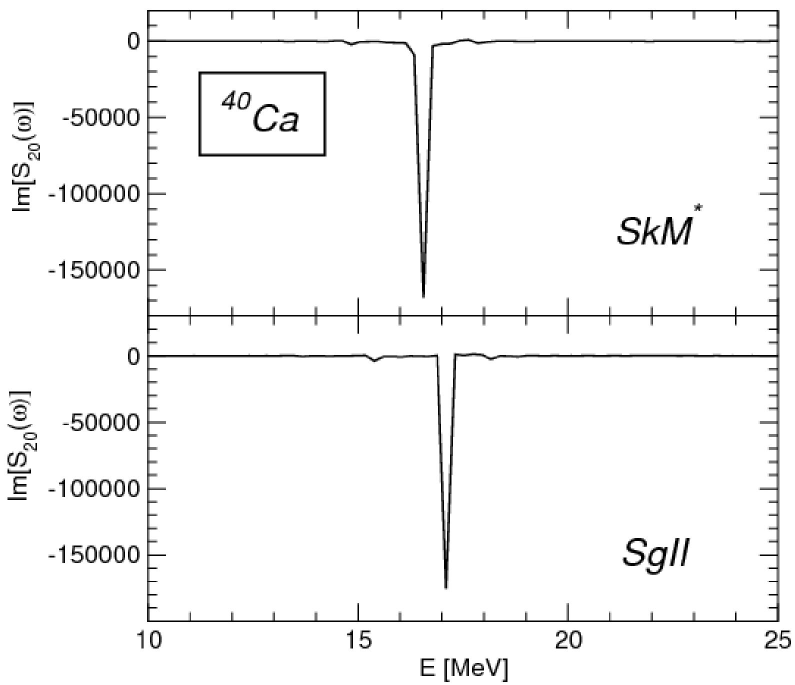
$$\delta\langle\hat{n}(\boldsymbol{x},t)\rangle=\langle\bar{\psi}_s(t)|\hat{n}_s(t)|\bar{\psi}_s(t)\rangle - \langle\psi_s(0)|\hat{n}_s(0)|\psi_s(0)\rangle$$

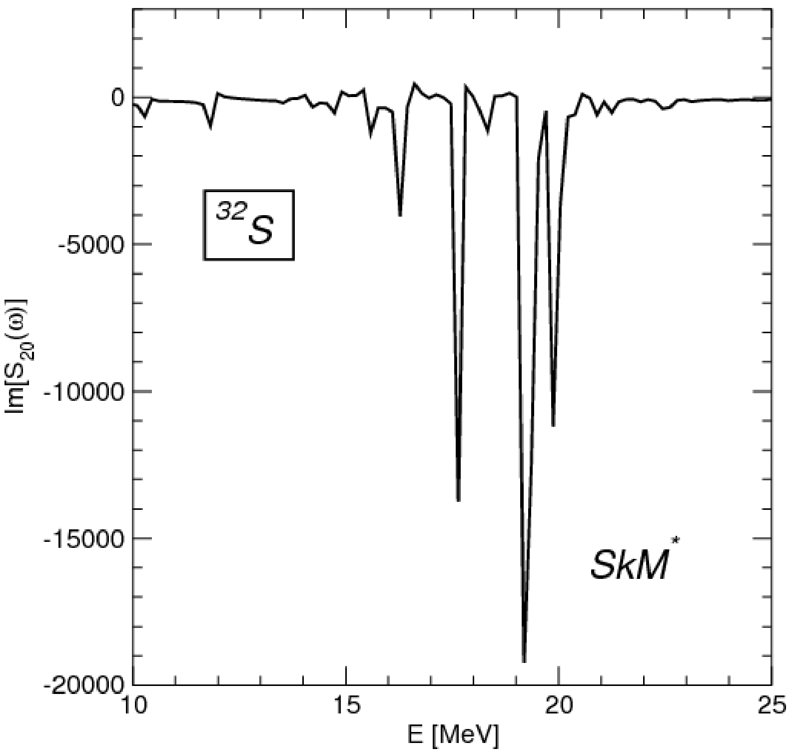
$$f(\omega)S(\omega)=\int d^3x\,\delta\langle F^\dagger(\boldsymbol{x})\,n(\boldsymbol{x},\omega)\rangle$$

