

Exploring universality with a many-body density functional

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and



In collaboration with

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Motivations

- Exploring systems from “**few**-body” to “**many**-body” within a unified picture
consider a very powerful approach: Energy Density Functional
- However, maintain translation/Galileian invariances
- here is a problem... but we will see how to overcome it
- Study systems that are close to the unitary limit and are suited for effective expansion of the interaction
we will see an example at the end

Summary

- Fast recall of Density Functional Theory (DFT) and Kohn-Sham (KS) equation
(systems of interacting particles placed in an external one-body potential)
- Self bound systems and Hyperspherical Coordinates
(interacting particles, no external one-body potential)
- Different formulation of DFT and KS equation
(the many-body hyperradial density)
- Application to bosons close to the unitary limit
(^4He atom clusters)

1: Fast recall of Density Functional Theory (DFT) and Kohn-Sham (KS) equation

(systems of interacting particles placed in an external one-body potential)

The EDF approach in a couple of slides:

P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964)

$$1) E(\mathbf{n}) \geq E_{\text{gs}} \quad 2) E(\mathbf{n}_{\text{gs}}) = E_{\text{gs}}$$

We have an Hamiltonian of interacting particles subject to an **external potential**

$$H = \sum_i^N \frac{p_i^2}{2m} + \sum_{i<j}^N V(\vec{r}_i - \vec{r}_j) + \sum_i^N v_{ext}(\vec{r}_i) \equiv \mathbf{T} + \mathbf{V} + \mathbf{v}_{ext}^{[1]}$$

$$E_{gs} = \langle \Psi_{gs} | \mathbf{T} + \mathbf{V} + \mathbf{v}_{ext}^{[1]} | \Psi_{gs} \rangle$$

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$\mathbf{n} \equiv \mathbf{n}(\vec{r})$ is the **one-body density**, namely the mean value of the one-body density operator $\sum_{i=1}^N \delta(\vec{r} - \vec{r}_i)$ on some N-body wave function

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$$\mathbf{n}(\vec{r}) = \frac{1}{N} \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_N \Psi^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \sum_{i=1}^N \delta(\vec{r} - \vec{r}_i) \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

And what is $E(\mathbf{n})$? It is a particular functional of the one-body density defined as

$$E[\mathbf{n}] = \langle \Psi^{\mathbf{n}} | T + V | \Psi^{\mathbf{n}} \rangle + \int d\vec{r} v_{\text{ext}}(\vec{r}) n^{[1]}(\vec{r})$$

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$$\langle \Psi^{\mathbf{n}} | T + V | \Psi^{\mathbf{n}} \rangle \equiv \min_{\Psi \rightarrow \mathbf{n}} \langle \Psi | T + V | \Psi \rangle \equiv F(\mathbf{n})$$

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2) $E(\mathbf{n}_{gs}) = E_{gs}$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r} v_{ext}(\vec{r}) n_{gs}^{[1]}(\vec{r}) \geq E_{gs} \text{ because of 1)}$$

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therefore $E_{gs} \geq F(\mathbf{n}_{gs}) + \int d\vec{r} v_{ext}(\vec{r}) n_{gs}^{[1]}(\vec{r})$



Equal!

The practical use of the theorem goes via the Kohn-Sham equation Phys. Rev. 140, A1133 (1965)

The **Kohn-Sham equation** is the Schroedinger equation of a **fictitious** system (the "Kohn-Sham system") of **independent** particles that generates the **same $n_{gs}(\mathbf{r})$** as any given system of **interacting** particles.

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Assuming the **W-representability** of $\mathbf{E}(\mathbf{n})$, namely

$$\mathbf{E}^{\text{W}}(\mathbf{n}) = \mathbf{E}(\mathbf{n})$$

→ solving the one-body **Kohn-Sham equation**

$$\left(-\frac{\nabla^2}{2m} + W_{KS}(\vec{r}) \right) \psi_i(\vec{r}) = \epsilon_i \psi_i(\vec{r})$$

$$\mathbf{E}^{\text{W}}(\mathbf{n}_{\text{gs}}) = \mathbf{E}(\mathbf{n}_{\text{gs}}) = \mathbf{E}_{\text{gs}}$$

By *reductio ad absurdum* one can show that

W_{KS} is unique!

But what is this one-body potential W_{KS} ???

At $n=n_{gs}$ E_{gs} is the minimum of $E(n)$ namely

$$dE^V(n)/dn = 0 \implies dT^{n,V}/dn + dV^n/dn + v_{ext}(r) = 0$$

$$dE^W(n)/dn = 0 \implies dT^{n,W}/dn + W(r) = 0$$

=

At $n=n_{gs}$ E_{gs} is the minimum of $E(n)$ namely

$$dE^V(n)/dn = 0 \implies dT^{n,W}/dn + dT^{n,V}/dn - dT^{n,W}/dn + dV^n/dn + v_{ext}(r) = 0$$

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$$dE^W(n)/dn = 0 \implies dT^{n,W}/dn + \boxed{W(r)} = 0$$

Formally:

$$W(r) = dT^{n,V}/dn - dT^{n,W}/dn + dV^n/dn + v_{\text{ext}}(r)$$

As to $V^n(\mathbf{n})$:

$$V(\mathbf{n}) \simeq U_H(\mathbf{n}) + V_{\text{exc}}(\mathbf{n}) + V_{\text{corr}}(\mathbf{n})$$

???

Moreover

$$dT^{n,V}/dn - dT^{n,W}/dn$$

???

The **KS** Hamiltonian is **not** translation/Galileian invariant
(as is not the original Hamiltonian that contains an external field)

So, what to do for self bound systems ??

2: Self bound systems and Hyperspherical Coordinates

*(interacting particles, **no** external one-body potential)*

For self-bound systems one requires
Translation / Galileian invariance

$$[H, \mathbf{P}_{\text{CM}}] = 0 \quad / \quad [H, \mathbf{R}_{\text{CM}}] = 0$$

$$H = \sum_i^N \frac{p_i^2}{2m} + \sum_{i < j}^N V(\vec{r}_i - \vec{r}_j) + \sum_i^N \cancel{V_{\text{ext}}(\vec{r}_i)} \equiv \mathbf{T} + \mathbf{V} + \cancel{V_{\text{ext}}}$$

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$$H = \frac{P_{CM}^2}{2Nm} + \frac{1}{2Nm} \sum_{i<j=1}^N |\vec{p}_i - \vec{p}_j|^2 + \sum_{i<j}^N V(\vec{r}_i - \vec{r}_j)$$

