Time-dependent Basis Function (tBF) approach to scattering

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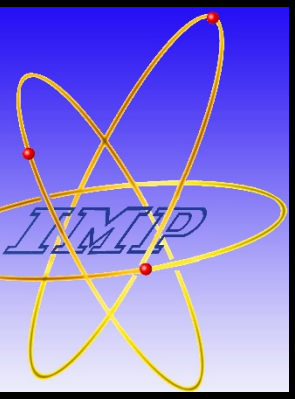
arXiv:1804.01156; Phys. Rev. C (in press)



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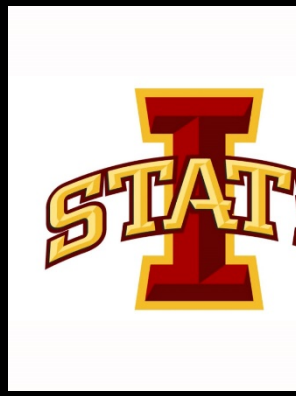


MSU, June 15, 2018

Motivations

Challenges in predicting nuclear structure and reactions, e.g.,

- Exotic nuclei, FRIB
- Astrophysics, radiative capture
- Fusion energy, ITER and NIF

These propel development of theories with predictive power:

- Fundamental, unified *ab initio* nuclear theory for nuclear structure and reactions

Background

Existing methods, e.g.,

- No-core Shell Model with Continuum
- No-core Shell Model/Resonating Group Method
- Gamow Shell Model
- Harmonic Oscillator Representation of Scattering Equations
- Green's Function Approaches
- Nuclear Lattice Effective Field Theory
- Many others

However, these successful methods may be challenged to retain full quantal coherence of all relevant nuclear processes

We introduce the time-dependent Basis Function (tBF) Method

- *Ab initio* approach
- Non-perturbative
- Retains full quantal interference
- Enables snapshots of dynamics
- Supercomputing directly applicable

Idea of tBF Method

1. *Ab initio* structure calculation

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$H_0 = T_{rel} + V$$

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

2. Scattering problem

$$i\frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

$$H(t) = T_{rel} + V$$ +V(t)

- Scattering state = time-dependent superposition of eige
- Operators become matrices in eigen-basis representatio

1. Solve for the "target" system's eigen-basis via *ab initio* calculation
2. Define the scattering state within this eigen-basis and evaluate H(t) in this basis
3. Solve the equation of motion in this eigen-basis

Ab initio Structure Calculation of Deuteron

Hamiltonian of the deuteron

$$H_{\mathrm{rel}} = T_{\mathrm{rel}} + V_{\mathrm{NN}}$$

with

- Intrinsic kinetic energy $T_{\mathrm{rel}} = \frac{P_{\mathrm{rel}}^2}{2m}$
- Realistic inter-nucleon interaction V_{NN}

HO Basis for NN Nuclear Structure Calculation

- Nuclear interaction conserves total angular momentum $\vec{J} = \vec{l} + \vec{S}$

$$|\beta_i\rangle \rightarrow |\{SJM_J T_z\}_i\rangle = \sum_{n,l} a^i_{nl} |nlSJM_J T_z\rangle$$

- Excitation quanta for basis space truncation:

$$N = 2n + l$$

- 3DHO basis wave function in coordinate space

$$\langle \vec{r} | nlSJM \rangle = R_{nl}(r) \sum_{m_l m_s} (lm_l Sm_s | JM) Y_{lm_l}(\Omega_{\hat{r}}) \chi_{Sm_s}$$

$$R_{nl}(r) = \sqrt{\frac{2n!}{r_0^3 \Gamma(n+l+\frac{3}{2})}} \left(\frac{r}{r_0}\right)^l \exp\left[-\frac{r^2}{2r_0^2}\right] L_n^{l+\frac{1}{2}}\left(\frac{r^2}{r_0^2}\right)$$

- Why 3DHO basis?
  - Respects the symmetries of the nuclear system
    - e.g., rotational and translational symmetries
  - The center of mass motion can be easily removed

SP16 interaction adopted for the initial application

Constructed by *J*-matrix inverse scattering theory

Reproduces NN scattering data

"16" means the interaction is fitted to reproduce some of the properties for ^{16}O

Reproduces selected properties of light nuclei

- e.g., ^{2}H, ^{3}H, ^{4}He

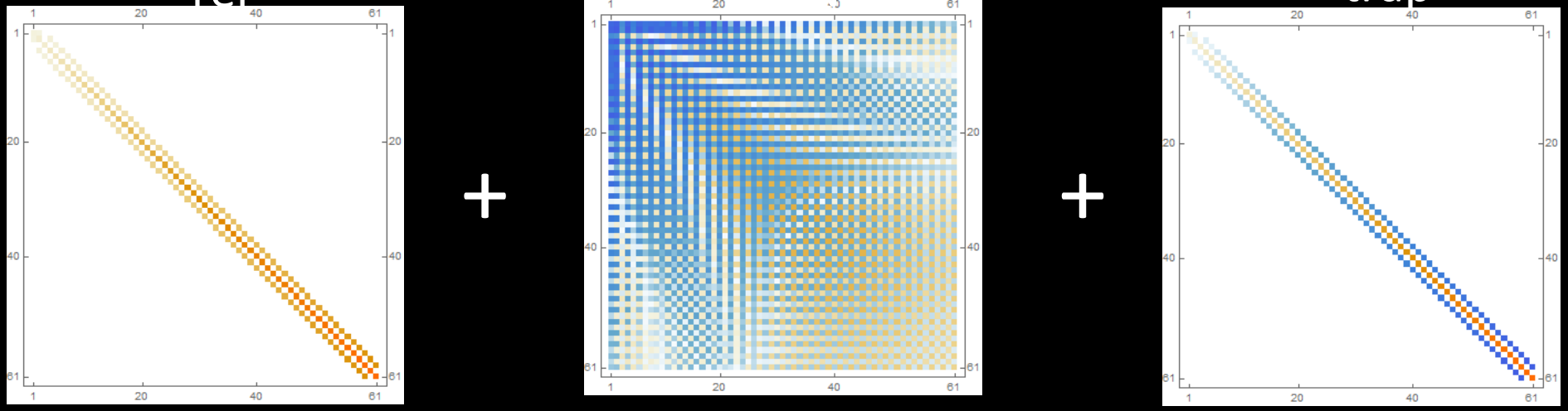
Includes two-nucleon (NN) interaction only

Non-local interaction

The interaction in 3DHO representation (matrix elements)

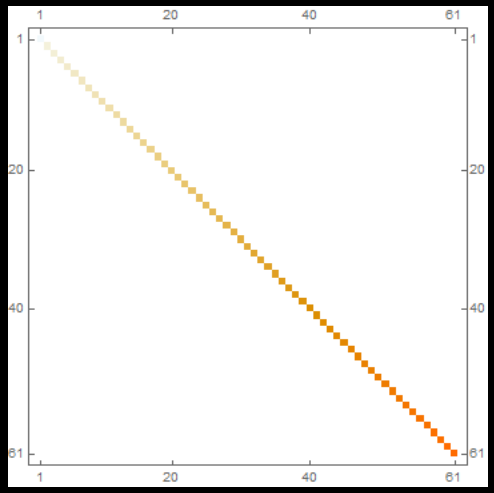
implify the “continuum” => add a HO confining interaction
amiltonian for Quasi-deuteron in 3DHO Representation

T_{rel} + V_{NN} + U_{trap}



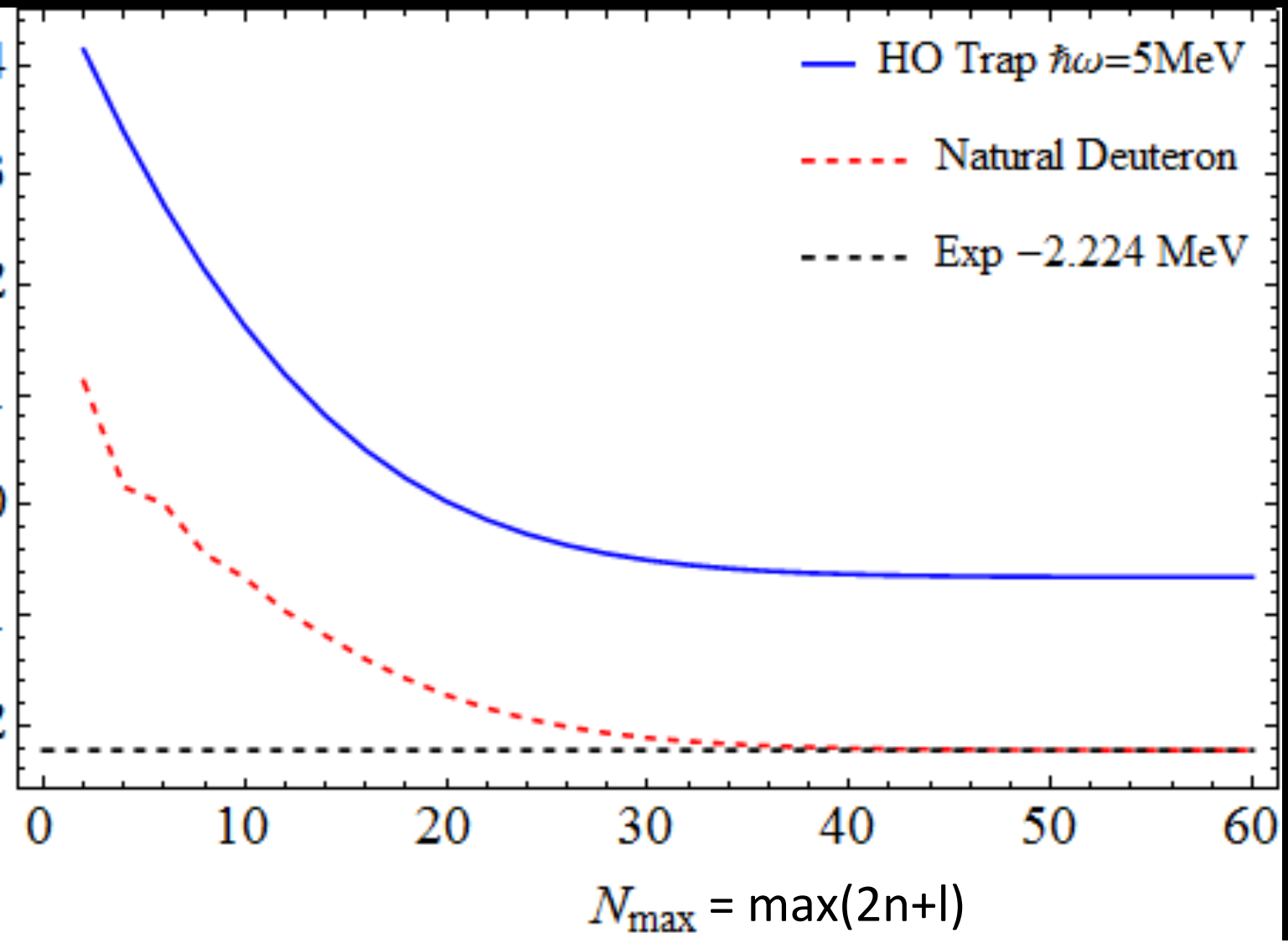
= Full Hamiltonian

Diagonalization



Eigen-energies on the diagonal

Results:
Ground State Energies for Natural and Quasi-Deuteron



- N_{max}=60;
- Basis strength=5

- As the basis spac
increases in dime
theoretical gs en
deuteron conver
the experimenta

