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Constrained Fermionic Dynamics of Nuclear Systems: Near Ground State Properties & the Isospin Symmetry

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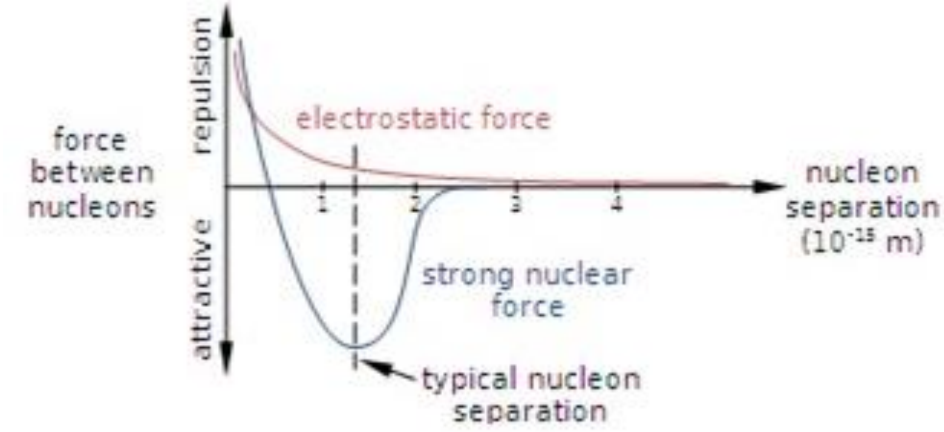
Content Overview

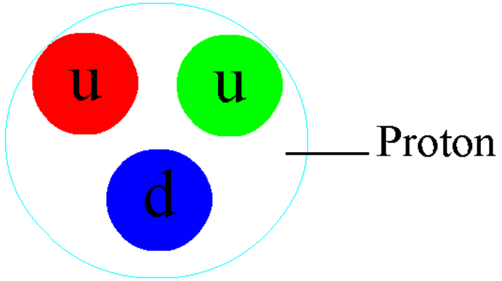
- PART I: CoMD & Initial Configurations
- PART II: CoMD & GDR
- PART III: CoMD & Isospin Symmetry

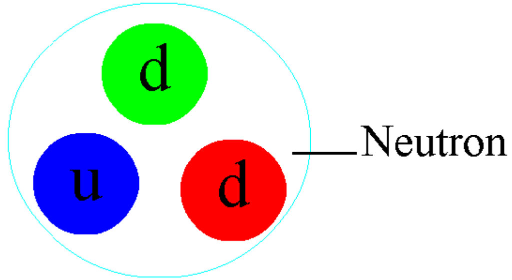
PART I: “CoMD and Initial Configurations”

The Nuclear N-Body Problem

- Nuclear Interaction → Fascinating, complicated and still unknown
- Results from the strong nuclear force between quarks & gluons of the nucleons
- Can be described by the exchange of pions or phenomenological
- Includes: central terms, spin-dependence, spin-orbit coupling, tensor terms, momentum and iso-spin dependence







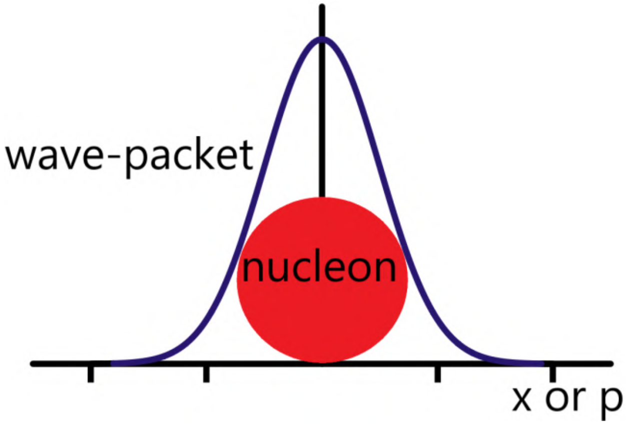
Constrained Molecular Dynamics Approach

- Hamiltonian: Skyrme Potential → Finite Range of interaction as momentum dependence

- Volume, surface, Coulomb, 3-Body and symmetry terms

$$V = V^{vol} + V^{surf} + V^{coul} + V^{sym} + V^{(3)}$$

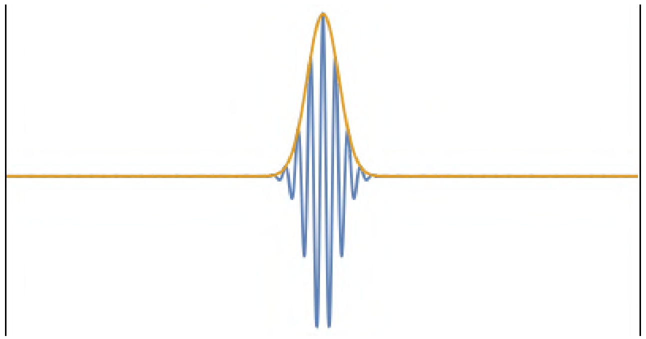
- Trial wavefunctions → parametrised gaussian wave-packets → Time Dependent Variational Principle → Hamiltonian Equations of Motion in Phase Space (Wigner Representation)



$$\frac{d}{dt}\langle\vec{p}_i\rangle = -\frac{\partial H}{\partial\langle\vec{r}_i\rangle}$$

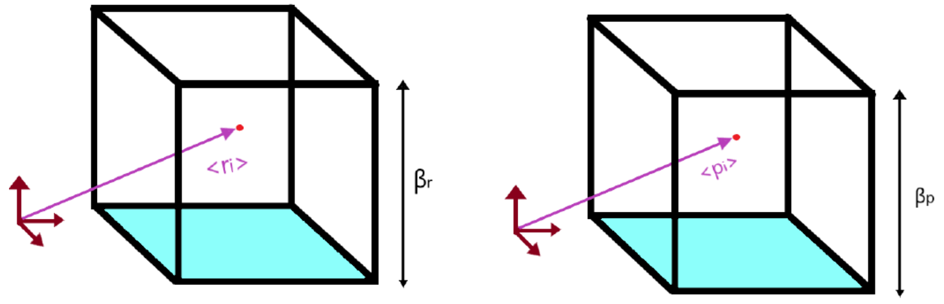
$$\frac{d}{dt}\langle\vec{r}_i\rangle = \frac{\partial H}{\partial\langle\vec{p}_i\rangle}$$

In CoMD σ_r and σ_p are constant!



