Exploring universality with a many-body density functional

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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, mantain 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 (^{4}He 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) $E(\mathbf{n}) \geq E_0$ 2) $E(\mathbf{n}) = E_0$

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1) $E(\mathbf{n}) \gtrsim E_0$ 2) $E(\mathbf{n}) = E_0$

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

n is the **one-body density:** the probability to find any of the N (indistinguishable) particles at position **r** , namely the following **integral**

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

What is E(**n**) ?

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

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

The proof of the Theorem (following Levy 1979):

1) $E(\mathbf{n}) \geq E_0$ Obvious! because of the Rayleigh–Ritz variational principle

2) $E(\mathbf{n}_{gs}) = E_0$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r}) \geq E_0$$

because of 1)

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

because it is a minimum

by definition

$$E_0 = \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r})$$

therefore

$$E_0 \leq F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r})$$

→ Equal!

The real 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 density as any given system of interacting particles.**

$$H_{KS} = T + \sum_i W_{KS}(\vec{r}_i)$$

$$n^{[1]}(\vec{r}) = \sum_i |\psi_i(\vec{r})|^2 = n^{[1]}_{gs}(\vec{r})$$

therefore **Kohn-Sham equation**

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

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Kohn-Sham equation

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$E(n) = E_W(n)$ at min

"W-representability"
of the functional

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By *reductio ad absurdum* one can show that

W_{KS} is unique!

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

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

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therefore **Kohn-Sham equation**

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

Since the n_{gs} is the **minimum** of the density functional **E(n),** the KS potential is defined by

$$\left.\frac{\delta E(\mathbf{n})}{\delta \mathbf{n}}\right|_{\mathbf{n}=\mathbf{n}_{gs}} = 0 \Longleftrightarrow W_{KS}(\vec{r}) = \frac{\delta V(\mathbf{n})}{\delta \mathbf{n}} + v_{ext}(\vec{r})$$

Therefore it is crucial to guess **V(n)**

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

???

The KS Hamiltonian is not translation/Galileian invariant

2: Self bound systems and Hyperspherical Coordinates

(interacting particles, no external one-body potential)

For self-bound systems one requires Translation / Galieian invariance

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

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

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

For self-bound systems one requires
Translation / Galieian invariance

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

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

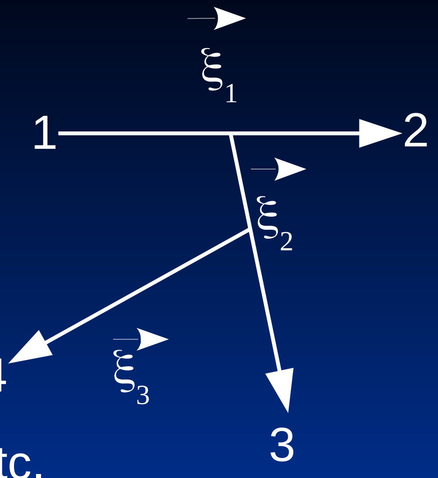
$$\rightarrow \quad H = \frac{P_{CM}^2}{2Nm} + \frac{1}{2Nm}\sum_{i<j=1}^N |\vec{p}_i - \vec{p}_j|^2 + \sum_{i<j}^N V(\vec{r}_i - \vec{r}_j)$$

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



$\vec{\xi}_i$ = distances between each particle "i" and the cm of the previous (N – i) particles

$\vec{r}_1$, $\vec{r}_2$, . . . $\vec{r}_N$ $\quad$ $\vec{p}_1$, $\vec{p}_2$, . . . $\vec{p}_N$ $\quad$ ⟵ transformation ⟶ $\quad$ $\vec{\xi}_0 = \vec{R}_{CM}$, ξ_1, . . . ξ_{N-1} $\quad$ $\vec{\pi}_0 = \vec{P}_{CM}$, π_1, . . . π_{N-1}

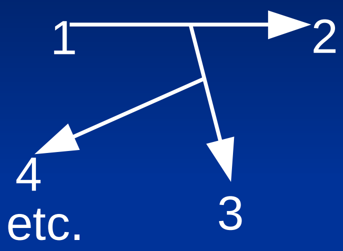
Remarks:

- 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



ξ_1
θ_1
ϕ_1
ξ_2
θ_2
ϕ_2
.
.
.
ξ_{N-1}
θ_{N-1}
ϕ_{N-1}

transformation →

ρ ← hyperradius
θ_1
ϕ_1
α_1
θ_2
ϕ_2
.
.
.
α_{N-2}
θ_{N-1}
ϕ_{N-1}

hyperangles (θ_1 … α_{N-2} … ϕ_{N-1})