Phys.Rev. C71, 034314 (2005)

Response via TDHF

$$\Im[S(\omega)] = -\frac{\pi}{\hbar}\sum_n \left| \int d^3x' \langle \psi_n | \tilde{n}(\boldsymbol{x}') | \psi_0 \rangle F(\boldsymbol{x}') \right|^2 \delta\left(\omega - \frac{E_n - E_0}{\hbar}\right)$$

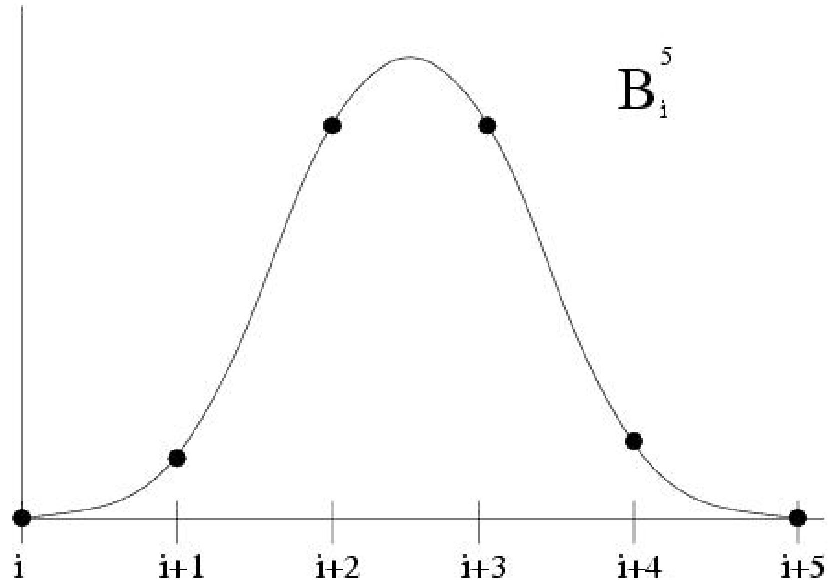




NUMERICAL METHODS

Discrete Mathematics – Basis-Spline Collocation

- Discretization is interpolation on the lattice
- Spline functions provide an optimal basis
- We develop the methodology of doing discrete mathematics on the lattice

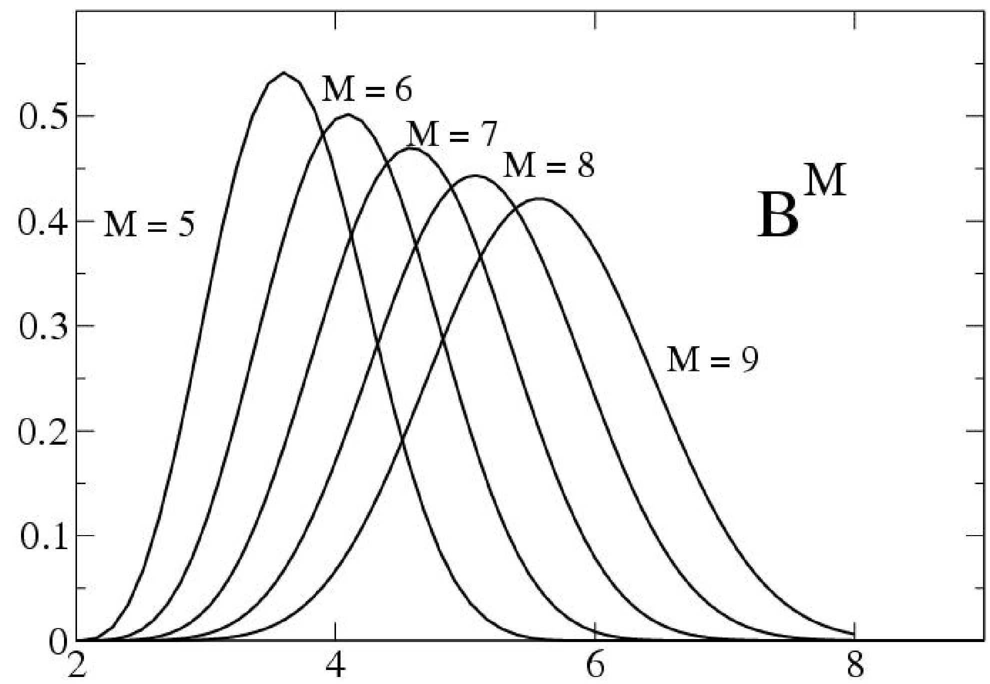


Basis Spline of order M=5
with "knots"