Constrained Molecular Dynamics Approach

- Pauli Antisymmetrisation Principle → Constrain of the Phase Space occupation fractions (= probabilities) → Pauli Correlation strength as free parameter *paulm*

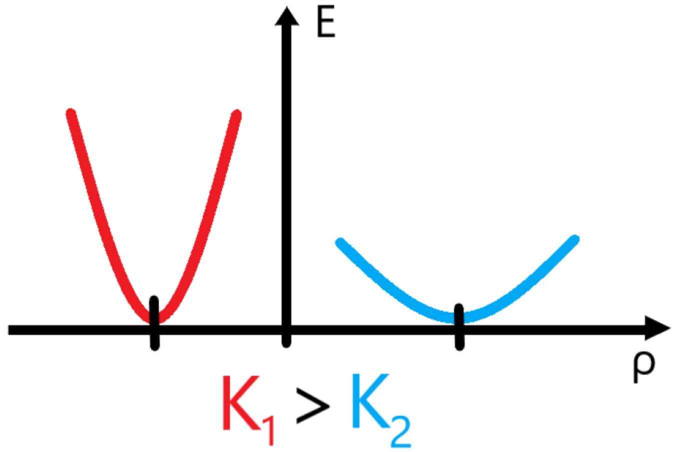


$$\bar{f}_i \leq \frac{paulm}{128}, \forall i$$

- Compressibility: The nuclear "compression susceptibility" parameter ("hardness of EOS")

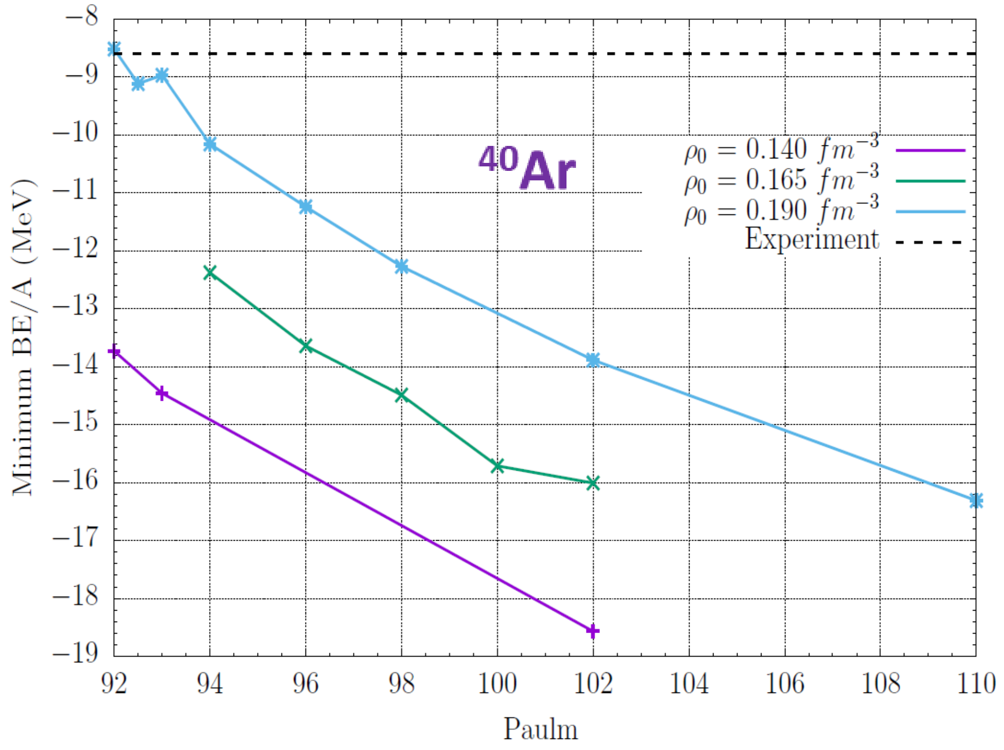
$$K_{NM} \equiv 9{\rho_0}^2 \left[\frac{\partial^2}{\partial \rho^2}\left(\frac{E}{A}\right)\right]_{\rho_0}$$

- Equations of Motion → 1st order differential equations → need initial conditions ! Three step calculation → Initialization, Evolution & Data Processing



Initial Configurations and Ground States

- Statistical Simulated Annealing → Initial Configurations (phase space centroids at t=0)
- Configuration Space → Depends heavily upon initial parameters
- Important parameters:
  - Strength of Pauli Correlations (*paulm*)
  - Wave-packet width (σ_r)
  - Saturation Density (ρ_0)
  - surface parameter ($C_{surface}$)
  - asymmetry parameter (a_{sym})
  - Compressibility (K) .
- Important characteristics: BE/A, neutron skin, rms radii, average density & occupation fraction