Time-Dependent Schrödinger Equation

Time-dependent full Hamiltonian

$$H(t) \quad = \quad H_0 + V_{\rm int}(t)$$

Equation of motion

- Schrödinger picture

$$i\frac{\partial}{\partial t}|\psi;t\rangle \quad = \quad H(t)|\psi;t\rangle$$

- Interaction picture

$$i\frac{\partial}{\partial t}|\psi;t\rangle_I \quad = \quad e^{iH_0t}\ V_{\rm int}(t)\ e^{-iH_0t}\ |\psi;t\rangle_I \ \equiv \ V_I(t)\ |\psi;t\rangle_I$$

Solve Time-dependent Schrödinger Equation

Equation of motion in interaction picture

$$i\frac{\partial}{\partial t}|\psi;t\rangle_I \quad = \quad V_I(t)\ |\psi;t\rangle_I$$

Formal solution

$$|\psi;\ t\rangle_I \quad = \quad U_I(t;t_0)|\psi;\ t_0\rangle_I$$

$$U_I(t;t_0) \quad = \quad \hat{T}\left\{\exp\left[-i\int_{t_0}^{t} V_I(t')\ dt'\right]\right\}$$

Transition Amplitudes of States

With the basis representation

$$H_0|\beta_i\rangle = E_i|\beta_i\rangle$$

$$\{|\beta_1\rangle, |\beta_2\rangle, \cdots, |\beta_n\rangle\}$$

the state vector for the system under scattering becomes

$$|\psi;\ t\rangle_I = \sum_{j=1}^{n} A_j^I(t)|\beta_j\rangle$$

$$|\psi;\ t_0\rangle_I \equiv |\beta_i\rangle$$

where the transition amplitude is

$$A^I_{i\to j}(t) \equiv A^I_j(t) = \langle\beta_j|U_I(t;t_0)|\beta_i\rangle$$

Numerical Method 1: Euler Method

Direct evaluation of the time-evolution operator

$$U_I(t;t_0) \quad = \quad T\ \exp\left[-i\int_{t_0}^{t} V_I(t)\ dt\right]$$

with

$$T\ \exp\left[-i\int_{t_0}^{t} V_I(t)\ dt\right]$$
$$\xrightarrow{\sum \delta t} \left[1 - iV_I(t_n)\delta t + O(\delta t^2)\right]\left[1 - iV_I(t_{n-1})\delta t + O(\delta t^2)\right]\ \cdots\ \left[1 - iV_I(t_1)\delta t + O(\delta t^2)\right]$$

- Fast in calculation
- Accurate up to $(\delta t)^2$
- Hence poor numerical stability

Numerical Method 2: Multi-Step Differencing

Multi-step differencing (MSD2) for the evolution:

$$|\psi; t+\delta t\rangle_I = e^{-iV_I(t)\delta t}|\psi; t\rangle_I = (1 - iV_I(t)\delta t + O(iV_I(t)\delta t)^2)|\psi; t\rangle_I$$

$$|\psi; t-\delta t\rangle_I = e^{iV_I(t)\delta t}|\psi; t\rangle_I = (1 + iV_I(t)\delta t + O(iV_I(t)\delta t)^2)|\psi; t\rangle_I$$

$$|\psi; t+\delta t\rangle_I = |\psi; t-\delta t\rangle_I - 2iV_I(t)\delta t|\psi; t\rangle_I + O(iV_I(t)\delta t)^3)|\psi; t\rangle_I$$

- MSD is an explicit method – it does not evaluate matrix inversions
- MSD2 is accurate up to $(\delta t)^3$
- MSD4 is accurate up to $(\delta t)^4$, however less efficient
- We employ MSD2 for better numerical stability and efficiency

T. Iitaka, Phys. Rev. E 49 46
Weijie Du et al., in preparat

For Comparison: First-Order Perturbation Theory

$$|\psi;\ t\rangle_I = T\ exp\left[-i\int_{t_0}^{t} V_I(t)\ dt\right]\ |\psi;\ t_0\rangle_I$$

$$\rightarrow \left[1 - i\ V_I(t_n)\delta t\right]\ \left[1 - i\ V_I(t_{n-1})\delta t\right]\ \cdots\ \left[1 - i\ V_I(t_1)\delta t\right]\ |\psi;\ t$$

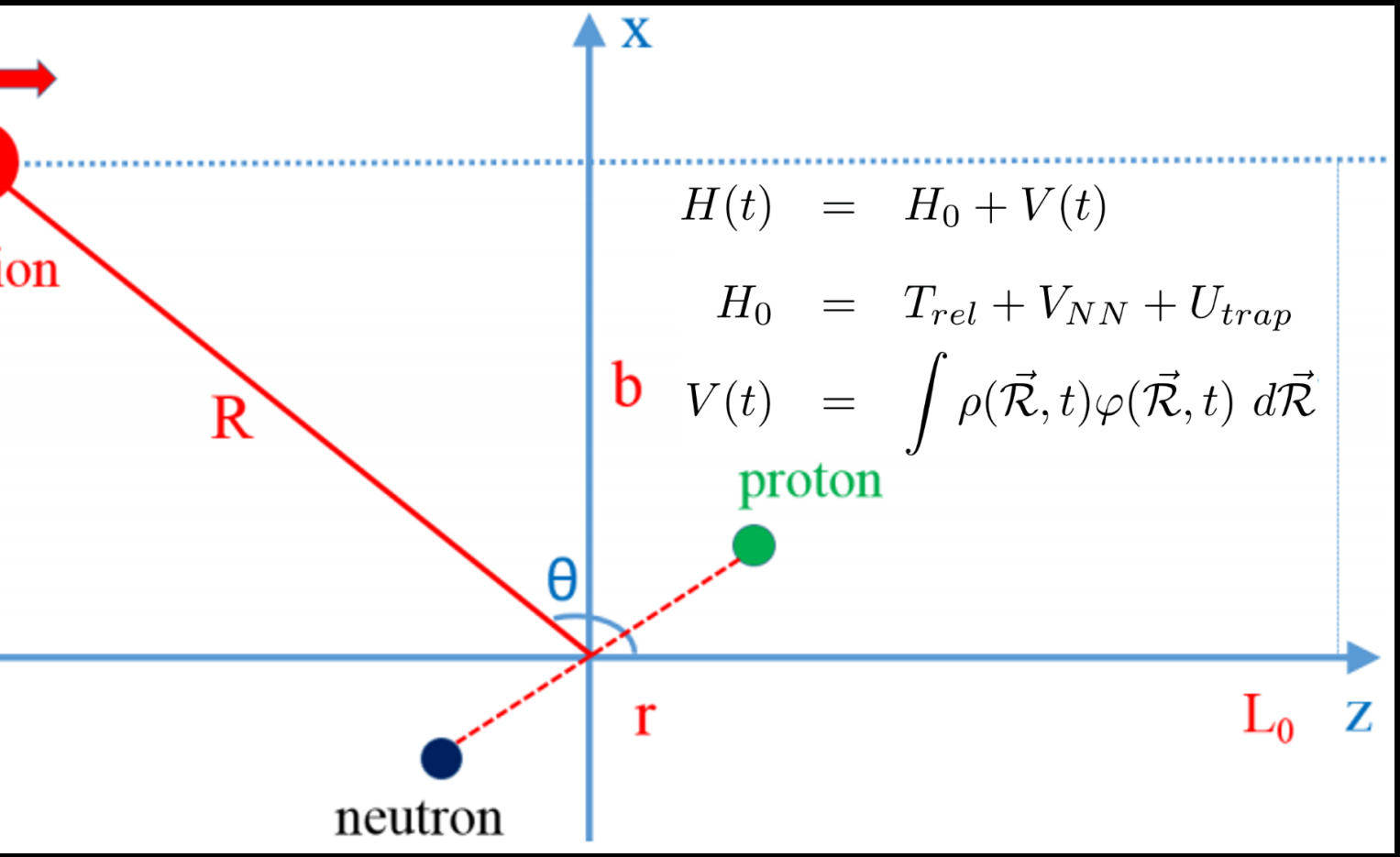
$$\rightarrow \left[1 - i\ \delta t\Big(V_I(t_n) + V_I(t_{n-1}) + \cdots + V_I(t_1)\Big)\right]|\psi;\ t_0\rangle_I$$

Purposes for this comparison

- tBF method is non-perturbative
- tBF method evaluates all the higher-order effects

First Model Problem: Coulomb Excitation of Deuterium System by Peripheral Scattering with Heavy Ion

Setup: Coulomb Excitation of Deuterium System



H_0: target Hamilt

φ: Coulomb field heavy ion

ρ: Charge density distribution of deuteron

Treatment of time-varying Coulomb field

In the basis representation, the operator for the Coulomb interactio becomes a matrix

We take a multipole decomposition for the Coulomb field and keep only the E1 multipole component

K. Alder et al., Rev. Mod. Phys. 28, 432 (1956)

$$\langle \beta_j | V_I(t) | \beta_k \rangle = \frac{4\pi}{3} Z e^2 \mathrm{e}^{i(E_j - E_k)t} \sum_\mu \frac{Y^*_{1\mu}(\Omega_{\hat{R}})}{|R(t)|^2} \langle \beta_j | \frac{r}{2} Y_{1\mu}(\Omega_{\hat{r}}) | \beta_k \rangle$$

E1 transition between bases

E1 Matrix Element in Basis Representation

E1 transition matrix element in the basis representation is evaluated by

- Basis functions from the *ab initio* structure calculation

$$|\beta_i\rangle \rightarrow |\{SJM_JT_z\}_i\rangle = \sum_{n,l} a^i_{nl} |nlSJM_JT_z\rangle$$