•M-1 order polynomials joined at knots
•M-1 derivatives exist
•Minimal support

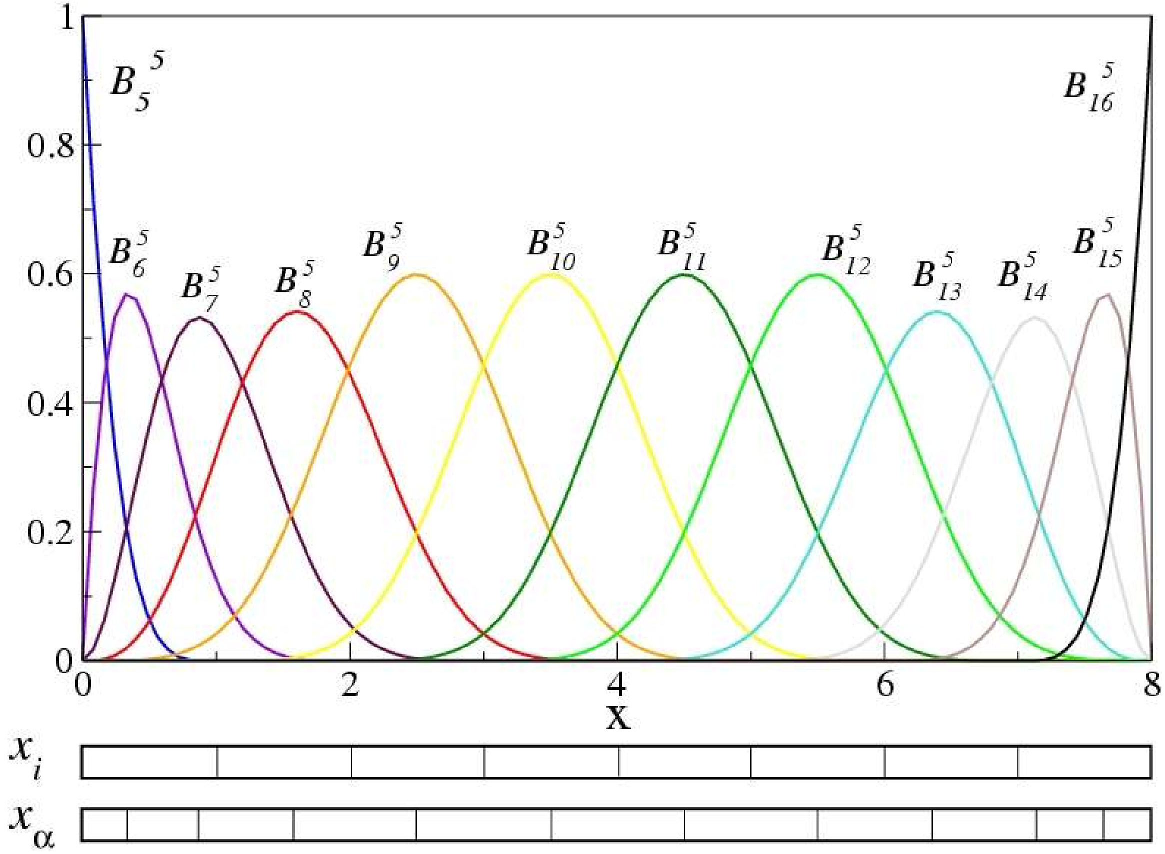
Umar et al, J. Comp. Phys., 93, 426 (1991)