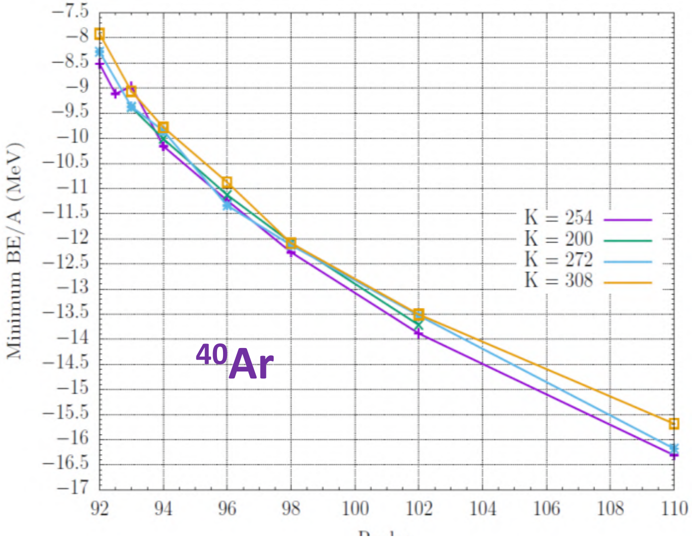


$$\frac{E_{Tot}}{A} = -\frac{BE}{A}$$

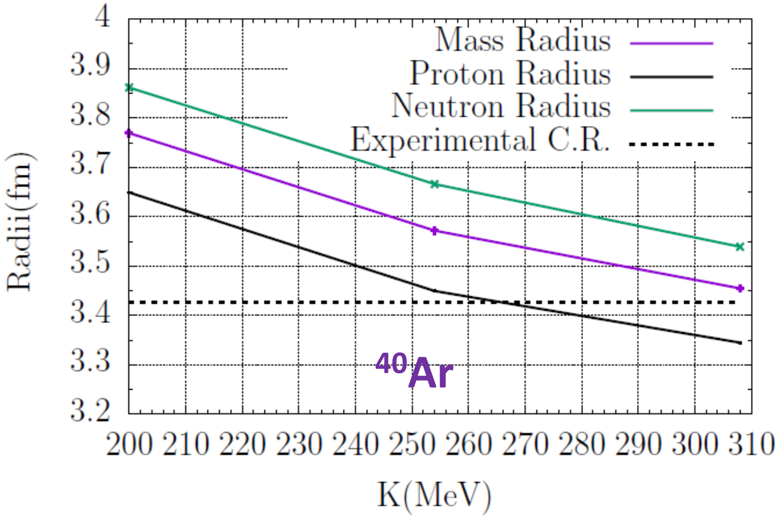
Effect of Important Model Parameters

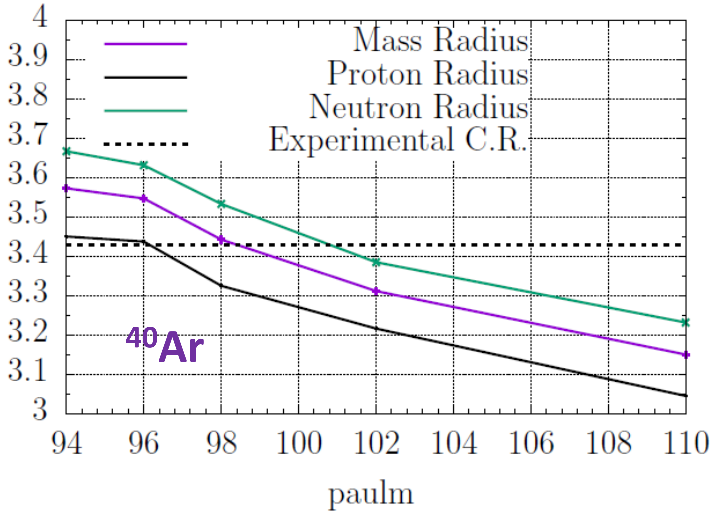
- Increase of K, σ_r, ρ_0 , a_{sym}
- Decrease of *paulm*

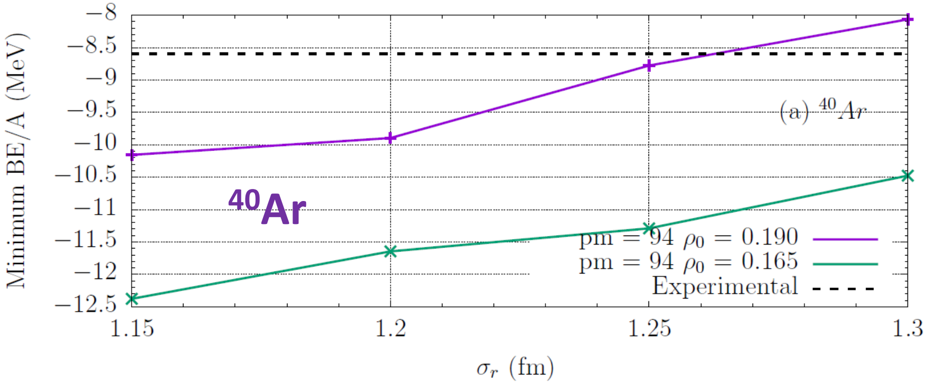
} Absolute Decrease of BE/A !



- Increase of K, *paulm* → Absolute Decrease radii & skin !







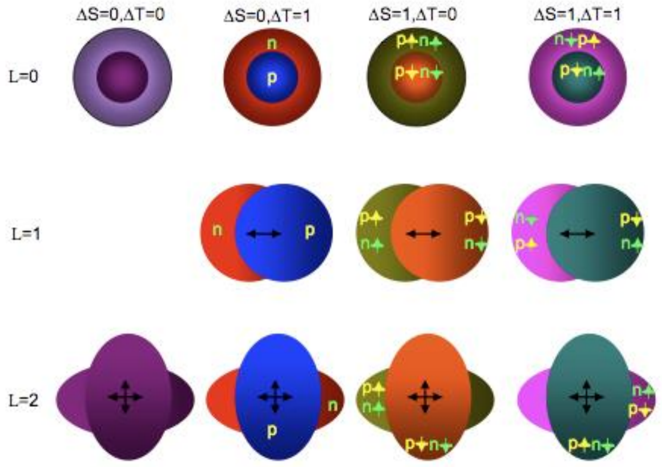
Globally Optimized Configurations

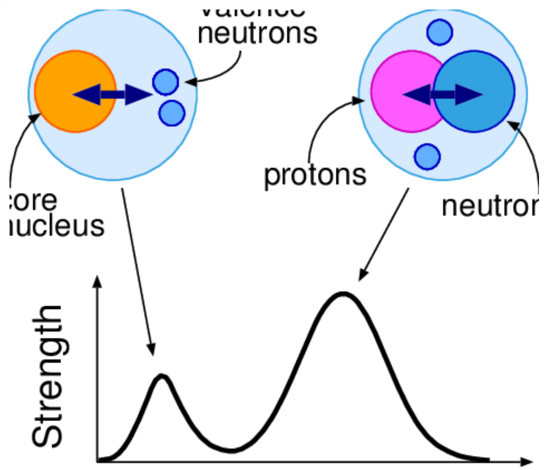
- Configurations are characterized by:
  - Binding Energy
  - Average Occupation Fractions
  - Radius
  - Average Density
- Usually as one characteristic is improved, the others worsen → Effort for Global Optimization !
- Optimization algorithm → Use of Skyrme-Hartree-Fock calculations, experimental data and empirical parametrizations
- Results so far: better over-all configuration and characteristics, more stable giant dipole resonances and reactions !