- And the analytic form of the E1 operator in 3DHO representation

$$\begin{aligned}
&\langle n_j l_j S_j J_j M_j | \frac{r}{2} Y_{1\mu}(\hat{r}) | n_k l_k S_k J_k M_k \rangle \\
&= \sqrt{\frac{1}{4m\Omega}} \sum_{m_{l_j} m_{s_j}} \sum_{m_{l_k} m_{s_k}} \delta_{S_j S_k} \delta_{m_{s_j} m_{s_k}} (l_j m_{l_j} S_j m_{s_j} | J_j M_j)(l_k m_{l_k} S_k m_{s_k} | J_k M_k) \\
&\times (-1)^{m_{l_j}} \sqrt{\frac{3(2l_j+1)(2l_k+1)}{4\pi}} \begin{pmatrix} l_j & 1 & l_k \\ -m_{l_j} & \mu & m_{l_k} \end{pmatrix} \begin{pmatrix} l_j & 1 & l_k \\ 0 & 0 & 0 \end{pmatrix} \\
&\times \begin{cases} \sqrt{n_j + l_j + \frac{3}{2}}\, \delta_{n_j n_k} - \sqrt{n_j} \delta_{n_j, n_k+1} & \text{for } l_k = l_j + 1 \\ \sqrt{n_k + l_k + \frac{3}{2}}\, \delta_{n_j n_k} - \sqrt{n_k} \delta_{n_k, n_j+1} & \text{for } l_j = l_k + 1 \\ 0 & \text{else} \end{cases}
\end{aligned}$$

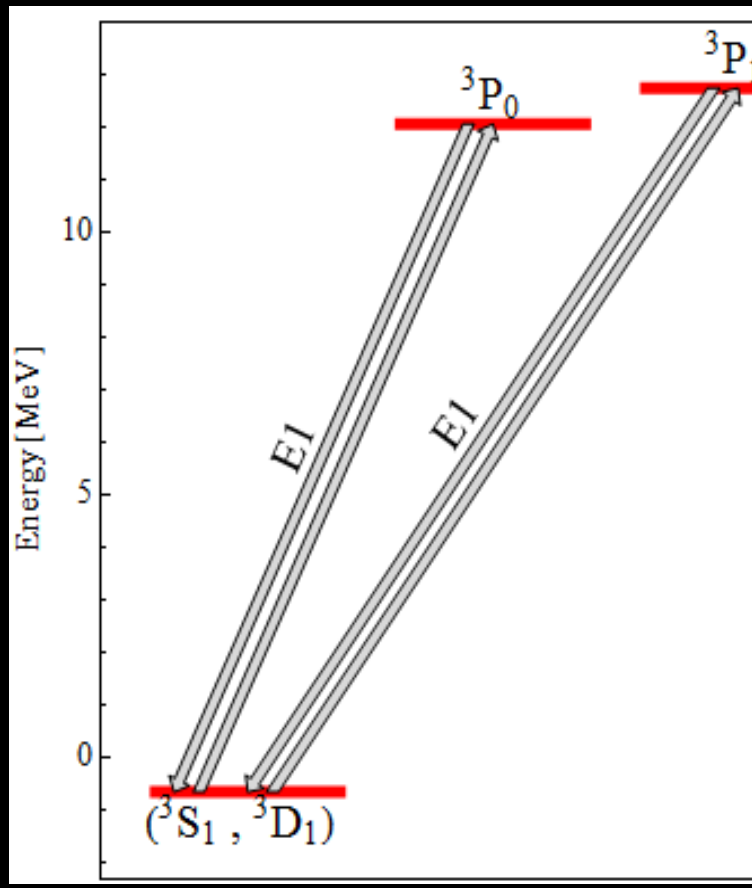
sis Set for Deuteron in Current Calculation

7 basis states are solved via *ab initio* method

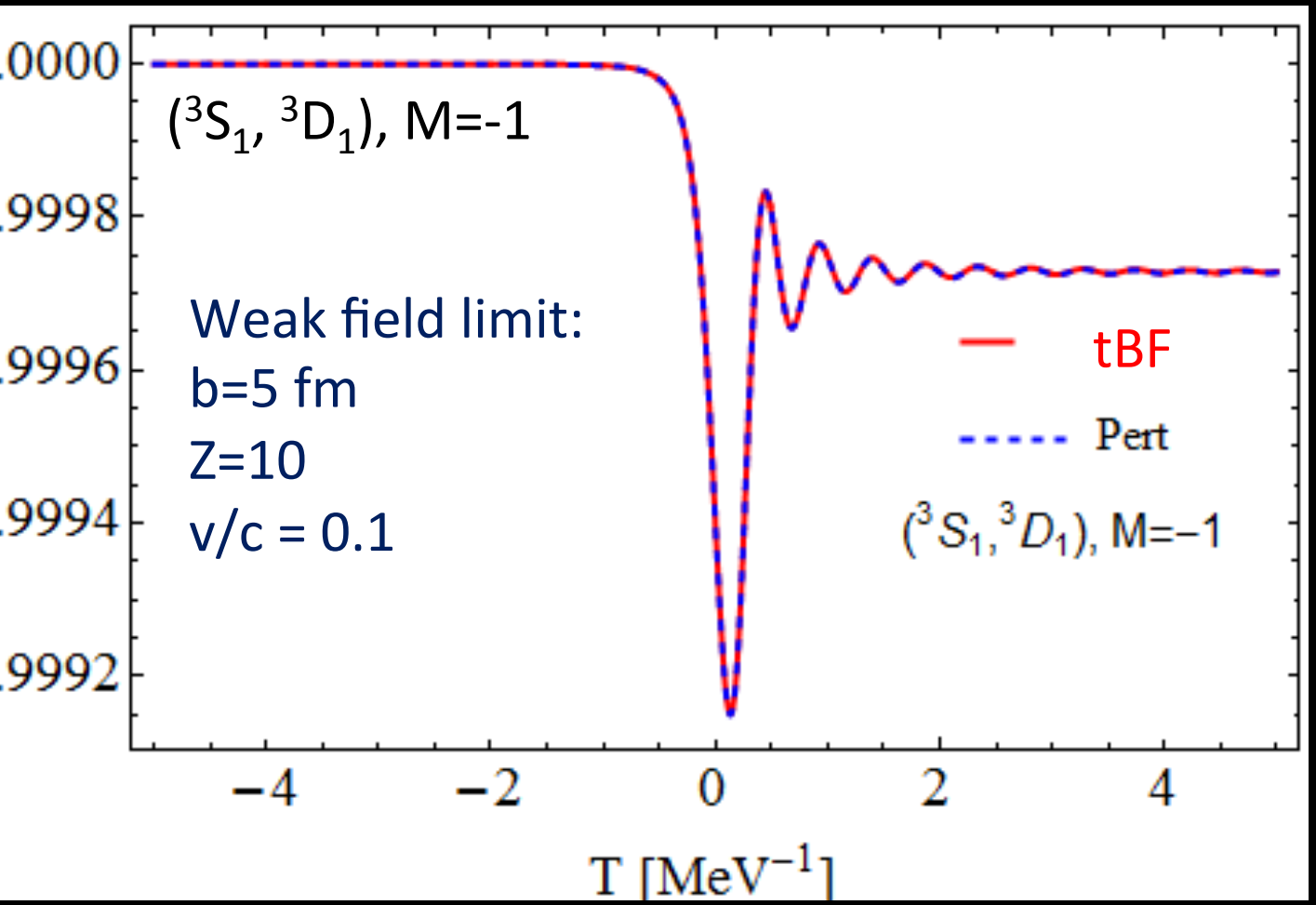
$(^3S_1, ^3D_1)$	$M = -1$	-0.65289 MeV
$(^3S_1, ^3D_1)$	$M = 0$	-0.65289 MeV
$(^3S_1, ^3D_1)$	$M = +1$	-0.65289 MeV
$^3P_0$	$M = 0$	12.0733 MeV
$^3P_1$	$M = -1$	12.7585 MeV
$^3P_1$	$M = 0$	12.7585 MeV
$^3P_1$	$M = +1$	12.7585 MeV

NTSE proceeding, Weijie Du et al. 2017

- Initial state
- Polarization antiparallel to z-ax
- E1 radiative transitions



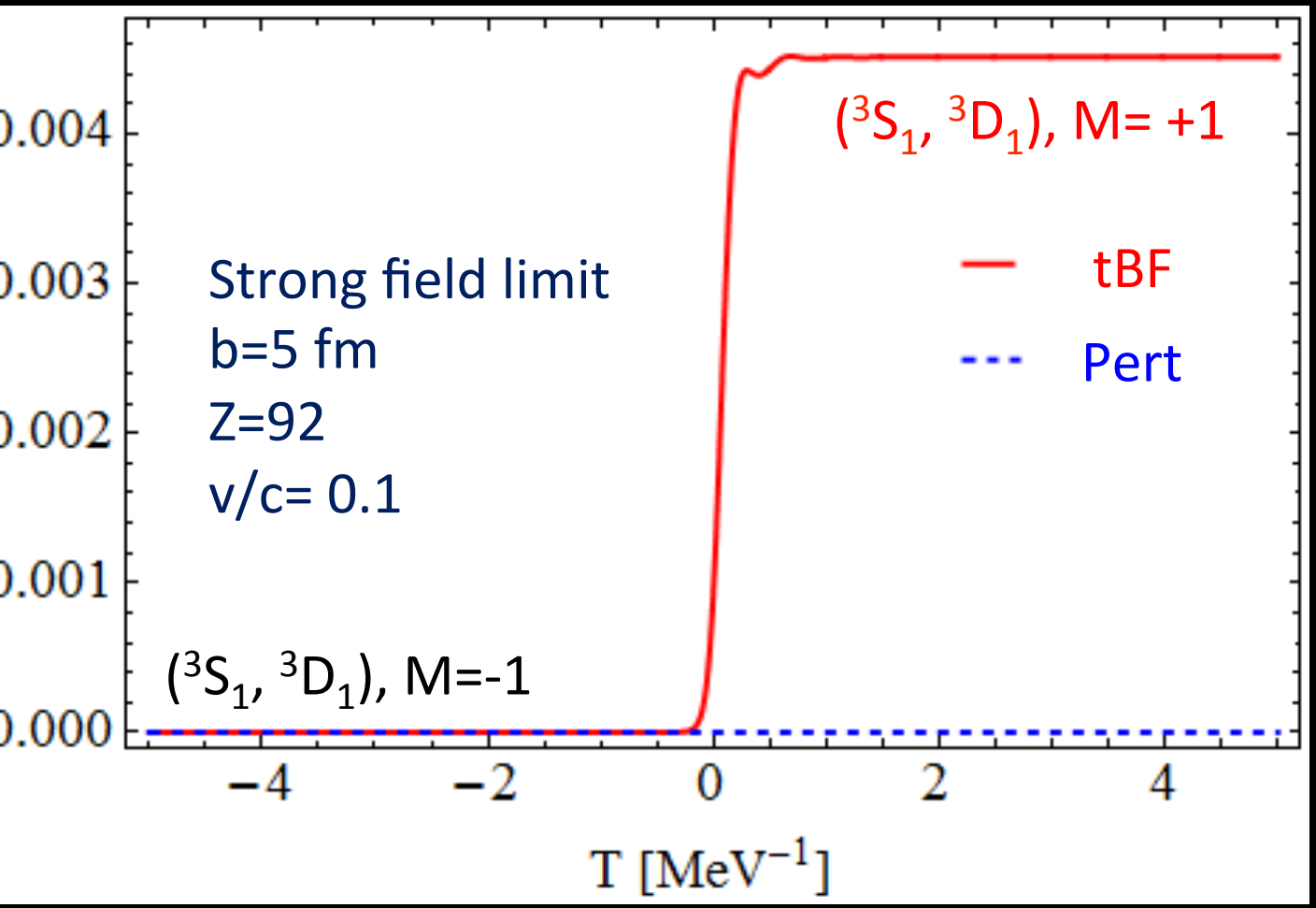
Transition Probabilities



Validity:

When the Coulomb f
is weak , tBF method
matches with first or
perturbation theory (

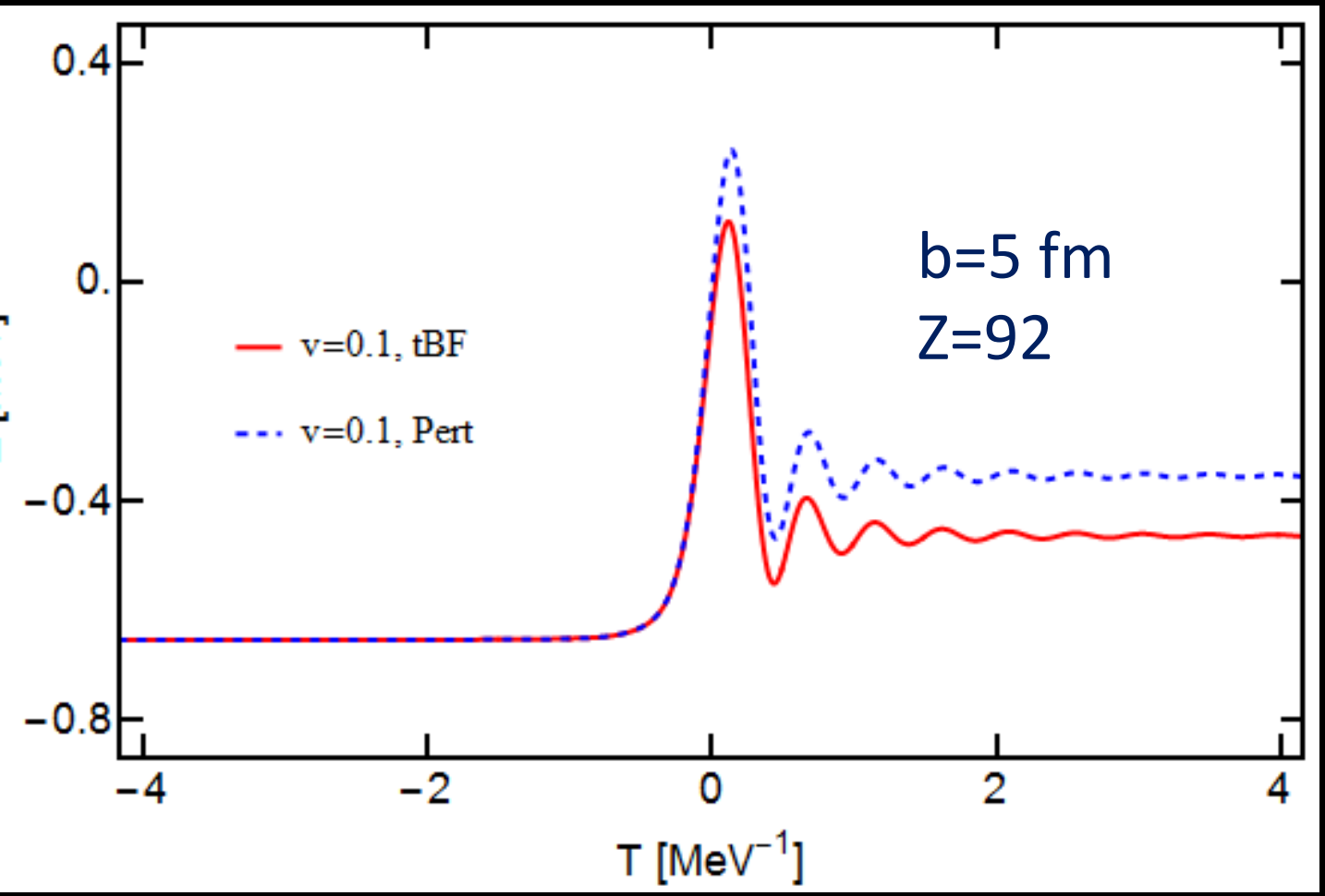
Higher-Order Effects



Forbidden transitio

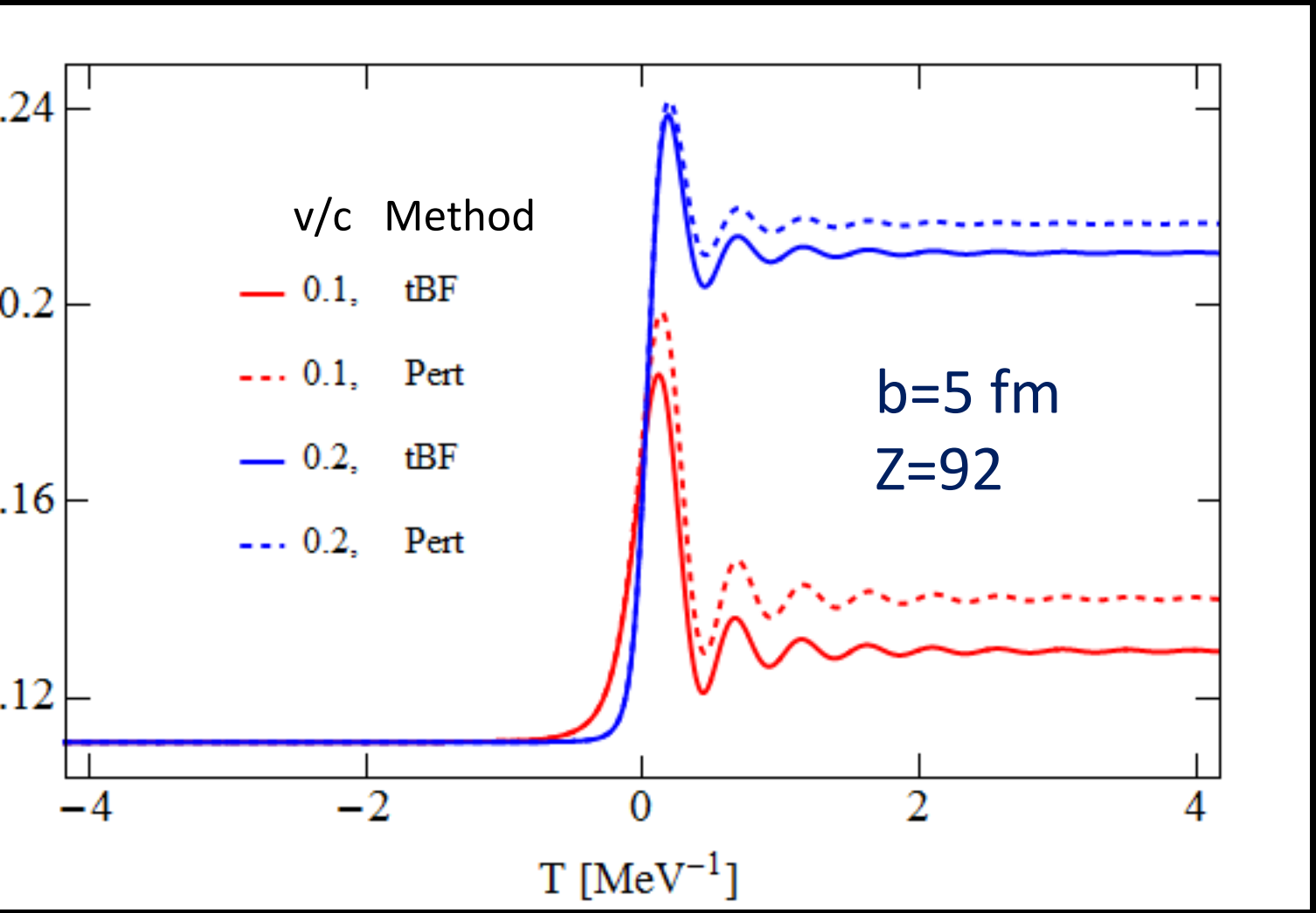
- Revealed by non-perturbative tBF

Excitation of Intrinsic Energy



- Observables as functions of time
- Quantum fluctuatio are taken care at th amplitude level