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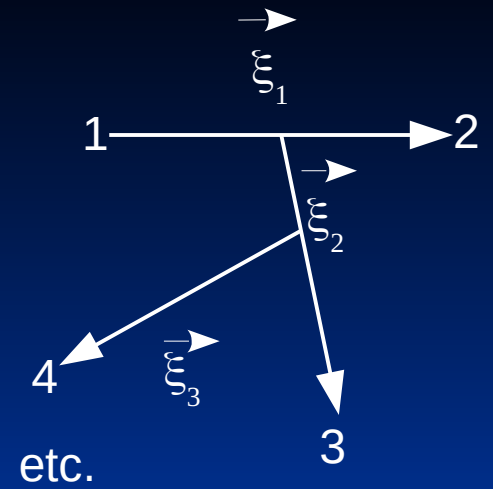
Invariant H_{inv}

Having eliminated the CM coordinate we need a set of N-1 vectors i.e. 3N-3 independent coordinates:

Jacobi coordinates

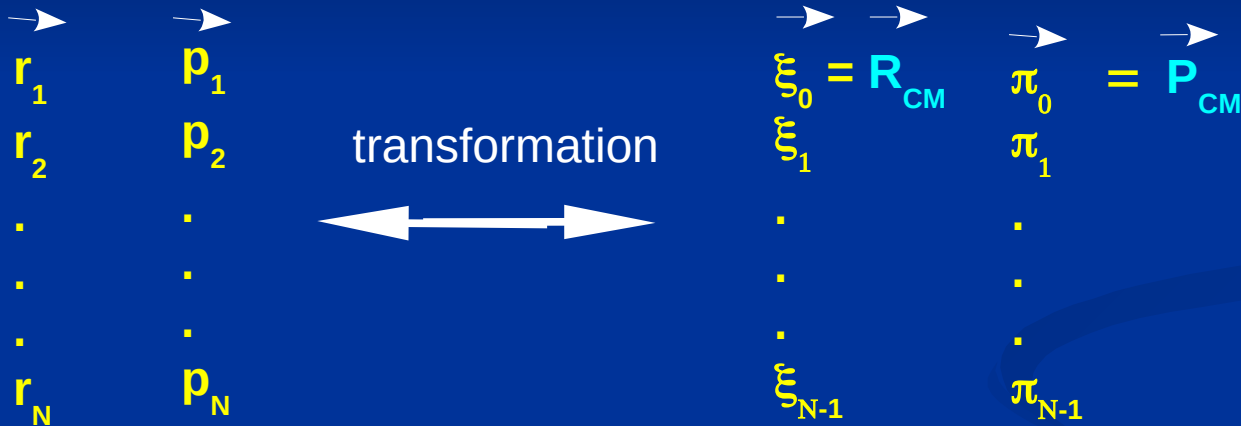
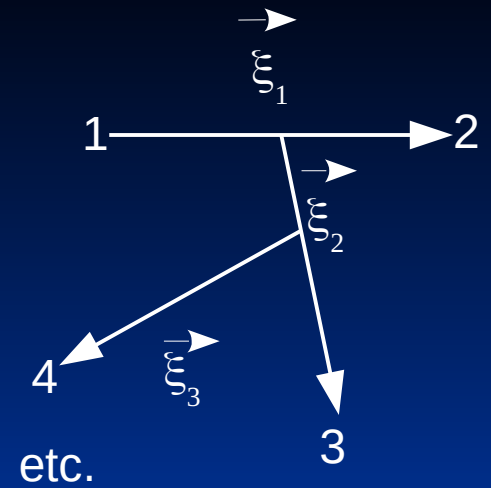
Jacobi coordinates

ξ_i = distances between each particle “ i ” and the cm of the previous $(N - i)$ particles



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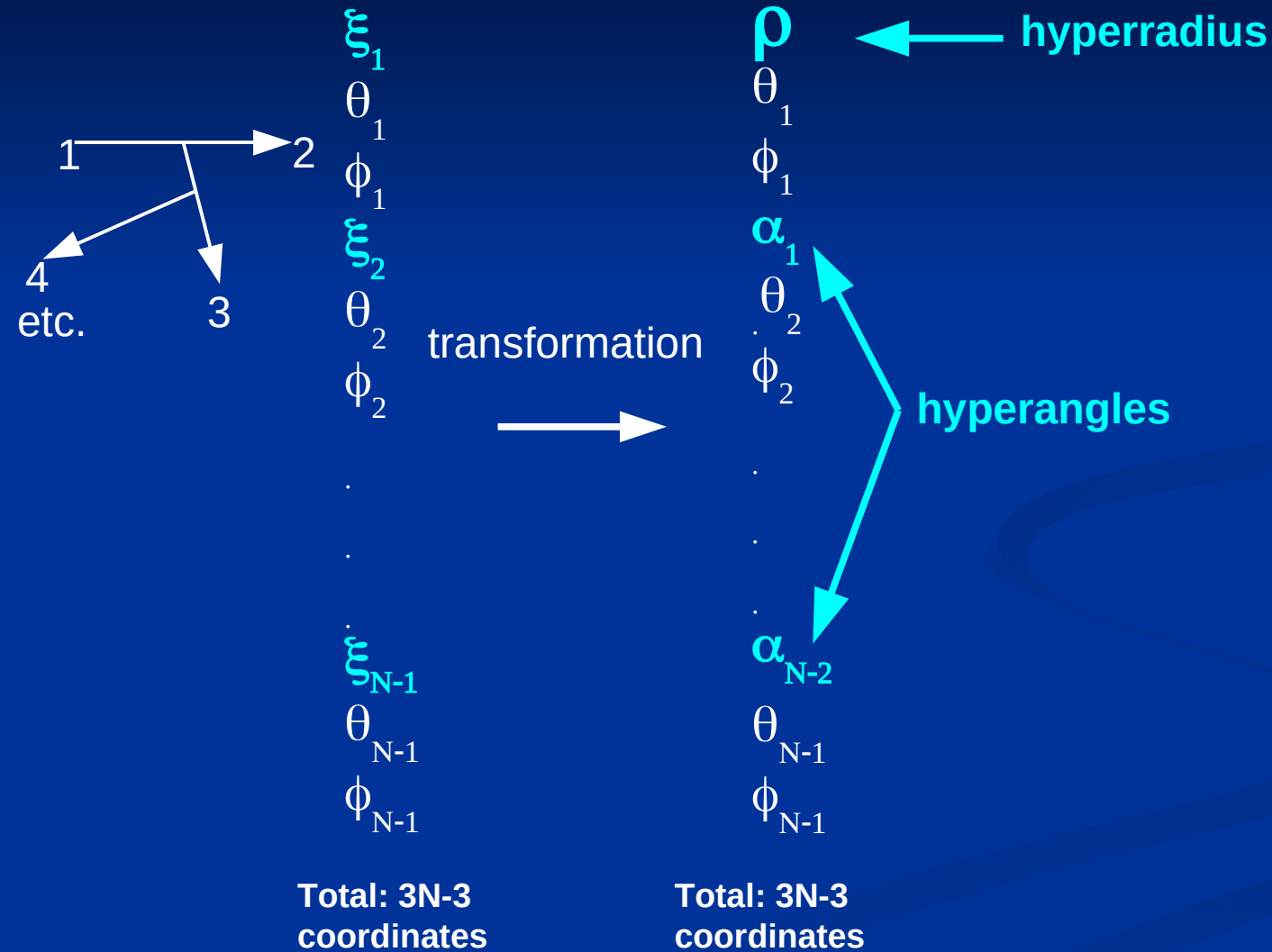