PART II: “CoMD & IVGDR”

Isovector Giant Dipole Resonance (GDR)

- Low lying excited states → Collective Vibrations! (= modes of rotations and vibrations, like in molecules)
- GDR → oscillation of proton center of mass against neutron center of mass
- Results in fission, peripheral, photonuclear reactions, …
- Give important information for the nuclear interaction and EoS (= function of energy vs density)





GDR in the CoMD Formalism

- Perturbation of the initial configurations → Damped oscillation (i.e. *D(t)*) → Lorentzian Fourier Spectrum
- Spectrum depends upon the parameters of the effective interaction (K, *paulm*, …)
- Width mostly depends on in-medium NN scattering cross-section

$$\sigma_{NN} = a_{redc}\left(T_{cm}, \overline{\rho}\right)\sigma_{free}$$

- Development of a simple model: CoMD based GDR equations of motion

$$\ddot{D} + b\dot{D} + \omega_0^2 D = 0$$

$$b = \frac{\Gamma}{\hbar} \sim \sigma_{NN}$$

$$\omega_0 = \sqrt{\frac{a_{sym}\rho_{np}}{2\rho_0 m\sigma_r^2}\frac{A}{NZ}}$$

$$\omega = \sqrt{\omega_0^2 - \left(\frac{b}{2}\right)^2}$$

$$\rho_{ij} \sim e^{-\frac{\left(\langle\vec{r}_i\rangle - \langle\vec{r}_j\rangle\right)^2}{4\sigma_r^2}}$$

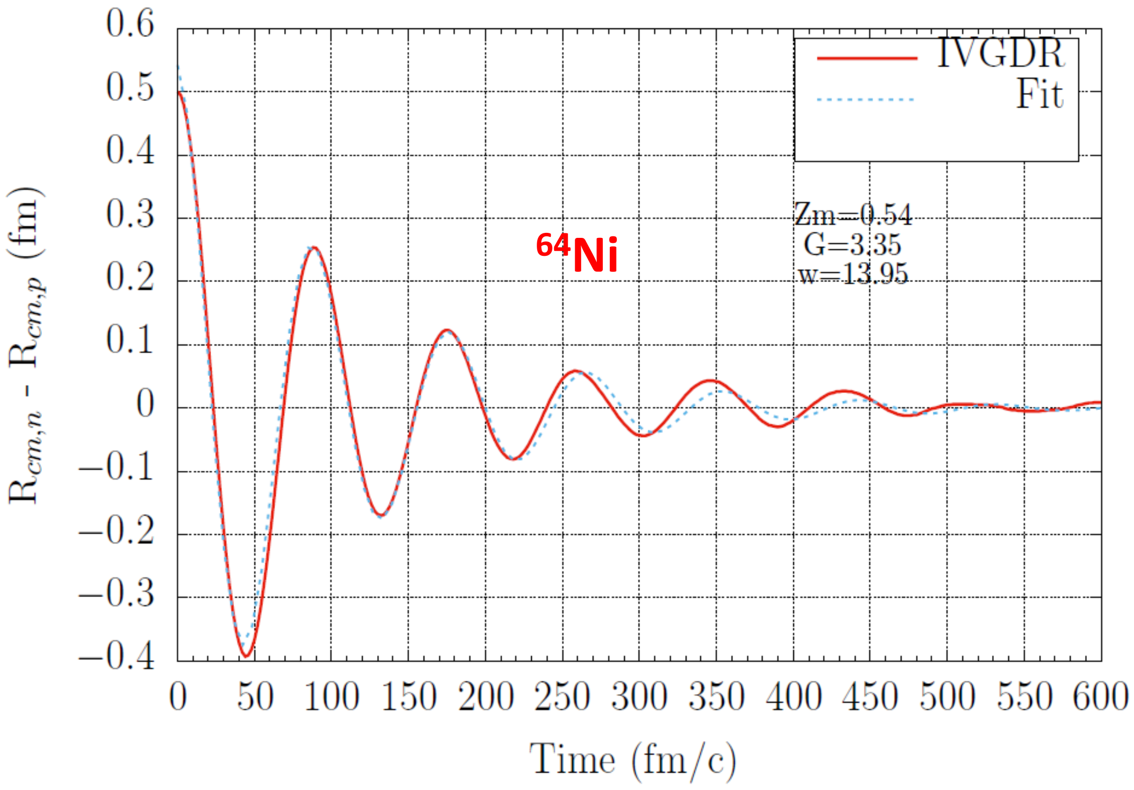
$$\rho_{np} = \sum_{i\to p}\sum_{j\to n}\rho_{ij}$$