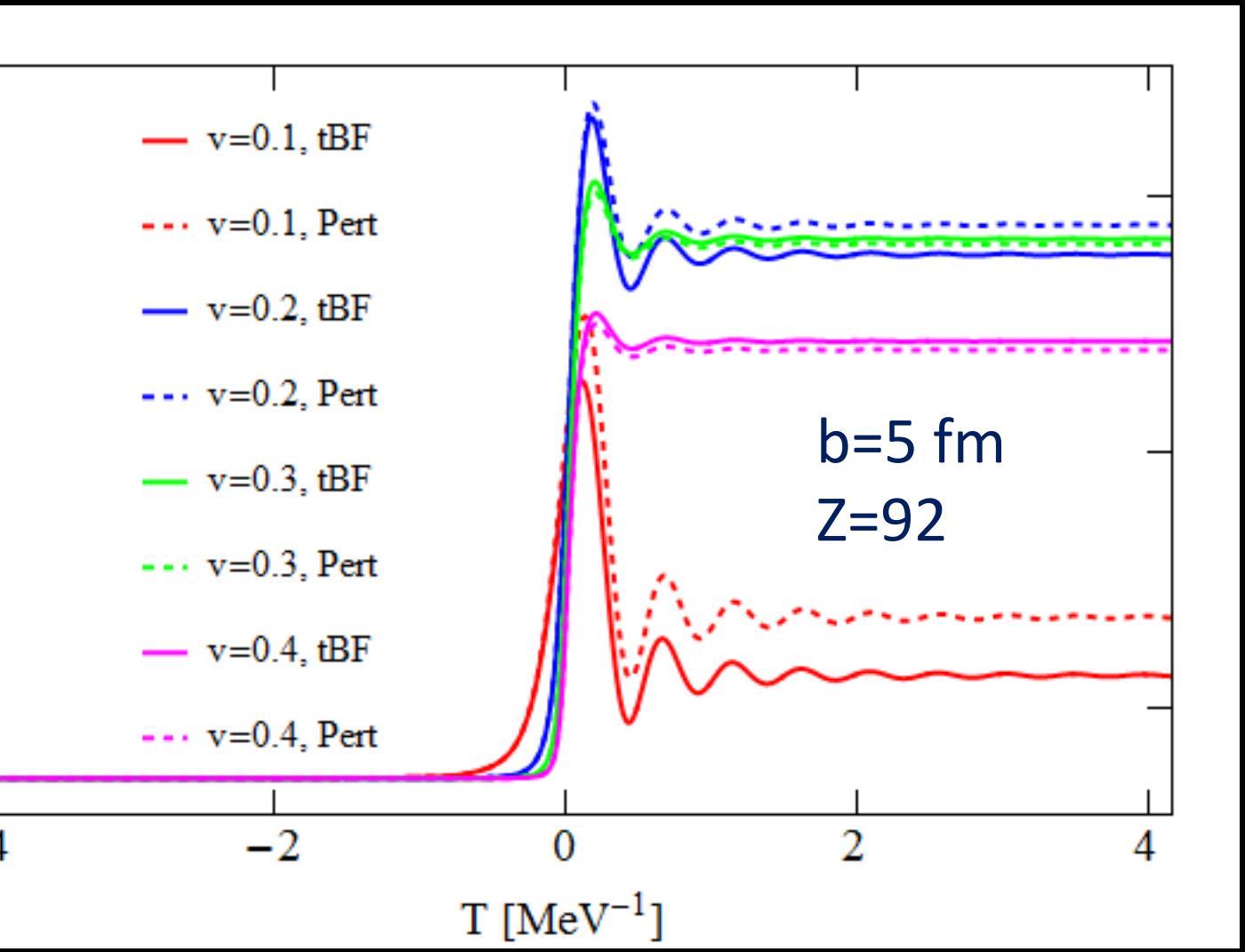
Excitation of Orbital Angular Momentum



Observable's dependence on

- time
- incident spe

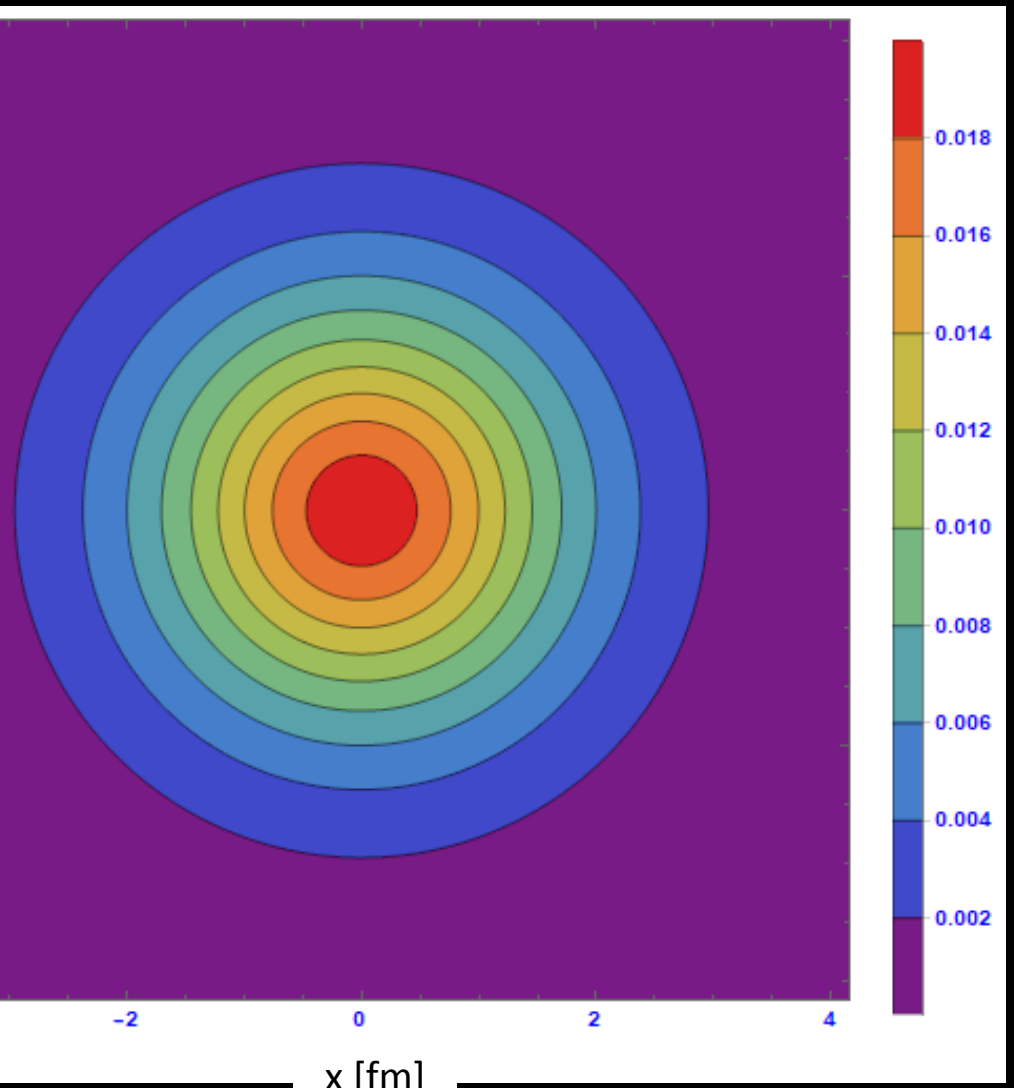
Expansion of r.m.s. Point Charge Radius

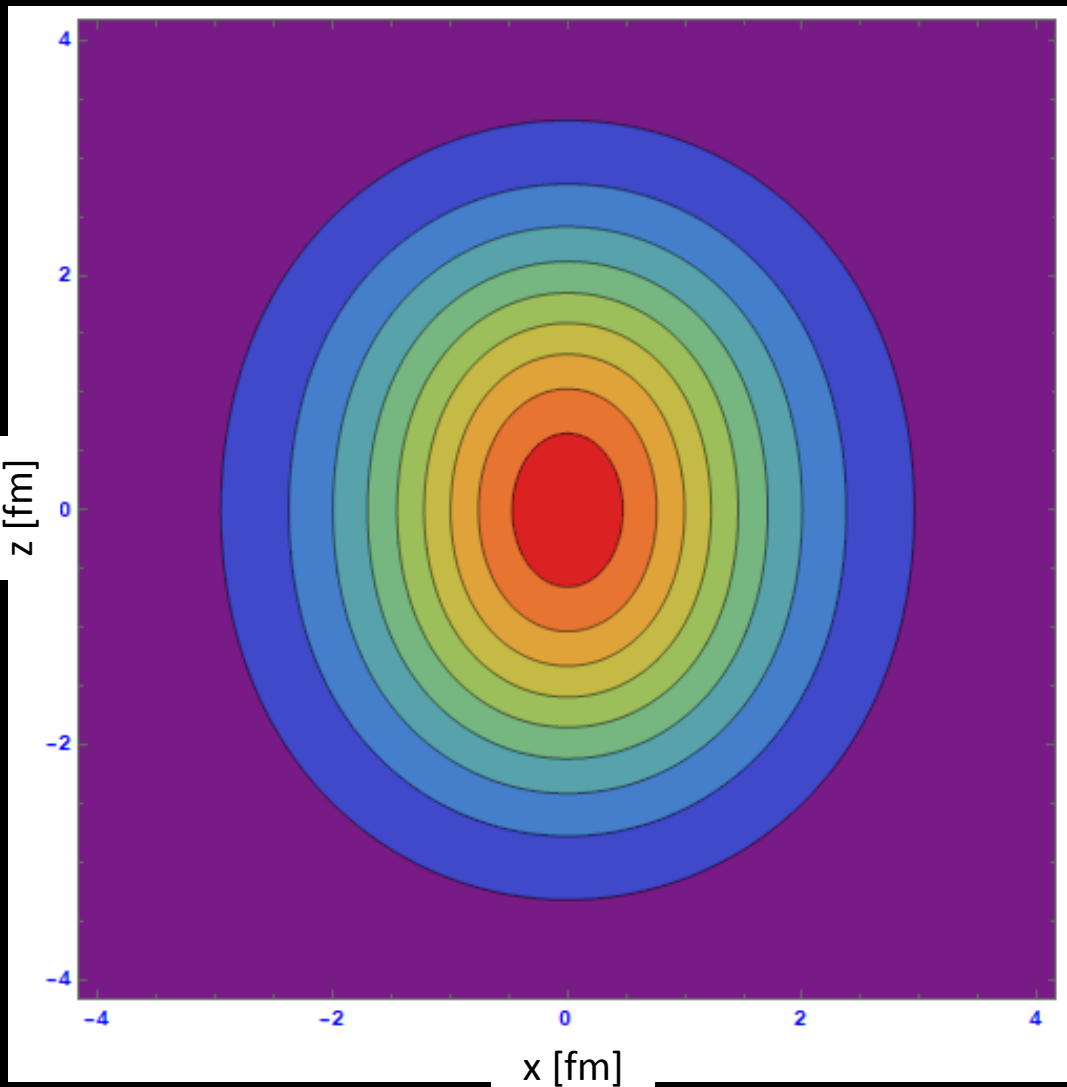


r.m.s. radius of the deuterium system during the scatterin a function of

- time
- incident spee

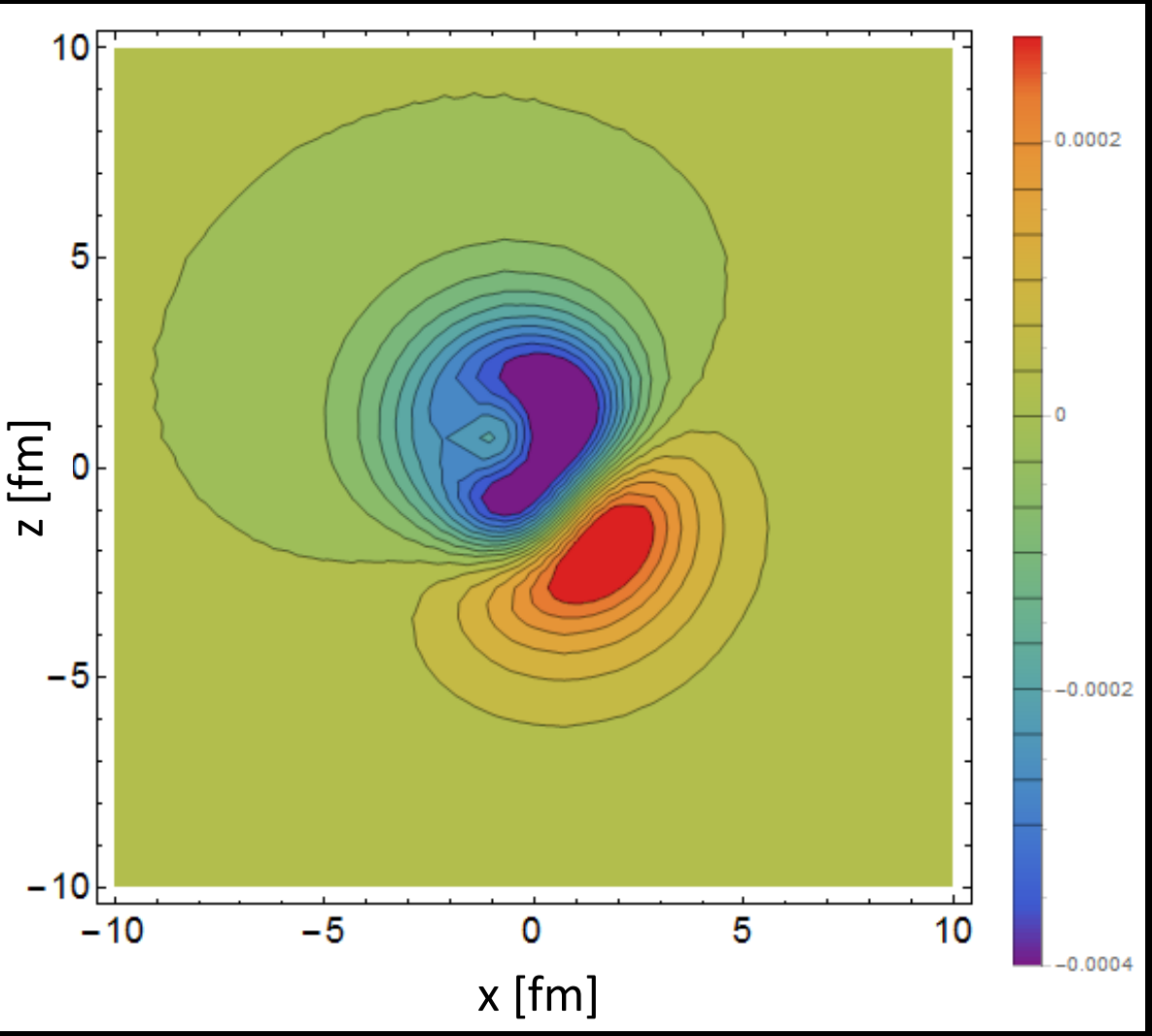
Dynamics: Charge Density Distribution of Initial np syste





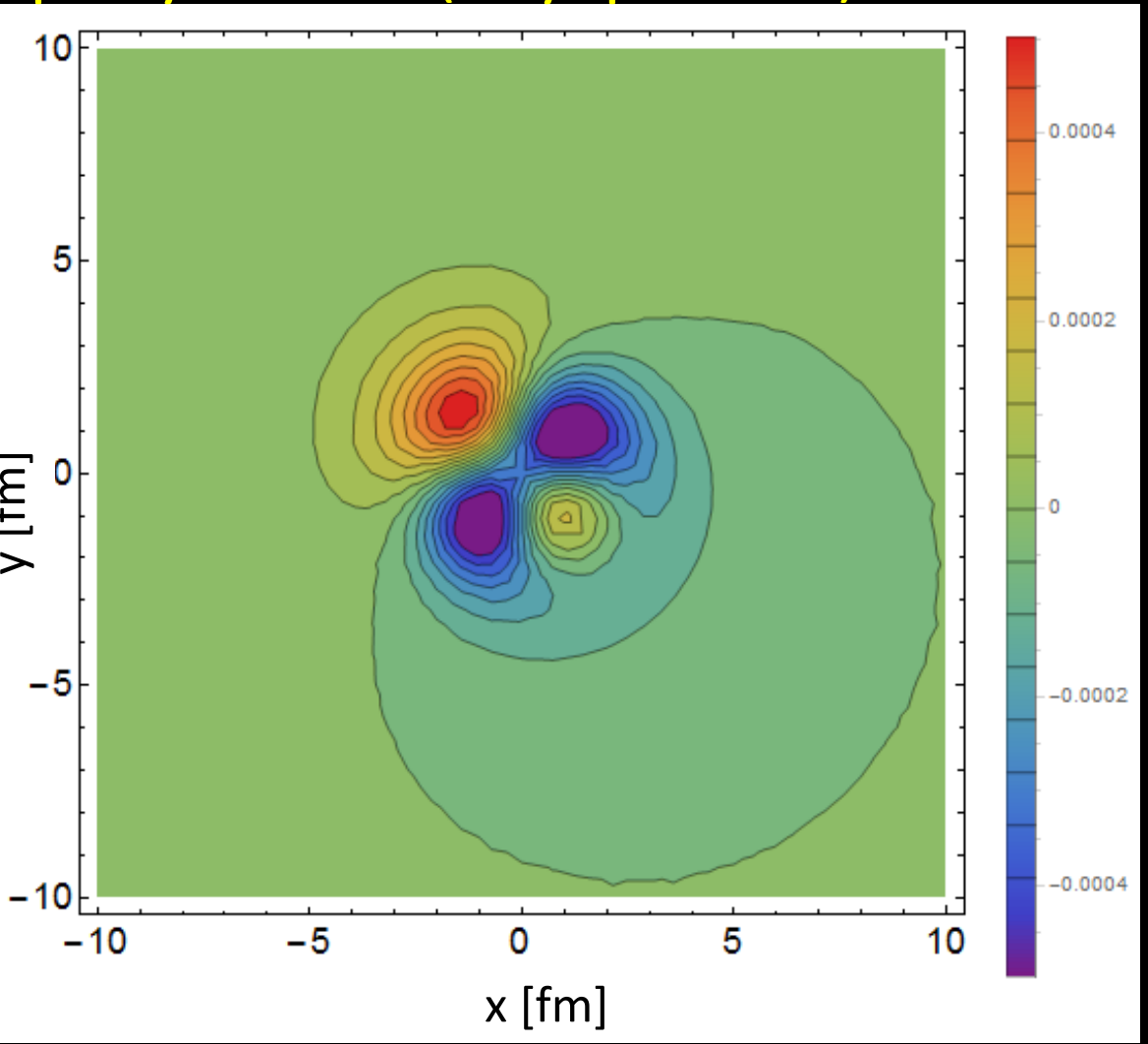