Remarks:

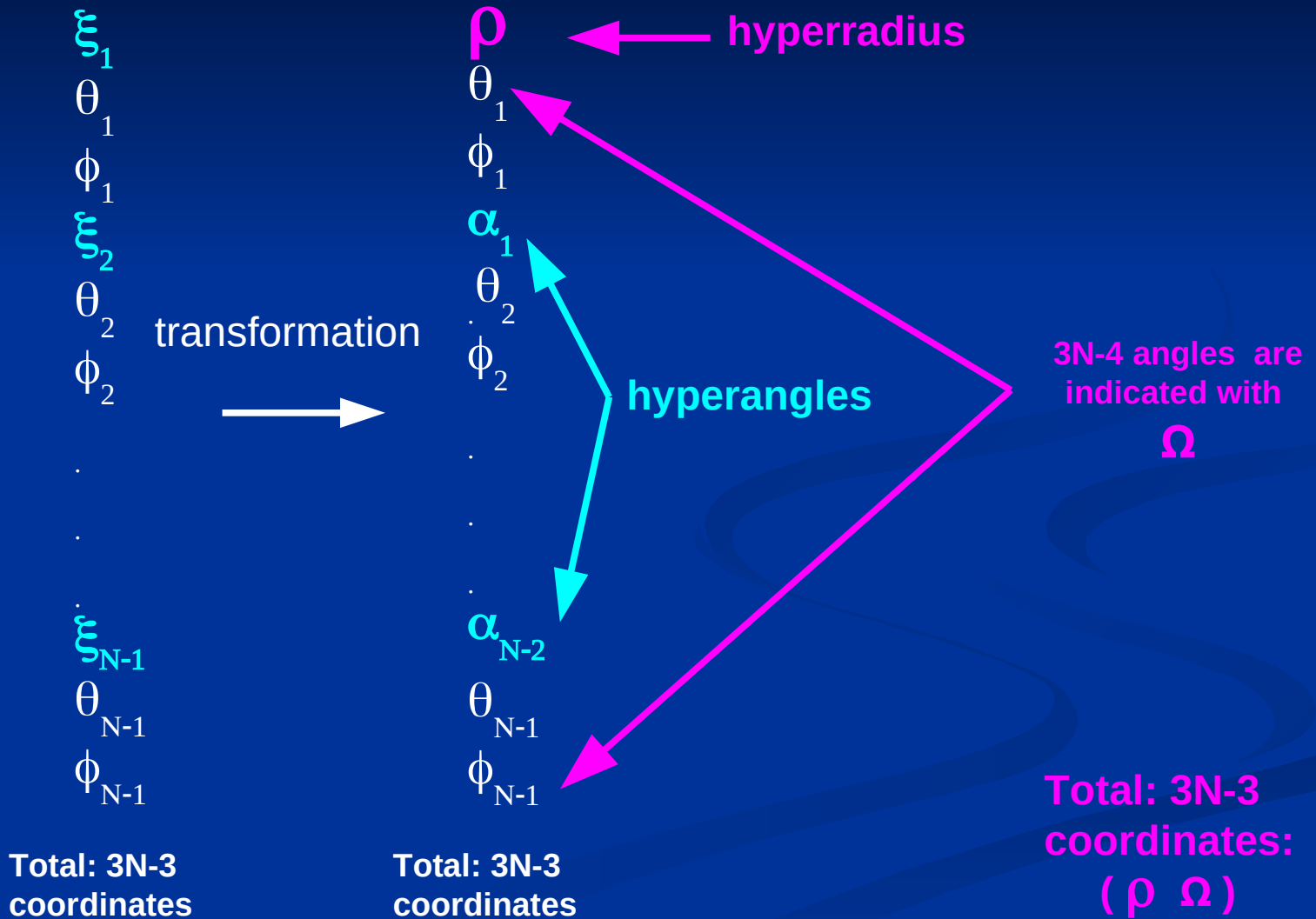
- When expressed in terms of Jacobi coordinates, any 1-body or 2-body potential becomes of “N-body nature”
- The translation invariant wave function is highly *correlated* (i.e. particles are not independent) beyond the correlation due to the dynamics

**One can further transform the Jacobi
coordinates into a new set of coordinates
called **Hyperspherical Coordinates****

HYPERSPHERICAL COORDINATES



HYPERSPHERICAL COORDINATES



HOW ARE HYPERRADIUS ρ AND HYPERANGLES α_i DEFINED ???

e.g. for **3** particles

ξ_1
 θ_1
 ϕ_1
 ξ_2
 θ_2
 ϕ_2

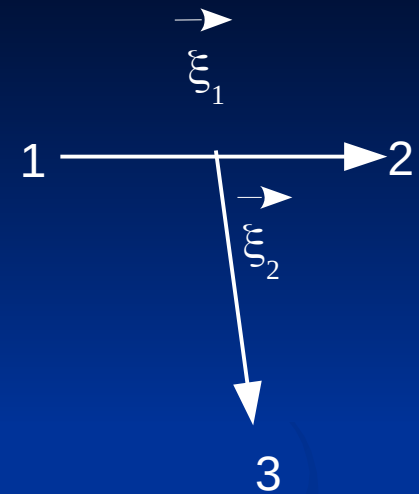
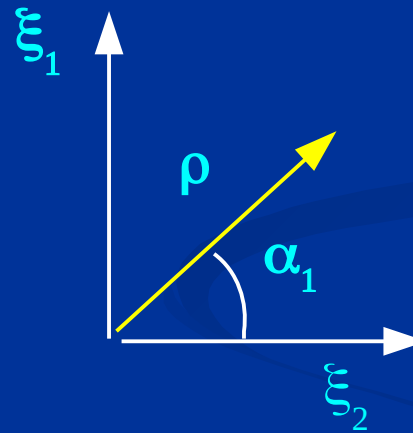
transform



$$\rho = \sqrt{\xi_1^2 + \xi_2^2}$$

$$\alpha_1 = \arccos(\xi_2 / \rho)$$

θ_1
 ϕ_1
 θ_2
 ϕ_2



HOW ARE HYPERRADIUS ρ AND HYPERANGLES α_i DEFINED ???