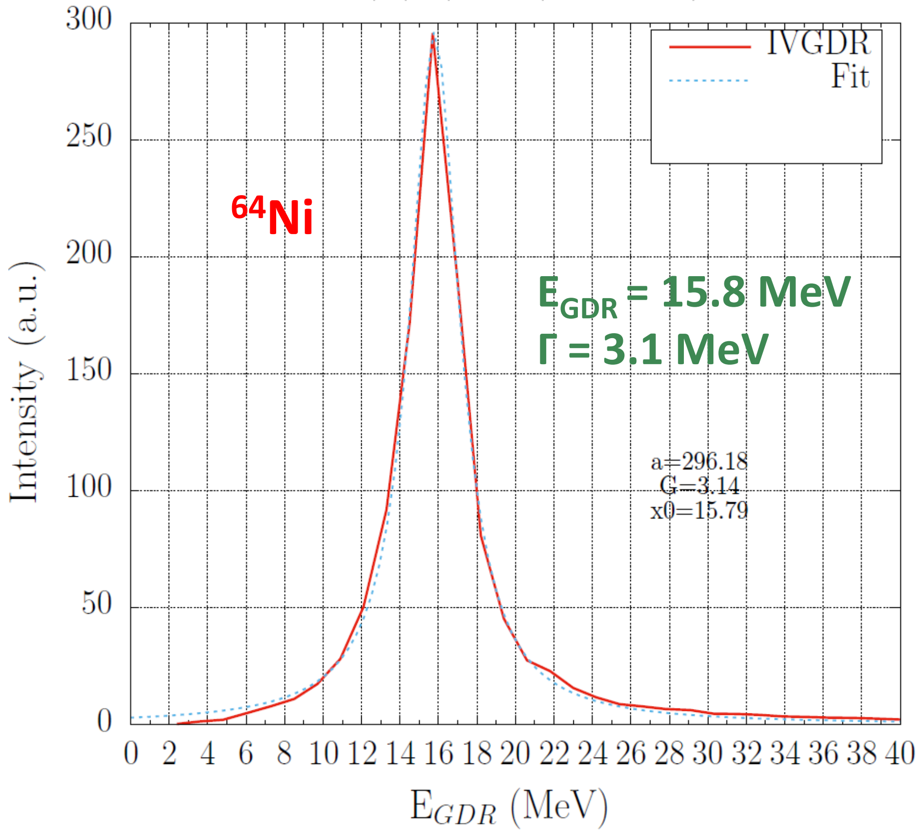
GDR in the CoMD Formalism

$$D(t) = D_0 e^{bt/2} \cos \omega t$$

$$b = \frac{\Gamma}{\hbar} \sim \sigma_{NN}$$

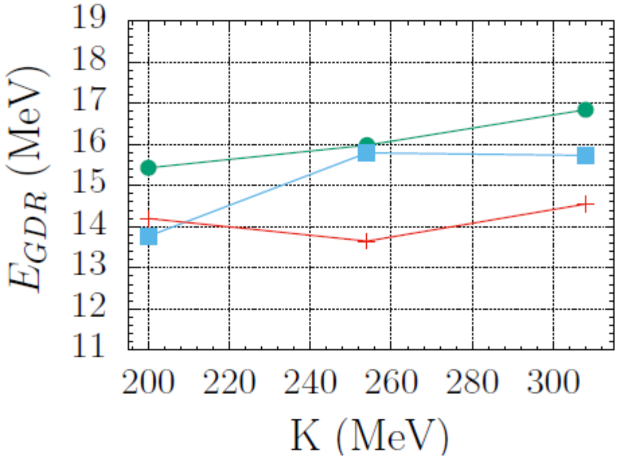
$$I = \frac{(\Gamma/2)\, D_0 \hbar}{(\Gamma/2)^2 + (E - E_D)^2}$$



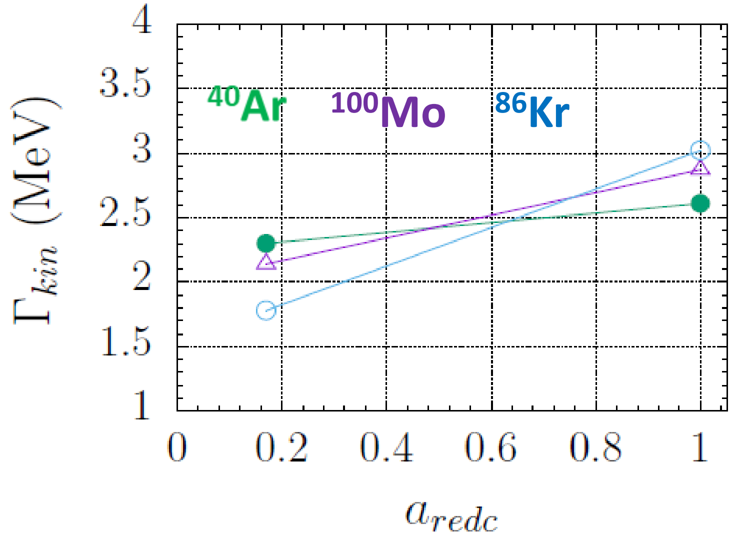


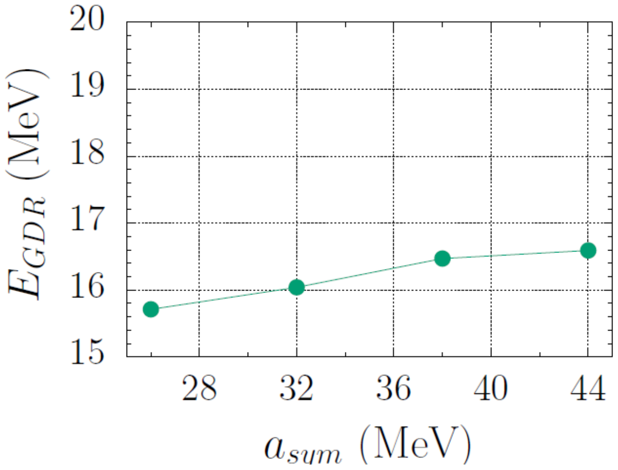
Effect of Model Parameters

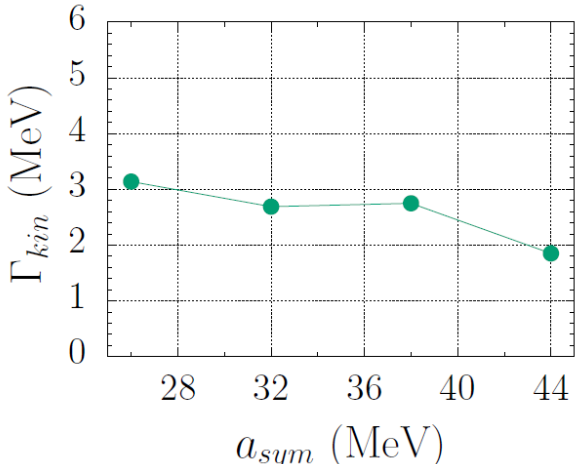
- Increase of K, a_{sym} ⟶ Increase of E_{GDR} !
- Increase of NN cross section → Increase of Γ !