- The Initial polarization is anti-parallel to the z-axis

Change in Charge Density Distribution of Scattered np System (x-z plane) at T= 0.23 MeV^{-1}



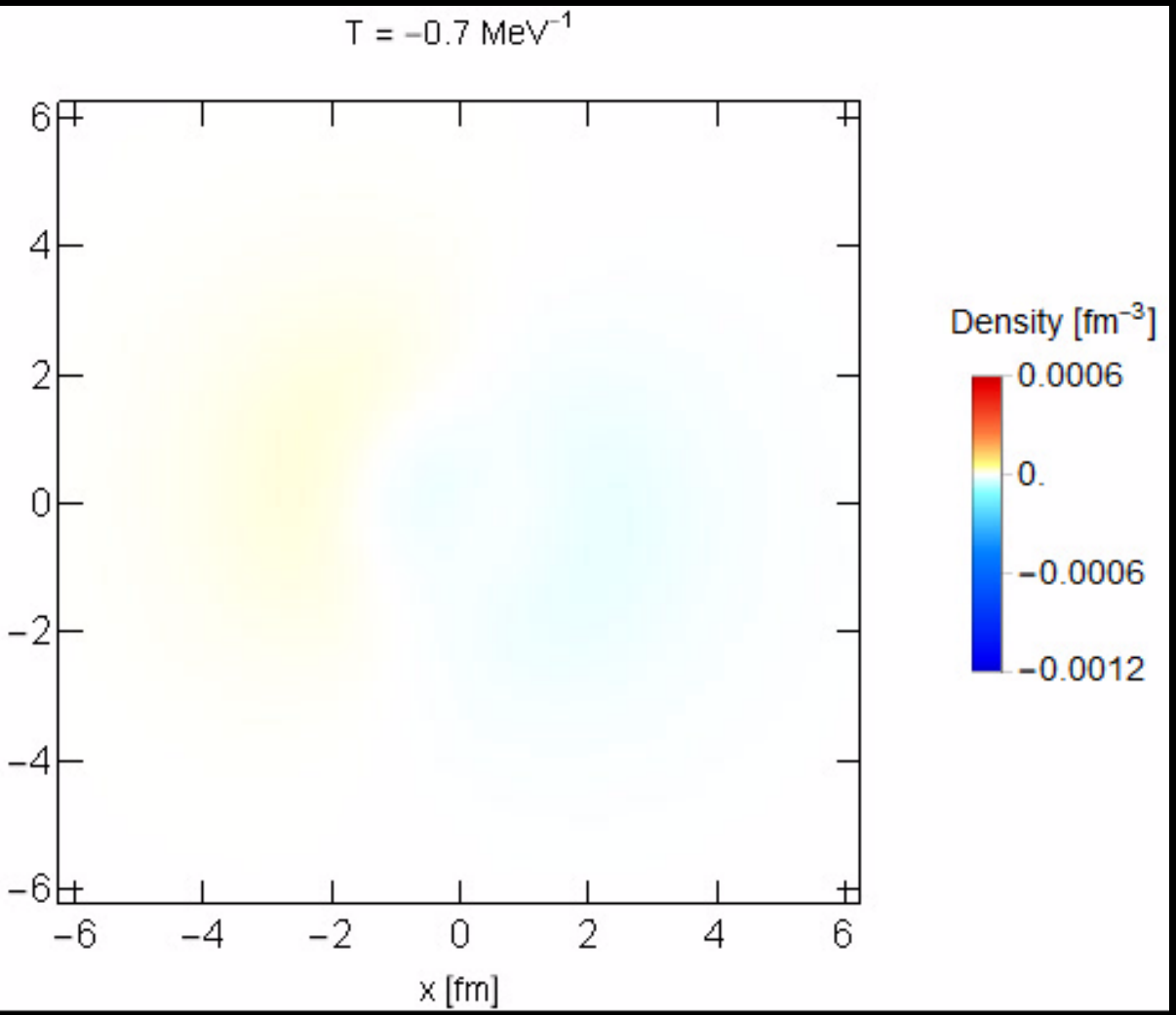
- The difference in charge density distributions between the evolved and the initial np system
- Note the polarization of the charge density distribution

Change in Charge Density Distribution of Scattered np System (x-y plane) at T= 1.975 MeV^{-1}



- Density fluctuation
- Excitation of orbita angular momentun

Dynamics Revealed by Animation (x-y Plane)