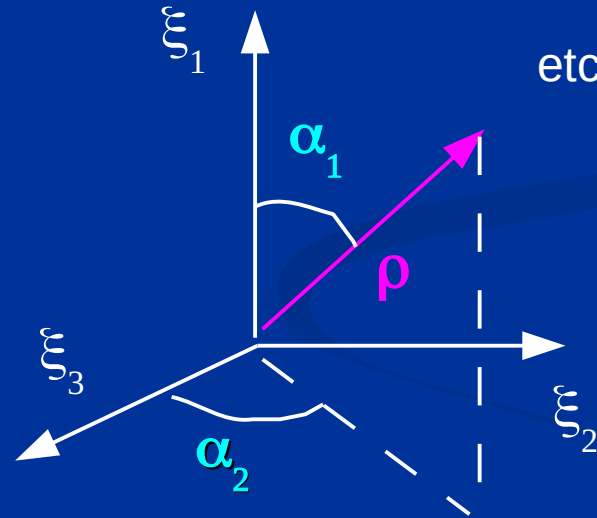
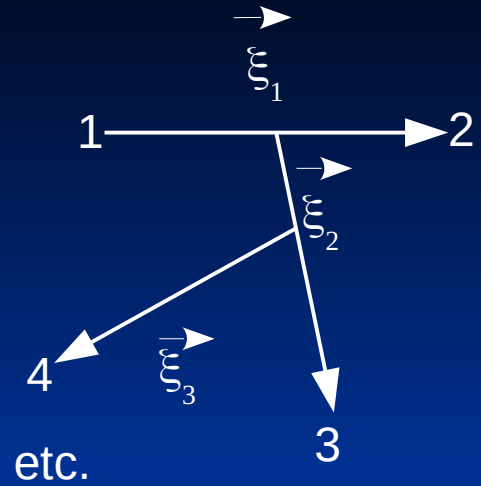
e.g. for 4 particles

ξ_1
 θ_1
 ϕ_1
 ξ_2
 θ_2
 ϕ_2
 ξ_3
 θ_3
 ϕ_3

transformation



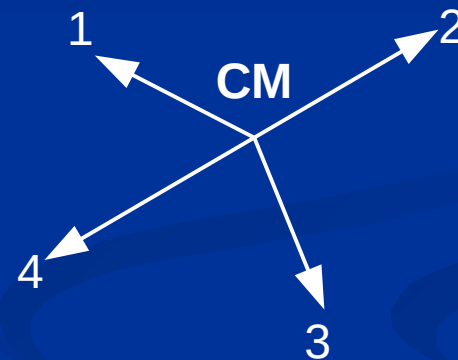
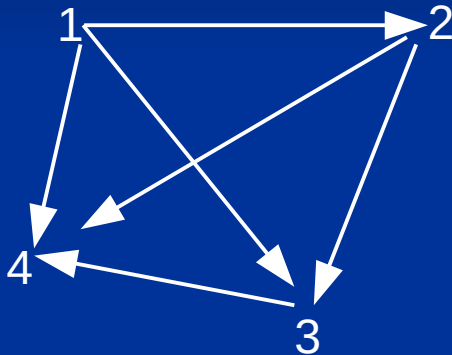
$\rho = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}$
 α_1
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 ϕ_1
 α_2
 θ_2
 ϕ_2
 θ_3
 ϕ_3



LET'S FOCUS ON THE HYPERRADIUS ρ :

$$\rho^2 \sim \sum_{ij} (\vec{r}_i - \vec{r}_j)^2$$

$$\rho^2 \sim \sum_i (\vec{r}_i - \vec{R}_{\text{CM}})^2$$



ρ can be considered as a highly
“collective” variable

***Very interesting feature of
Hyperspherical Coordinates (HC):***

***With HC the expression of the 2 body invariant
kinetic energy expressed in spherical coordinates
is generalized to the N-body case***

2 body: Kinetic Energy in **SPHERICAL** coordinates

$$T = \Delta_r - \frac{L^2}{r^2} = -\frac{1}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{L^2}{r^2}$$

The **spherical** harmonics $Y_{lm}(\theta, \phi)$ are the eigenfunctions of the **angular momentum** L^2

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N body: Kinetic Energy in **HYPERSPHERICAL** coordinates

$$T = \Delta_\rho - \frac{K^2}{\rho^2} = -\frac{1}{2m} \left(\frac{\partial^2}{\partial \rho^2} + \frac{(3N-4)}{\rho} \frac{\partial}{\partial \rho} \right) + \frac{K^2}{\rho^2}$$

The **hyperspherical** harmonics $Y_{K \dots}(\Omega)$ are the eigenfunctions of **hyperangular momentum** K^2

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2 body: SPHERICAL HARMONICS

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$$L^2 Y_{lm}(\theta, \phi) = L(L+1) Y_{lm}(\theta, \phi)$$

N body: HYPERSPHERICAL HARMONICS

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$$K^2 Y_{K\dots}(\Omega) = K(K+3N-5) Y_{K\dots}(\Omega)$$

In terms of Hyperspherical coordinates the invariant Hamiltonian becomes

$$H_{inv} = (\Delta_{\rho} - K^2 / \rho^2) + V(\rho, \theta_1 \phi_1, \theta_2 \phi_2, \dots, \alpha_1, \alpha_2, \dots)$$


The diagram shows the symbol Ω at the top, with two arrows pointing downwards to the angular coordinates $\theta_1 \phi_1$ and $\theta_2 \phi_2$ in the potential function V of the equation above. This indicates that Ω is a function of these angular coordinates.

$$= (\Delta_{\rho} - K^2 / \rho^2) + V(\rho, \Omega)$$

Remark:

- When expressed in terms of Jacobi coordinates, even a 1-body operator becomes of “N-body nature”

Remarks in view of EDF:

- In H_{inv} there is no “real” one-body (IPM) density
- But one may define an analogous “many-body” density

$$n(\mathbf{r}) \longrightarrow \nu(\rho)$$

$$r^2 n^{[1]}(r) = \int d\Omega_r d\vec{r}_2 \dots d\vec{r}_N \Psi^*(\vec{r}, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, \dots, \vec{r}_N)$$



$$\rho^{3N-4} \nu(\rho) = \int d\Omega \Psi^*(\rho, \Omega) \Psi(\rho, \Omega)$$

**The idea is to try an EDF
approach for $\nu(\rho)$**

3: Different formulation of DFT and KS equation

(the many-body **hyperradial density**)

The EDF approach for $v(\rho)$

The **ANALOGOUS** of the Hohenberg Kohn statement:

$$1) E(v) \geq E_{gs} \quad 2) E(v_{gs}) = E_{gs}$$

The EDF approach for $v(\rho)$

The **ANALOGOUS** of the Hohenberg Kohn statement:

$$1) E(v) \geq E_{gs} \quad 2) E(v_{gs}) = E_{gs}$$

Given the invariant H $H_{inv} = (\Delta_{\rho} - K^2/\rho^2) + V(\rho, \Omega)$

What is $E(v)$?

$$E[v] = \langle \Psi^v | T + V | \Psi^v \rangle \equiv \min_{\Psi \rightarrow v} \langle \Psi | T + V | \Psi \rangle$$

The proof goes along the same line as before....