^{40}Ar







Effective Mass and Momentum Dependence

- Finite Range of interaction → Momentum dependence
- Skyrme-like Potential of CoMD → Contact force
- Gaussian ansatz of momentum dependent term:

$$V^i_{mom} = Ae^{-c\langle\overrightarrow{p_i}\rangle^2}$$

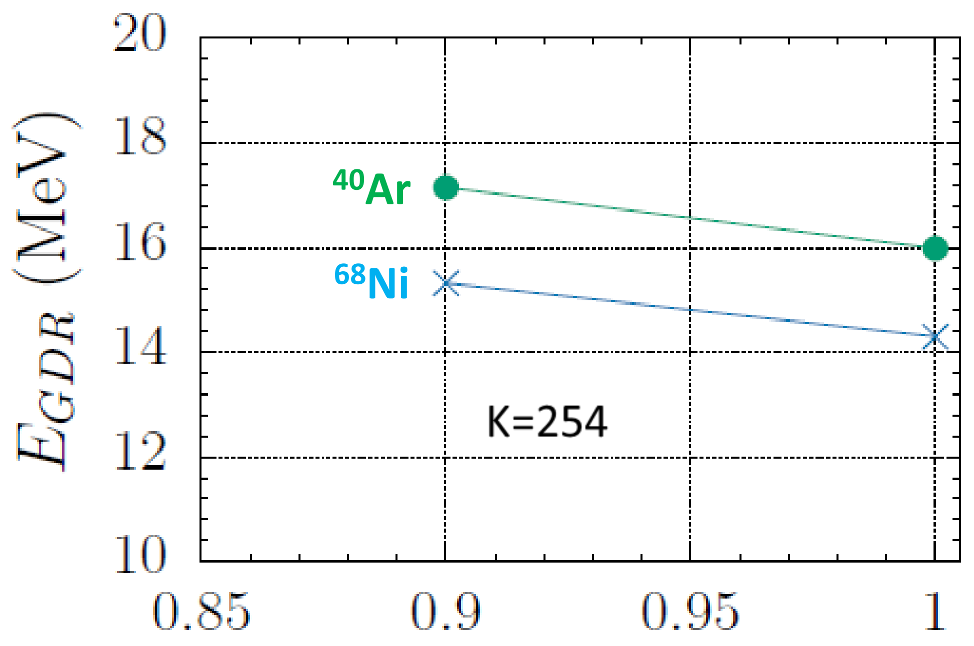
- Low energy limit → p^2 dependence → "Effective mass"

$$V^i_{mom} \approx A\left(1 - c\langle\overrightarrow{p_i}\rangle^2\right) \longrightarrow T^i = \frac{\langle\overrightarrow{p_i}\rangle^2}{2m}(1 - cA) \equiv \frac{\langle\overrightarrow{p_i}\rangle^2}{2m^*}$$

- Parametrization though free parameter:

$$m^* \equiv f_{mass} \cdot m$$

- Decrease of mass → Increase of E_{GDR}

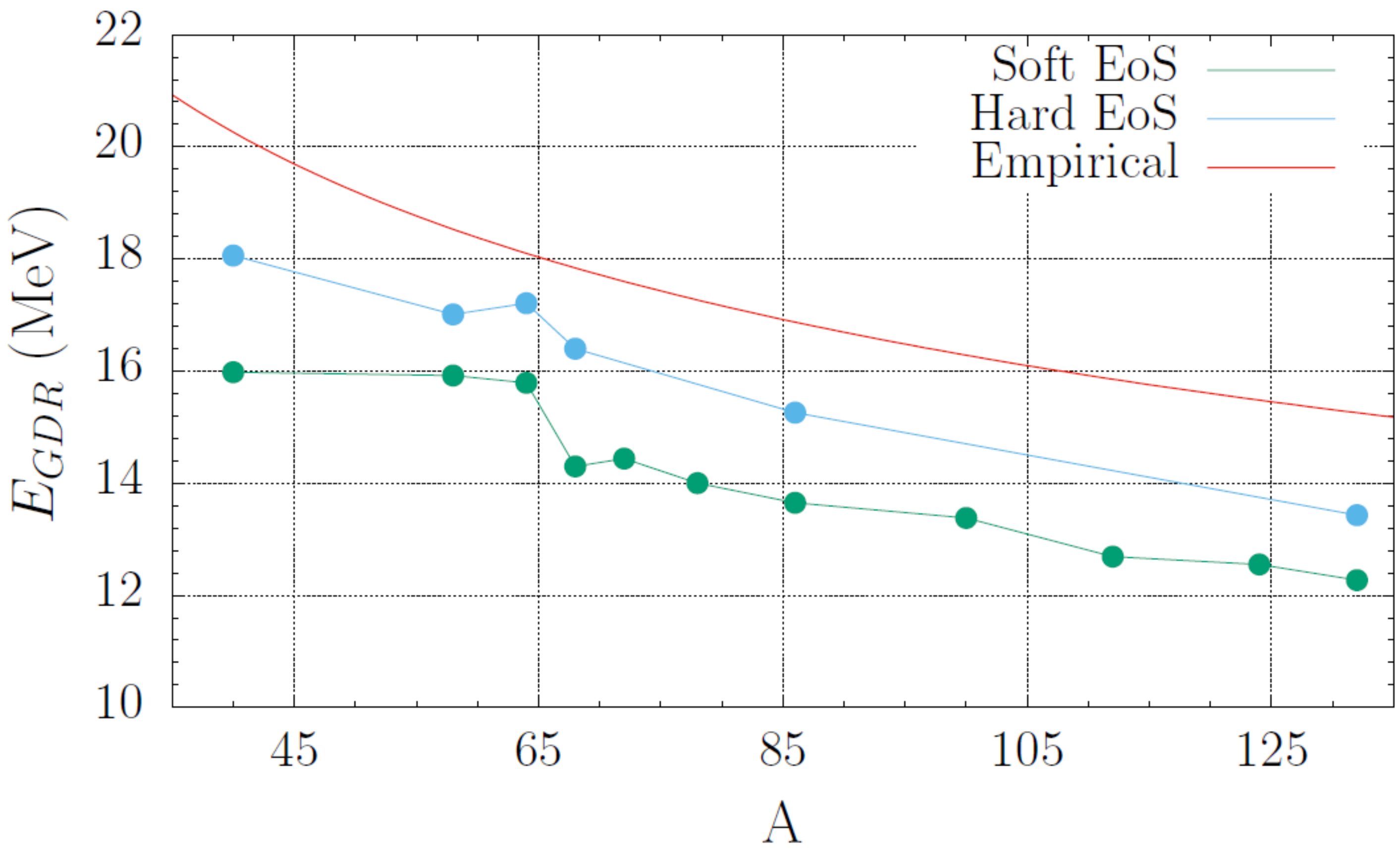


Mass Dependence of GDR & Skin in CoMD

- GDR → Correct dependency upon A

$$E_{GDR} = 31.2A^{-1/3} + 20.6A^{-1/6}$$

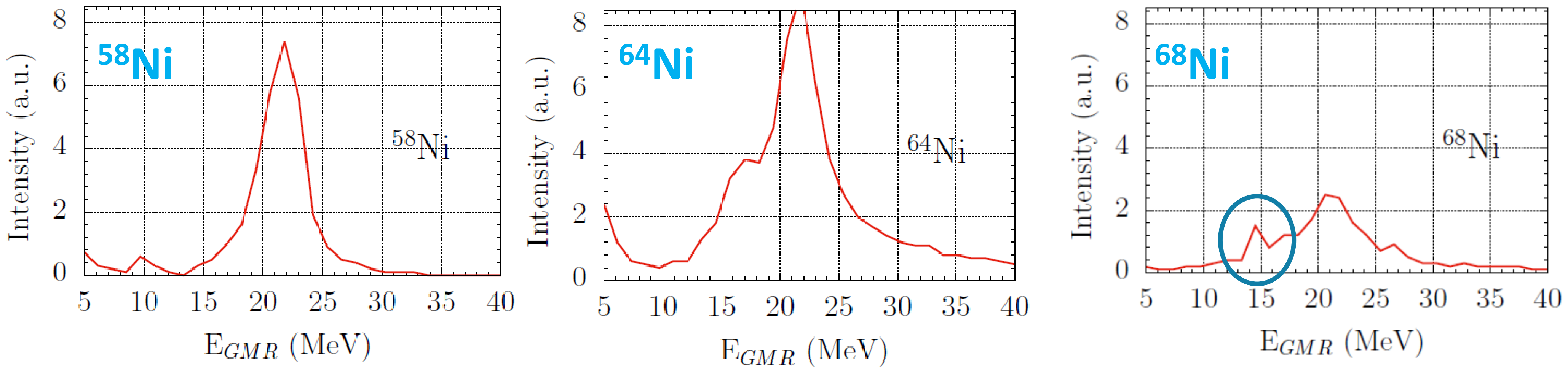
- Soft EOS→K=254, a_{sym}=32 MeV & m*/m=1
- Difference from empirical parameterization by about 3-4 MeV
- Hard EOS→K=308, a_{sym}=38 MeV & m*/m<1
- Difference from empirical parameterization by about 1-2 MeV



G. Giuliani, H. Zheng, A. Bonasera *Prog in Part & Nuc Phys* **76**, pp 116-164 (2014).

Giant Monopole Resonances in CoMD

- Momentum Space Iso-Scalar Perturbation → Temperature
- Fourier Transform of Radius over time → GMR Spectrum !!
- ^{x}Ni (x=58,64,68) → E_{GMR} ~ 22 MeV (experimental 21.1 ± 1.9 MeV)
- Soft monopole for ^{68}Ni → E_{soft} ~ 14.5 MeV (experimental 12.9 ± 1.0 MeV)



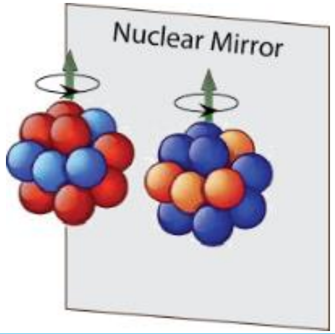
X. Sun, *Phys Rev C*, **103** 044603 (2021)

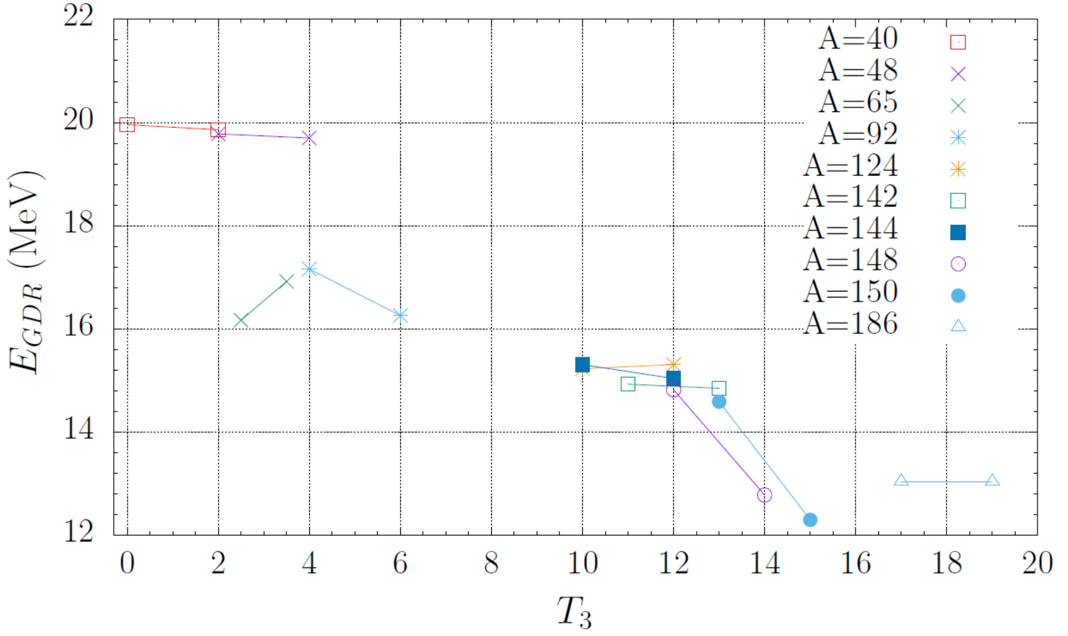
PART III: "CoMD & Isospin Symmetry"

Nuclear Isospin Symmetry

- Masses of proton-neutron almost equal → two states of the same "nucleon particle"
- Isospin quantum number → Identity of the particle → $\tau_n = 1/2$ & $\tau_p = -1/2$ → same algebra as s = 1/2 particles !
- Isospin Mirror Transformation→ exchange of protons and neutrons (i.e. n→p)
- Isospin Symmetry → Approximate Symmetry of the nuclear systems → Breaks due to Coulomb interaction → Isospin Symmetry Breaking (ISB), e.g. E_{GDR}
- Total Coupled Isospin quantum numbers

$$\widehat{T}^2|\Psi\rangle = \tau\,(\tau+1)\,|\Psi\rangle \qquad \widehat{T}_3|\Psi\rangle = \tau_3|\Psi\rangle = \frac{N-Z}{2}|\Psi\rangle$$





V.A. Plujko, O.M. Gorbachenko, R. Capote, P. Dimitriou, *At Dat Nuc Dat Tab* **123 & 124**, 1-85 (2018).