Basis-Splines of order M



Basis Splines of order M=5,...,9

Basis Splines with Fixed Boundary Conditions



Basis Splines of order M=5 with boundary conditions

Discrete Mathematics: Basis-Spline Collocation Method

- Expand functions in B-splines, discretize on collocation lattice

$$f(x)=\sum_{k=1}^{N} B_k^M(x)\,c^k \longrightarrow f_\alpha=\sum_{k=1}^{N} B_{k\alpha}^M c^k$$

- Solve for expansion coefficients by inverting B

$$c^k=\sum_{\alpha=1}^{N}[B_{k\alpha}]^{-1} f_\alpha \xrightarrow{\text{on lattice}} f(x)\to f_\alpha$$

- Action of an operator on a function

$$[Of(x)]=\sum_{k=1}^{N}[OB_k^M(x)]\,c^k \xrightarrow{\text{substitute } c^k} [Of(x)]_\alpha=\sum_{k=1}^{N}[OB_k^M(x)]_\alpha \sum_{\alpha'=1}^{N}[B_{k\alpha'}]^{-1} f_{\alpha'}$$

- Rewrite by defining collocation operator

$$[Of(x)]_\alpha\to\sum_{\alpha'} O_\alpha^{\alpha'} f_{\alpha'} \xrightarrow{\text{where}} O_\alpha^{\alpha'}\equiv\sum_{k=1}^{N}[OB_k(x)]_\alpha B^{k\alpha'}$$

- Lattice integration defined in a similar way

$$\int_a^b f(x)\,dx\to\sum_\alpha \omega^\alpha f_\alpha \xrightarrow{\text{with}} \omega_\alpha\equiv\sum_k h_k c^k$$

3-D Discrete TDHF Equations

- Expand single-particle states in B-spline basis

$$\phi_\lambda(x,y,z;t)=\sum_{ijk} B_i(x)B_j(y)B_k(z)c_\lambda^{ijk}(t)$$

- Discretize on the collocation lattice before variation

$$S=\int dt \sum_{\alpha\beta\gamma} \Delta V_{\alpha\beta\gamma}\left\{H(\alpha\beta\gamma)-\left[i\hbar\sum_\mu \phi_\mu^*(\alpha\beta\gamma)\frac{\partial\phi_\mu}{\partial t}(\alpha\beta\gamma)\right]\right\}$$

- After variation local terms are local

$$\frac{\delta\phi_\mu^*(\alpha\beta\gamma)}{\delta\phi_\lambda^*(\alpha'\beta'\gamma')}=\frac{1}{\Delta V_{\alpha\beta\gamma}}\delta_{\lambda\mu}\delta_{\alpha'\alpha}\delta_{\beta'\beta}\delta_{\gamma'\gamma} \longrightarrow \int d^3r\,\rho^2=\sum_{\alpha\beta\gamma}\omega^\alpha\omega^\beta\omega^\gamma|\rho(\alpha\beta\gamma)|^2$$

- Non-local terms look like

$$\left(\nabla\phi_\lambda\right)_{\alpha\beta\gamma}=\sum_{\alpha'} D_\alpha^{\alpha'}\phi_\lambda(\alpha'\beta\gamma)\hat{\imath}+\sum_{\beta'} D_\beta^{\beta'}\phi_\lambda(\alpha\beta'\gamma)\hat{\jmath}+\sum_{\gamma'} D_\gamma^{\gamma'}\phi_\lambda(\alpha\beta\gamma')\hat{k}$$

Numerical Solutions

$$\phi_\lambda(t+\tau) = \exp[-i\tau h(\tau)]\phi_\lambda(t)$$

Formal solution for a small time-step

$$\phi_\lambda(t+\tau) \approx \left[1+\sum_{n=1}^{N}\frac{(-i\tau h)^n}{n!}\right]\phi_\lambda(t)$$

Numerical approximation

$$\chi_\lambda^{k+1} = O\{\chi_\lambda^k - x_0 D[E_0](h^k - \epsilon_\lambda^k)\}$$

$$D(E_0) = \left[1+\frac{T_x}{E_0}\right]^{-1}\left[1+\frac{T_y}{E_0}\right]^{-1}\left[1+\frac{T_z}{E_0}\right]^{-1}$$

$E_0 = 20\,MeV \quad x_0 = 0.05$

Damped Gradient for static solution