Before:

The proof of the Theorem (following Levy 1979):

1) $E(\mathbf{n}) \geq E_{gs}$ Obvious! because of the Rayleigh-Ritz variational principle

2) $E(\mathbf{n}_{gs}) = E_{gs}$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r} v_{ext}(\vec{r}) n_{gs}^{[1]}(\vec{r}) \geq E_{gs} \text{ because of 1)}$$

$$F(\mathbf{n}_{gs}) \equiv \min_{\Psi \rightarrow \mathbf{n}_{gs}} \langle \Psi | T + V | \Psi \rangle \leq \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle$$

because it is a minimum

by definition

$$E_{gs} = \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle + \int d\vec{r} v_{ext}(\vec{r}) n_{gs}^{[1]}(\vec{r})$$

therefore $E_{gs} \geq F(\mathbf{n}_{gs}) + \int d\vec{r} v_{ext}(\vec{r}) n_{gs}^{[1]}(\vec{r})$



Equal!

Now:

The proof of the Theorem (following Levy 1979):

1) $E(\mathbf{v}) \geq E_{gs}$ Obvious! because of the Rayleigh-Ritz variational principle

2) $E(\mathbf{v}_{gs}) = E_{gs}$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r} \psi_{gs}(\vec{r}) n_{gs}^{[1]}(\vec{r}) \geq E_{gs} \text{ because of 1)}$$

$\mathbf{n} \rightarrow \mathbf{v}$

$$F(\mathbf{n}_{gs}) \equiv \min_{\Psi \rightarrow \mathbf{n}_{gs}} \langle \Psi | T + V | \Psi \rangle \leq \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle$$

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by definition

$$E_{gs} = \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle + \int d\vec{r} \psi_{gs}(\vec{r}) n_{gs}^{[1]}(\vec{r})$$

therefore

$$E_{gs} \geq F(\mathbf{n}_{gs}) + \int d\vec{r} \psi_{gs}(\vec{r}) n_{gs}^{[1]}(\vec{r})$$



Equal!

The practical use of the theorem goes via the “Analogous” of the Kohn-Sham equation

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Solving the one-variable **A K S** equation

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...provided the **W-representability** of the functional $E(\nu)$

By *reductio ad absurdum* one can show that

W_{KS} is unique!

One assumes that two hypercentral potentials, $W_1(\rho)$ and $W_2(\rho)$, differing by more than a constant, exist in such a way that the two Hamiltonians $H_1^W = T + W_1(\rho)$ and $H_2^W = T + W_2(\rho)$ have the same $v(\rho)$. Let us call $|\Phi_1\rangle$ and $|\Phi_2\rangle$ the respective wave functions and \mathcal{E}_1 and \mathcal{E}_2 the corresponding energies. From the Rayleigh-Ritz variational principle the following condition holds:

$$\mathcal{E}_1 < \langle \Phi_2 | H_1^W | \Phi_2 \rangle = \langle \Phi_2 | H_2^W | \Phi_2 \rangle + \langle \Phi_2 | H_1^W - H_2^W | \Phi_2 \rangle, \quad (28)$$

$$\mathcal{E}_1 < \mathcal{E}_2 + \int d\rho \rho^{3(N-4)} [W_1(\rho) - W_2(\rho)] v(\rho). \quad (29)$$

The same can be repeated starting from \mathcal{E}_2 arriving at

$$\mathcal{E}_2 < \mathcal{E}_1 + \int d\rho \rho^{3(N-4)} [W_2(\rho) - W_1(\rho)] v(\rho). \quad (30)$$

Summing both inequalities we arrive at the following contradiction, $\mathcal{E}_1 + \mathcal{E}_2 < \mathcal{E}_1 + \mathcal{E}_2$, proving that the first assumption was wrong. Accordingly, it is proven that the density $v(\rho)$ uniquely determines the hyper-radial potential $W(\rho)$ that generates it.

The practical use of the theorem goes via the “Analogous” of the Kohn-Sham equation

$$\left[\Delta_{\rho} + \frac{\mathbf{K}^2}{\rho^2} + W_{AKS}(\rho) \right] \Phi_{[\mathbf{K}_{min}]}(\rho) = E_{gs} \Phi_{[\mathbf{K}_{min}]}(\rho)$$

$$\rho^{(3N-4)} v_w(\rho_{gs}) = |\Phi_{[\mathbf{K}_{min}]}(\rho)|^2$$

$K_{min} = 0$ for bosons $K_{min} \neq 0$ for fermions

for KS:

$$W_{KS}(\rho)$$

???

for AKS:

$$W_{AKS}(\rho)$$

???

At $v=v_{gs}$ E_{gs} is the minimum of $E(v)$ namely

$$dE^V(v)/dv = 0 \implies dT^{n,V}/dn + dV^n/dn = 0$$

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=

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=

Simplest guess:

remember

$$H_{inv} = (\Delta_{\rho} - K^2 / \rho^2) + V(\rho, \Omega) \\ = V^{[2]}(\rho, \Omega) + V^{[3]}(\rho, \Omega) + \dots$$

Try integral on the hyperangular part of the ground state wave function

Sort of “mean field” for the ρ coordinate!

$$W_{AKS}(\rho) = N(N-1)/2 \int d\Omega V^{[2]}(\rho, \Omega) |Y_{[Kmin]}(\Omega)|^2 + \\ N(N-1)(N-2)/6 \int d\Omega V^{[3]}(\rho, \Omega) |Y_{[Kmin]}(\Omega)|^2 + \dots$$

4: Application to bosons close to the unitary limit (^4He atoms)

Helium clusters

Remarks:

The dimer of ${}^4\text{He}$ has a binding energy of about **1 mK**, three orders of magnitude less than the typical energy scale of $\hbar^2 / m r_{\text{vdW}}^2 = \mathbf{1.677\text{ K}}$,

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Moreover, the two-body scattering length has been estimated to be **$a \approx 190 a_0$** , twenty times larger than **$r_{\text{vdW}} = 5.08 a_0$** . In the limiting case, **$a \rightarrow \infty$** , the system is located at the **unitary limit** well suited for an **effective expansion** of the interaction

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The **first term** of this expansion is a **contact interaction** between the two helium atoms. However, as it is well known, the three-body system (as well as larger systems) collapses, even if the contact interaction is set to produce an infinitesimal binding energy. This phenomenon is known as the **Thomas collapse** and it is remedied by the introduction of a contact **three-body force** set to correctly describe the trimer energy

Accordingly, the **leading order (LO)** of this effective theory has two terms,

$$V_{LO}^{[2]} = \sum_{i < j} A e^{-r_{ij}^2 / a^2}, \quad V_{LO}^{[3]} = \sum_{i < j < k} B e^{-r_{ijk}^2 / \beta^2},$$

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A and **α** are fitted to scattering length and effective range,

Several choices are possible for **B** and **β** , for exemple

- a)** fit to **trimer** and **tetramer** binding energies
- b)** in view of the fact that $W(\rho)$ has to account for energies at any N , one can obtain couples **(B, β) values**, all fitting the **tetramer** binding energy.