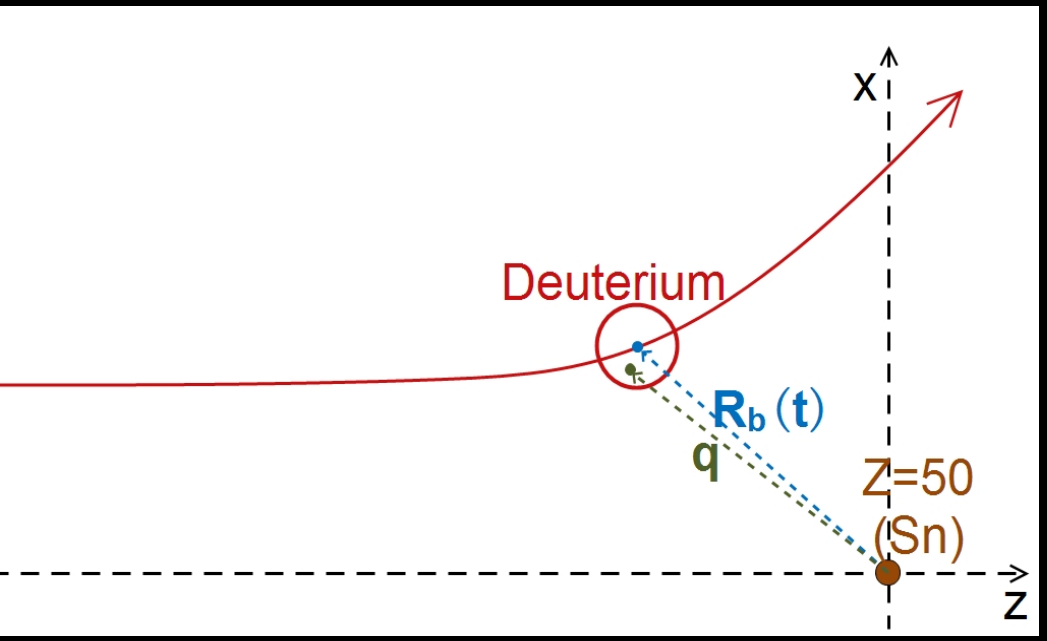


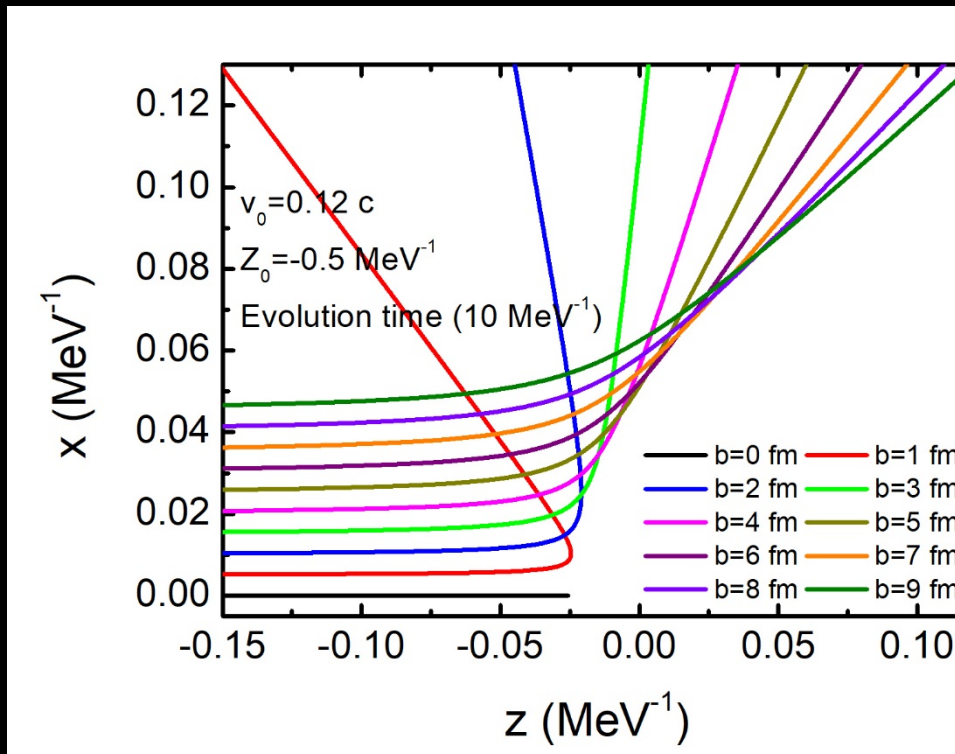
How to interpret?

- The polarization of charg distribution when HI approaches
- The excitation of rotatio degree of freedom
- The excitation of oscillational degree of freedom