Isospin Symmetry of the CoMD

- Ground state → Approximate symmetry → Explicit Symmetry Breaking → Coulomb interaction in CoMD Lagrangian

$$V = V^{vol} + V^{surf} + V^{coul} + V^{sym} + V^{(3)}$$

- Absolute Neutron Skin → Approximately isospin symmetric

$$|skin| = \left| \sqrt{\langle r_n^2 \rangle} - \sqrt{\langle r_p^2 \rangle} \right|$$

$$L = \frac{e^{bt}}{2} \left(\dot{D}^2 - \omega_0^2 D^2 \right)$$

- Extension of GDR theoretical treatment → GDR Lagrangian <u>totally isospin symmetric</u> !

$$\omega_0 = \sqrt{\frac{a_{sym} \rho_{np}}{2 \rho_0 m \sigma_r^2} \frac{A}{NZ}}$$

$$\rho_{ij} \sim e^{-\frac{(\langle \vec{r}_i \rangle - \langle \vec{r}_j \rangle)^2}{4\sigma_r^2}}$$

- GDR energy depends on A & τ_3^2

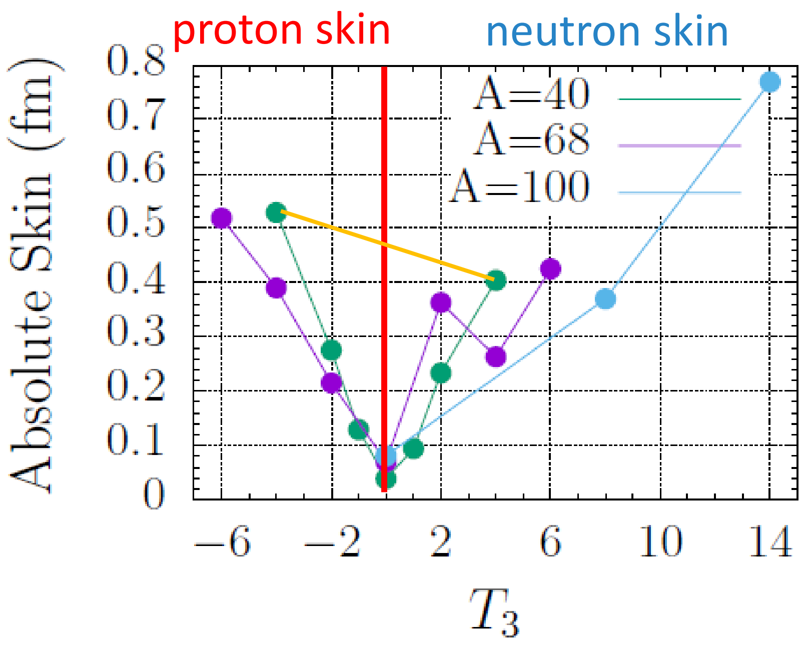
$$\frac{A}{NZ} = \frac{A}{4} - \frac{\tau_3^2}{A}$$

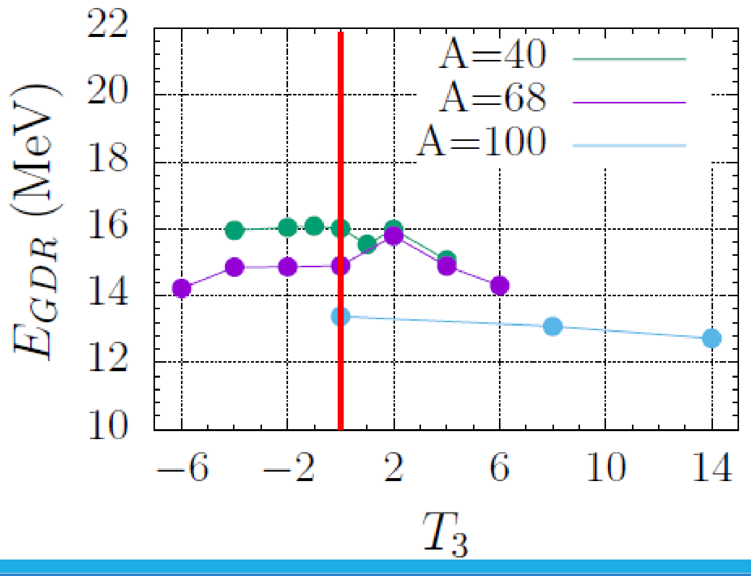
$$\rho_{np} = \sum_{i \to p} \sum_{j \to n} \rho_{ij}$$

Isospin Symmetric !!

Isospin-T_3 Symmetry Behavior of the CoMD

- Absolute Skin → Symmetric "well" near N=Z line → Explicit Symmetry Breaking
- GDR :
  - Explicit mass dependence around N=Z
  - $T_3>0$ → Descending Trend





$$T_3 = \frac{N - Z}{2}$$

Summary & Conclusions

- Extensive use of the CoMD description of the nuclear N-body problem & dynamics
- Algorithm for selection of optimum configurations → better overall results in calculations
- Higher K, wave-packet width & Lower *paulm,* saturation density → Higher Total E/A (Less bound nucleus)
- Higher K, symmetry energy parameter & Lower *paulm*, effective mass → Higher GDR Energy
- Higher N-N Scattering Cross Section → Greater Width
- Study of Monopole modes for ^{x}Ni, x = 58, 64, 68
- Examined Isospin symmetry behavior in CoMD:
  - Protons slightly larger than neutron skins (mirror pairs)
  - Lower of E_{GDR} with increasing T_3
- Further Investigations are on going
- Future Goals: Use of K=308, Explicit Momentum Dependence & Development of E_{GDR} parameterization f(A,Z).

I WOULD LIKE TO THANK DR. G. SOULIOTIS FOR HIS GUIDANCE AND SUPPORT AND THE OTHER MEMBERS OF THE GROUP AND YOU FOR YOUR ATTENTION !