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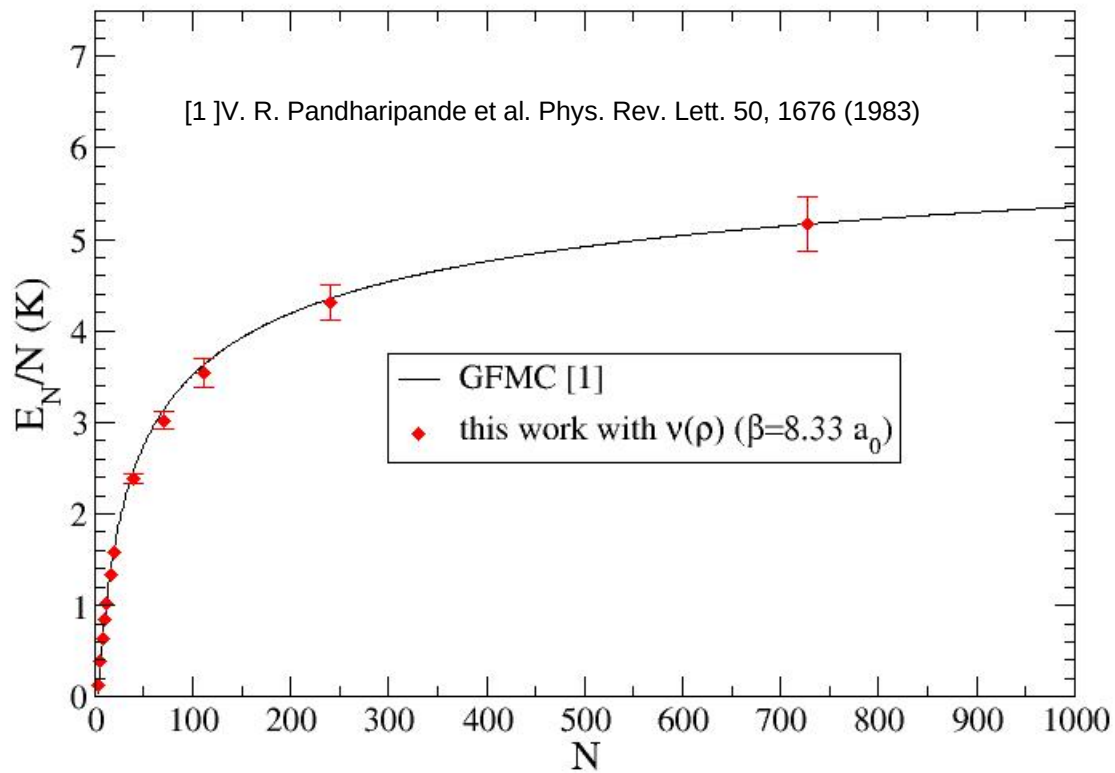
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RESULTS FOR BINDING ENERGIES
FOR ANY NUMBER N OF PARTICLES

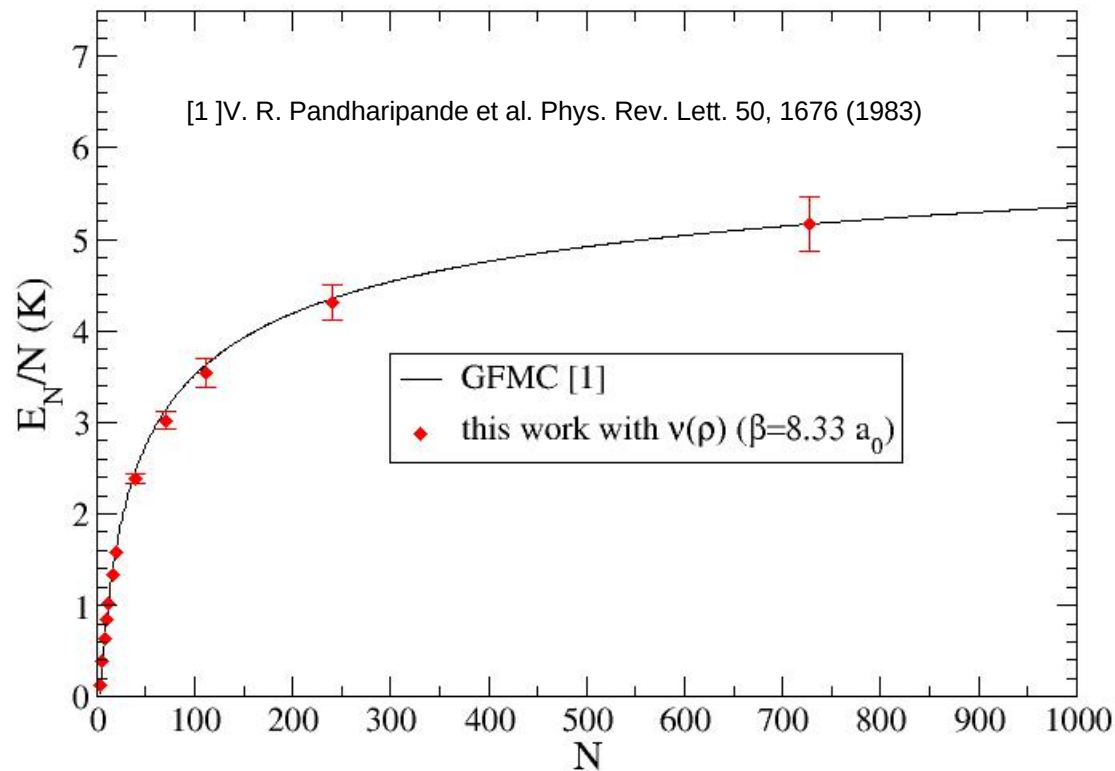
Binding energy per particle for any N

Phys. Rev. A 104, 030801 (2021)