Recent Progress
Peng Yin, et al., in preparation

Implement Rutherford Trajectories





$$\frac{d^2\vec{R}}{dt^2} = F_C(R) = Ze^2\frac{\vec{R}}{R^3}$$

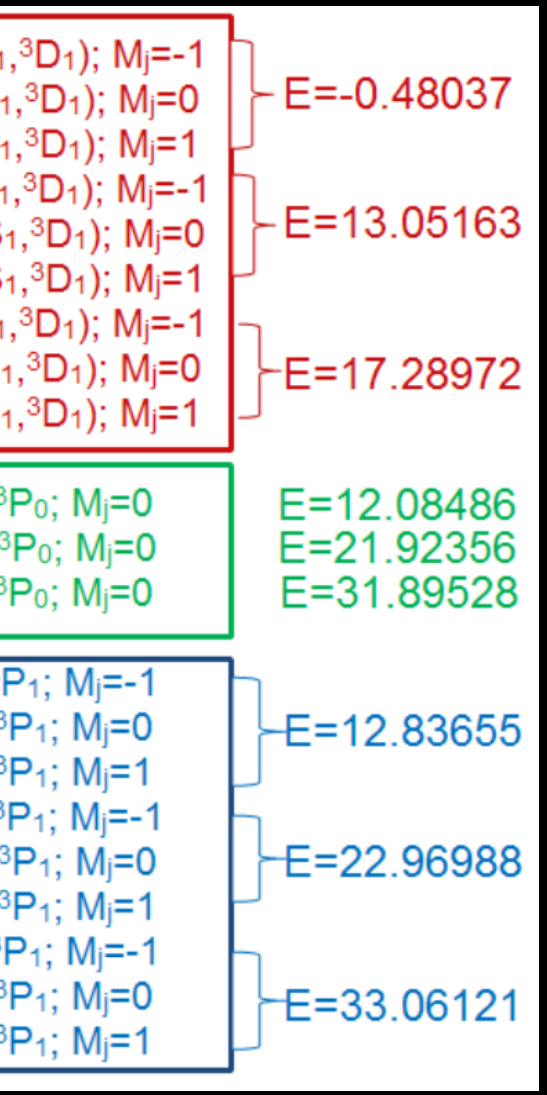
quation of Motion

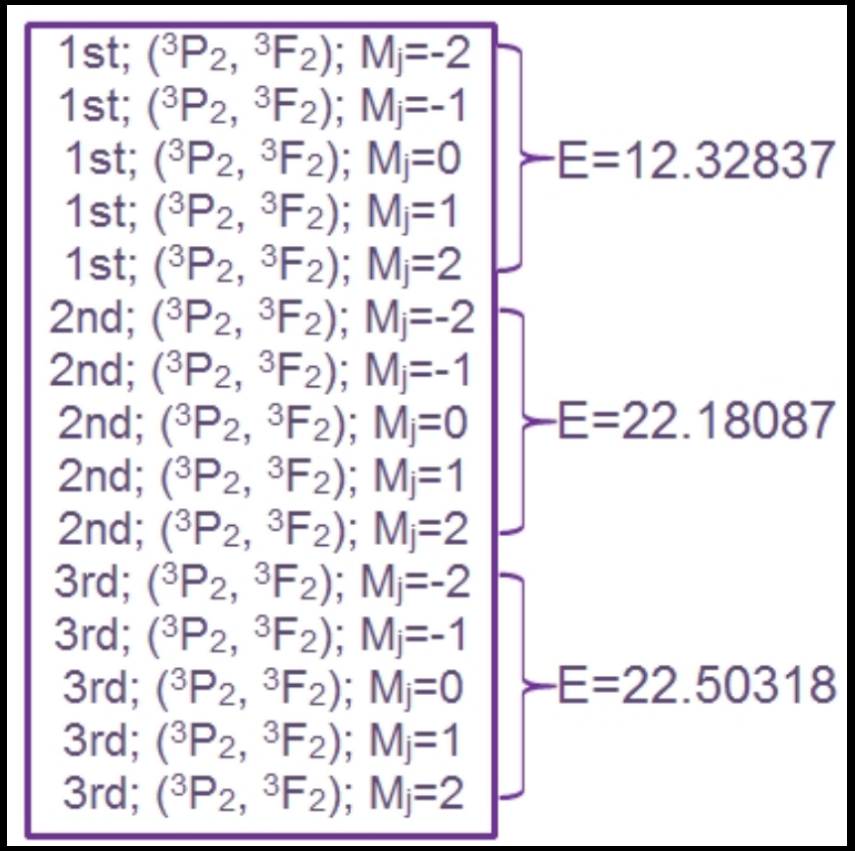
$$\vec{v}(t=0) = \vec{v}_0;$$

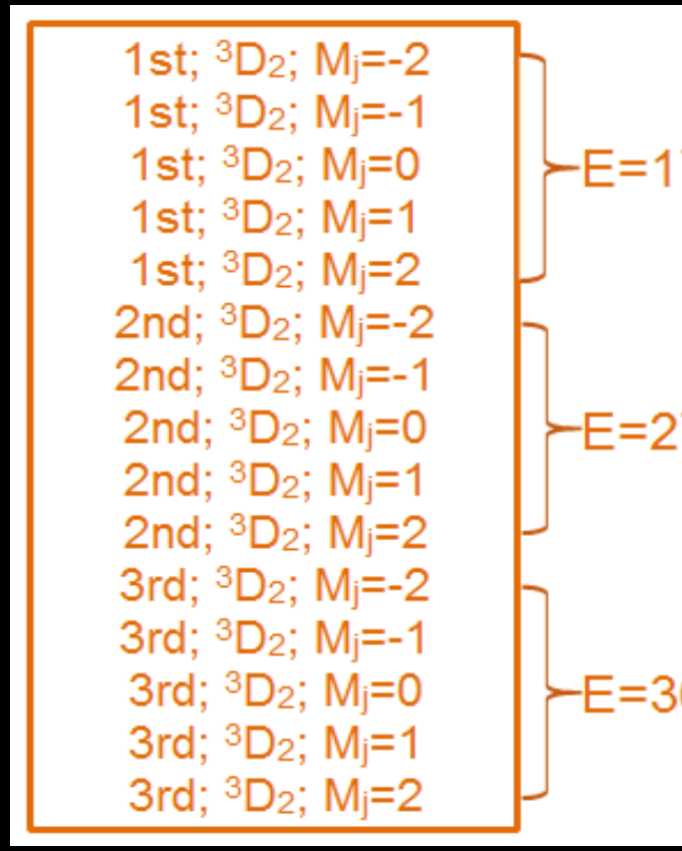
$$(x(t=0), z(t=0)) = (b, z_0)$$

Initial Condition

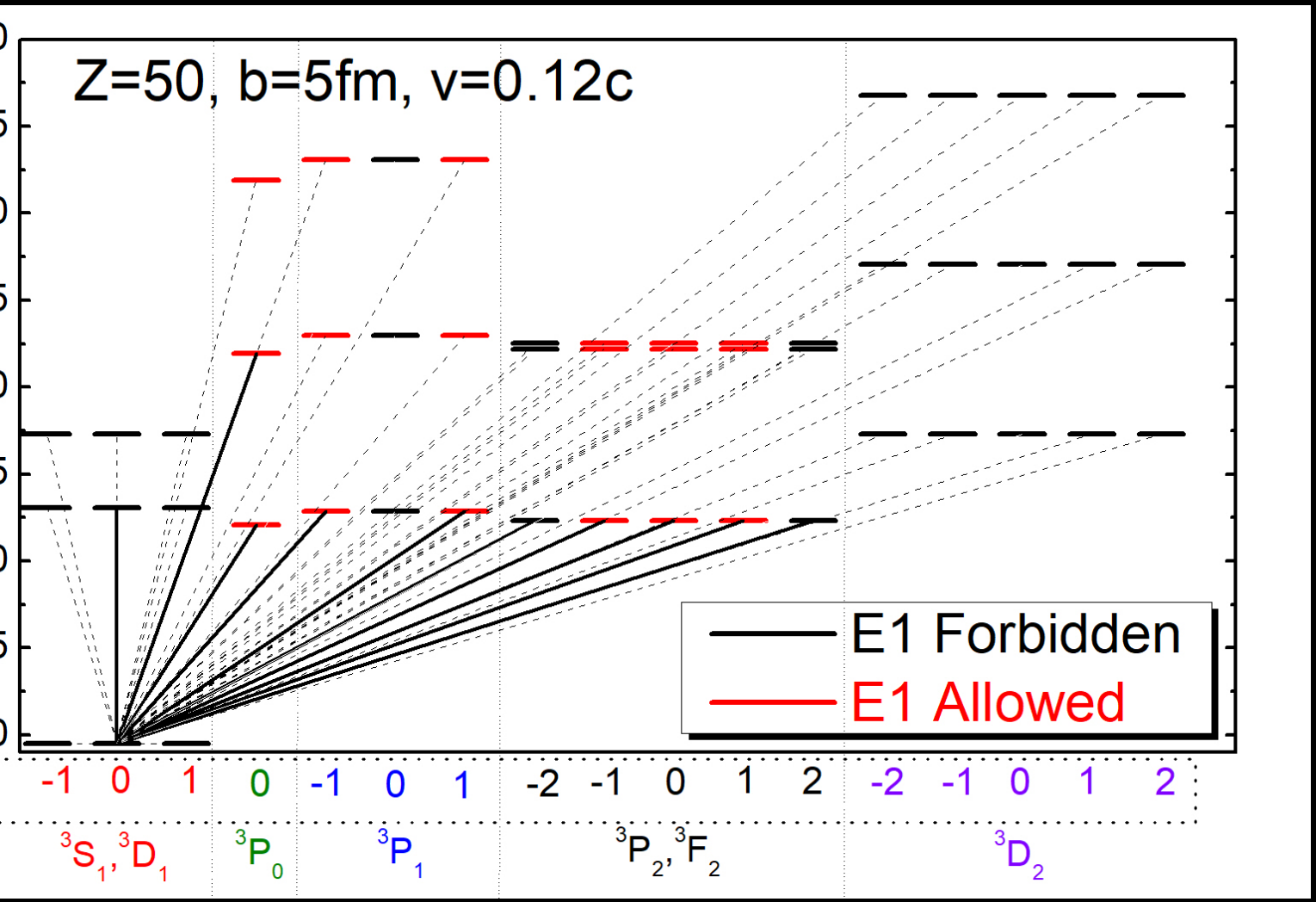
51 States Implementing Daejeon16 *NN*-interaction





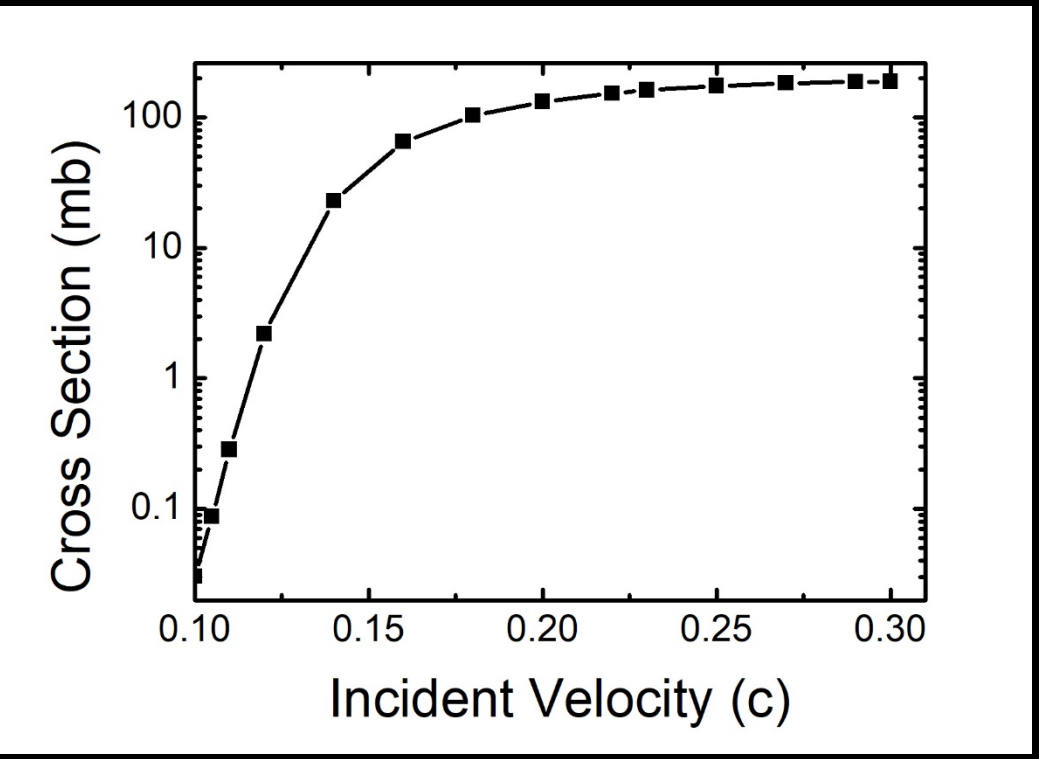


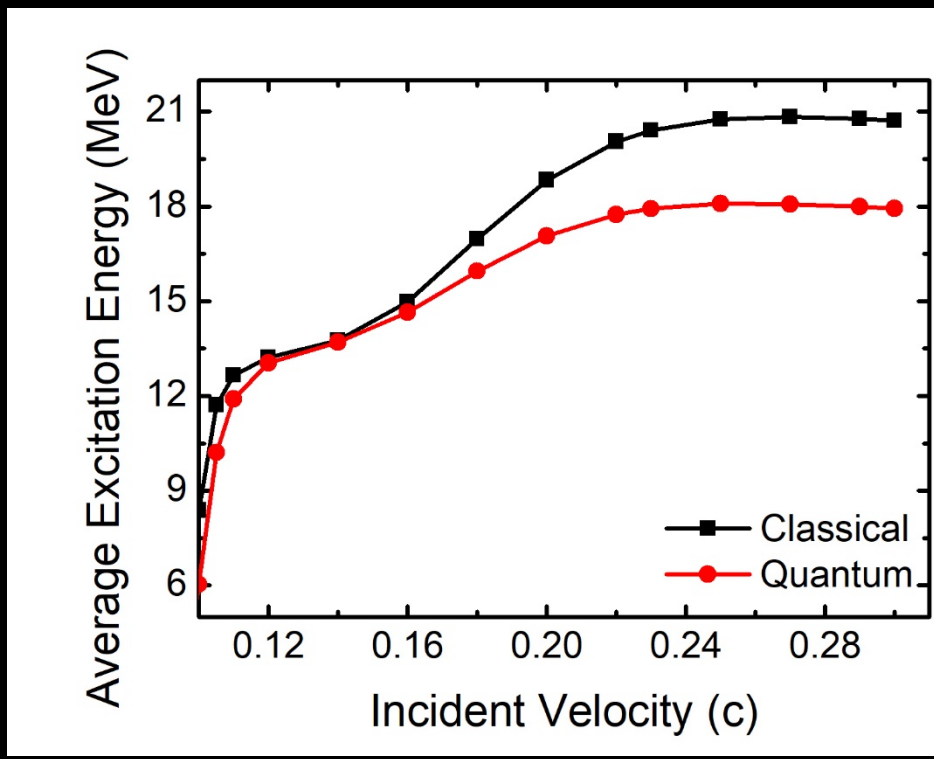
Population in 51 States After Scattering



- Rutherford Scat
- First Order Perturbation th vs. MSD2

astic Cross Section and Average Excitation Ene





ss section and average excitation energy increases with incident veloc
h cross section and average excitation energy reach saturation at
ficiently high incident velocity

Summary

Time-dependent Basis Function (tBF) is motivated by progress both in experimental nuclear physics and in supercomputing techniques

tBF is a non-perturbative *ab initio* method for time-dependent problem

tBF is particularly suitable for strong, time-dependent, field problems

tBF evaluates at the amplitude level - full quantal coherence is retained

tBF is aimed to provide insights into fundamental structure/reaction issues in a detailed and differentiated manner for nuclear reactions

Outlook

Observables: differential cross sections with polarization, inclusive non-line inelastic response, contributions of 2-body currents, higher-order electromagnetic couplings, . . .

Perform calculation in larger basis space and study convergence with respec to density of states in the continuum

Study the sensitivity with respect to the nuclear Hamiltonian

Include strong force in the background field

More realistic center of mass motion

- Trajectory from QMD
- Direct computation of relative motion of the two nuclei (e.g. RGM)

Extend investigations on constraints for the symmetry energy from scatterin

Announcement

New faculty position in Nuclear Theory at Iowa State University with

support from the DOE Fundamental Interactions Topical Collaboration

Daejeon, South Korea
October 29 – November 2, 2018

https://indico.ibs.re.kr/event/216/

Thank you!