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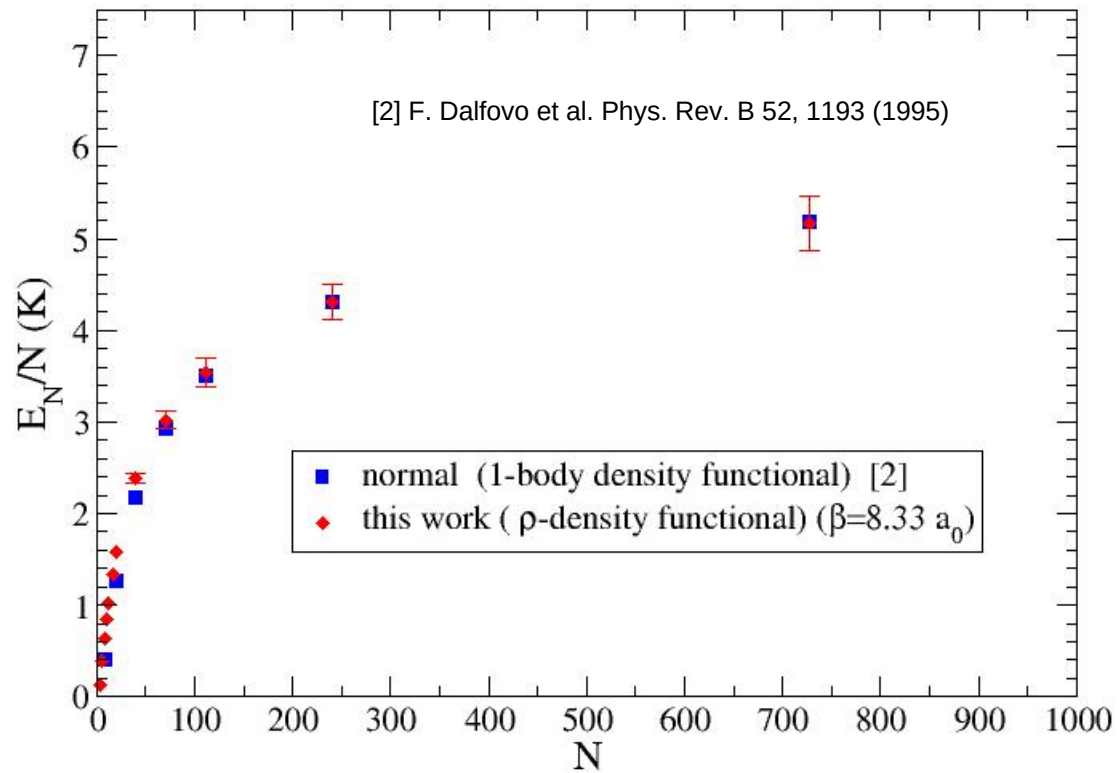
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For the **lowest N** values we observe **substantial independence** from the three-body range β with the overall best description inside the interval $7.5 a_0 < \beta < 9.0 a_0$

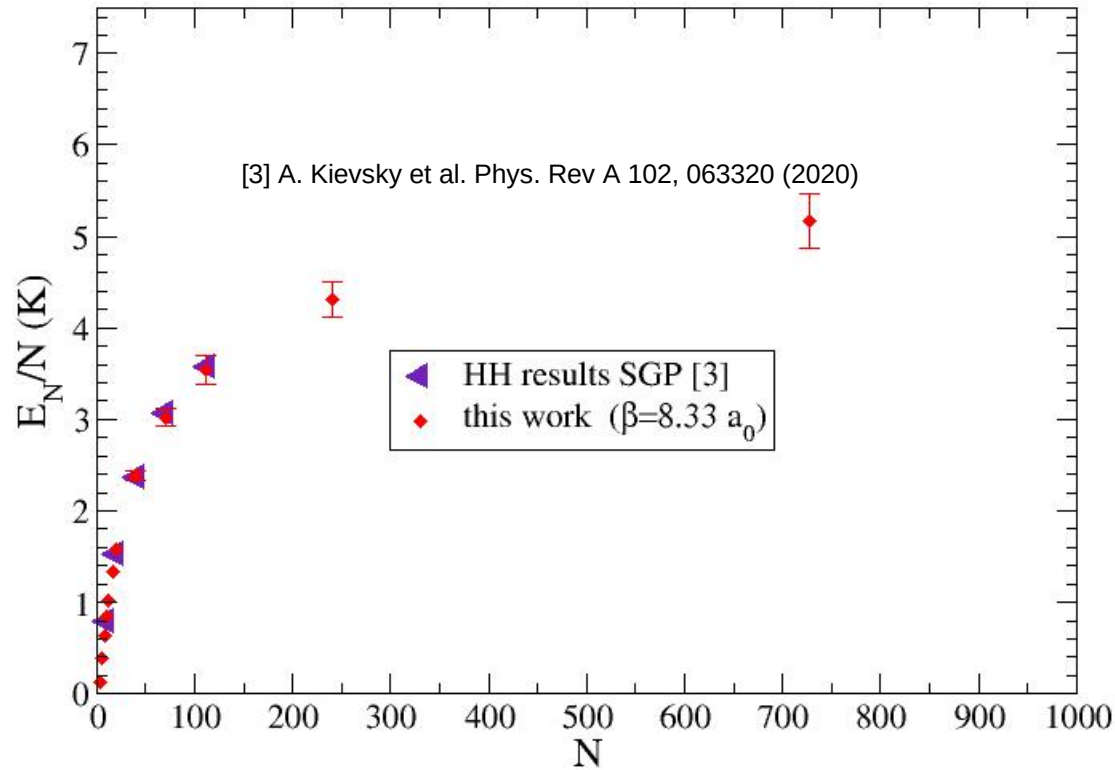
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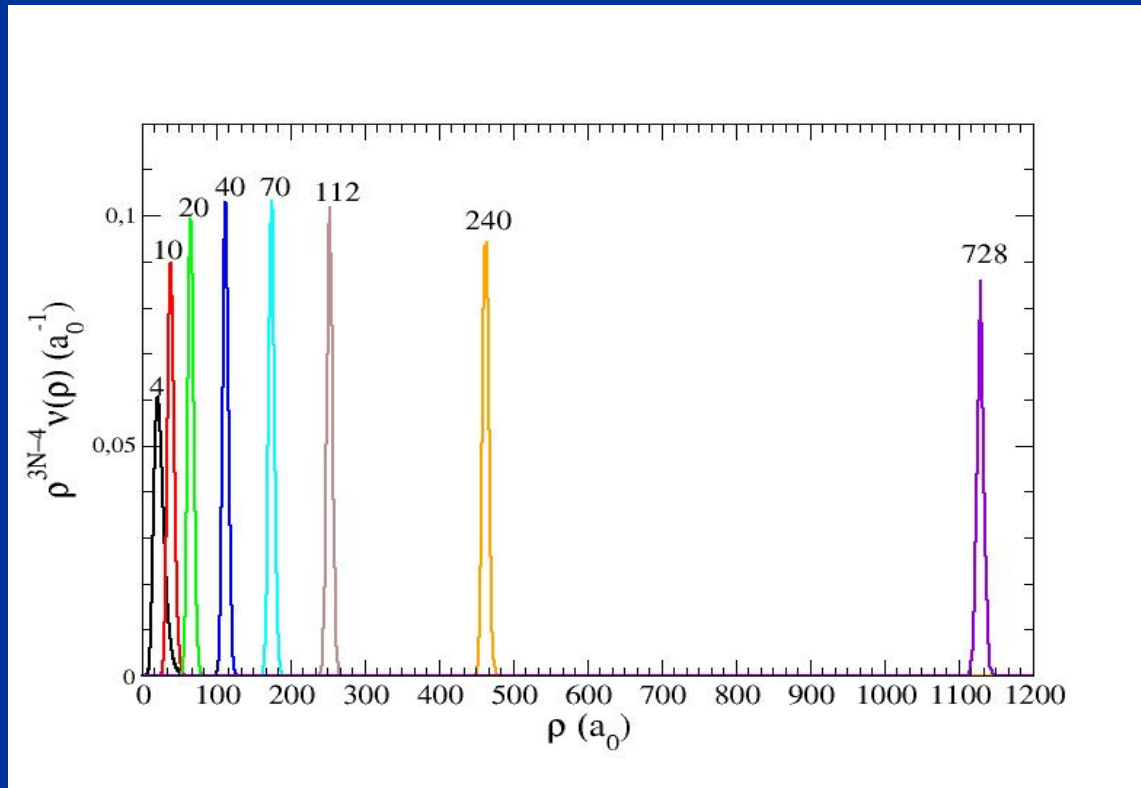
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(reduced) many-body density $v(\rho)$ for selected number of particles

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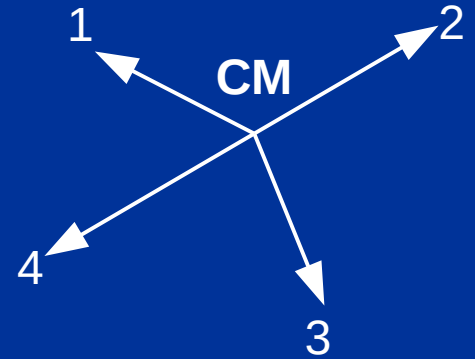
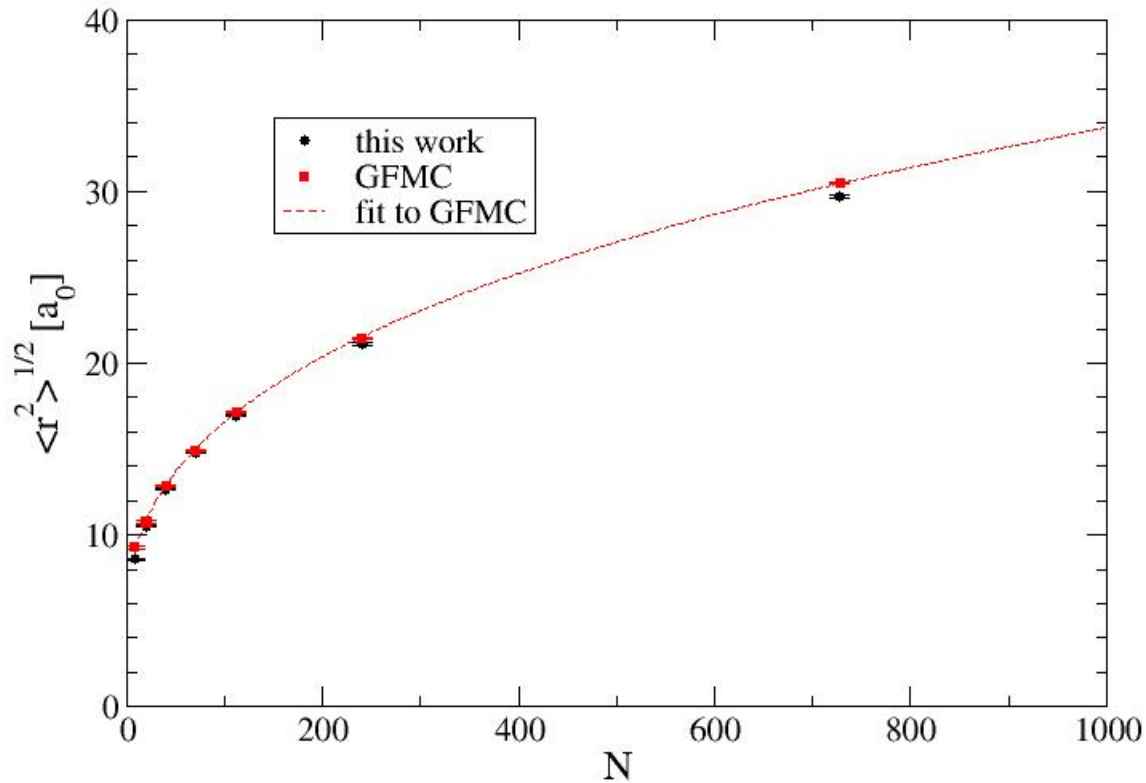
Extremely **localized density** around a value almost **linear with N** .

Very compact object. Closer particles are discouraged (incompressible?)
Also larger values are discouraged.

Mean square radius

$$\rho^2 \sim \sum_i (\vec{r}_i - \vec{R}_{\text{CM}})^2$$

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CONCLUSIONS

- An energy density functional approach has been formulated in terms of the density $\nu(\rho)$ where ρ is a translation invariant variable of collective nature
- It has been shown that the functional $E[\nu]$ is governed by a **unique** (unknown) **hyperradial potential $W(\rho)$** .
- The solution of a **single hyperradial equation** with such an hyperradial potential allows to determine the **binding energy for any N** in a straightforward way.
- We have applied this framework to the bosonic case focusing on **^4He clusters**.
- The guess for **$W(\rho)$** has been **inspired by the effective theory** approach together with a **generalization of the mean field** concept.
- Extremely satisfying results have been found. The key point has been **using the range of the three-body interaction β** , to fine tune the **$W(\rho)$** .

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OUTLOOK

- Extension to **trapped systems**
- Extension to **Fermions**. In Nuclear Physics: **$W(\rho)$??? EFT ???**

And much more to explore with the **AKS** equation and
the **Many-Body Density Functional $E(v(\rho))$** !!!