Total: 3N-3 coordinates

Total: 3N-3 coordinates

HYPERSPHERICAL COORDINATES

ξ_1
θ_1
ϕ_1
ξ_2
θ_2
ϕ_2
.
.
.
ξ_{N-1}
θ_{N-1}
ϕ_{N-1}

Total: 3N-3 coordinates

transformation →

ρ ← **hyperradius**
θ_1
ϕ_1
α_1
θ_2
ϕ_2
.
.
.
α_{N-2}
θ_{N-1}
ϕ_{N-1}

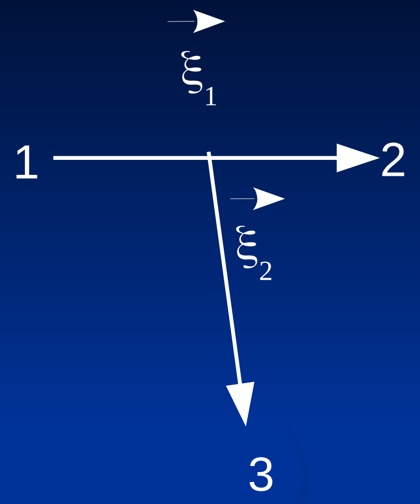
Total: 3N-3 coordinates

hyperangles

3N-4 angles are indicated with Ω

Total: 3N-3 coordinates: (ρ Ω)

HOW ARE HYPERRADIUS ρ AND HYPERANGLES α_ι DEFINED ???

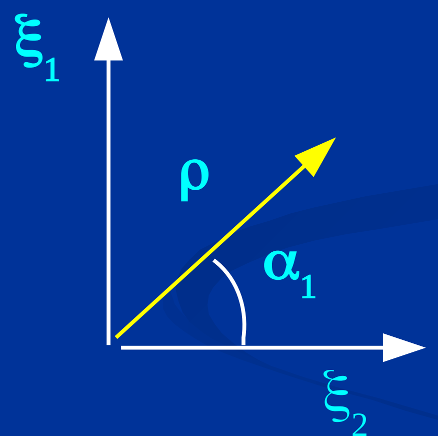


e.g. for **3** particles

ξ_1
θ_1
ϕ_1
ξ_2
θ_2
ϕ_2

transform →

$$\rho = \sqrt{\xi_1^{\,2} + \xi_2^{\,2}}$$
θ_1
ϕ_1
$$\alpha_1 = \arccos(\xi_2/\rho)$$
θ_2
ϕ_2



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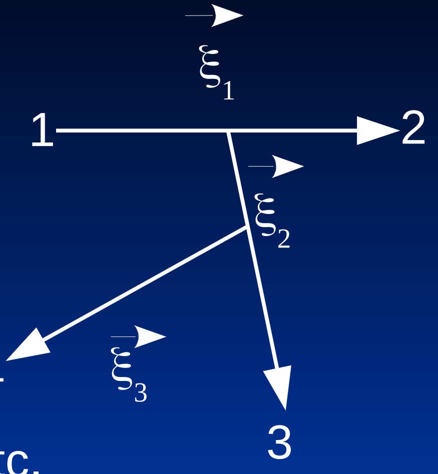
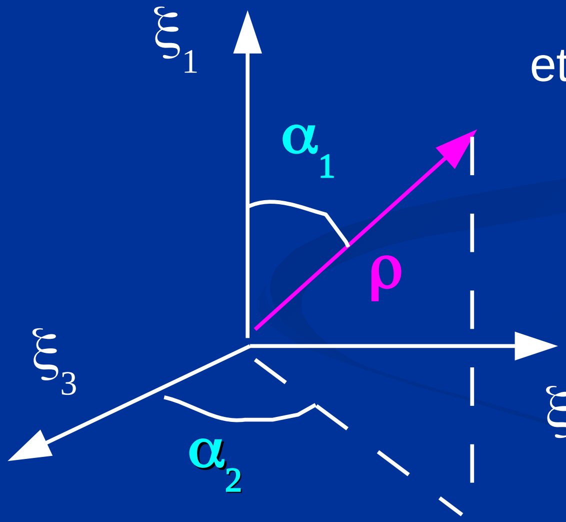


etc.

e.g. for **4** particles

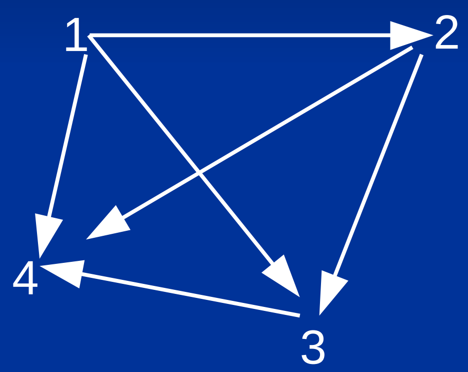
	transformation	
ξ_1		$\rho = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}$
θ_1		θ_1
ϕ_1		ϕ_1
ξ_2	$\longrightarrow$	α_1
θ_2		θ_2
ϕ_2		ϕ_2
ξ_3		α_2
θ_3		θ_3
ϕ_3		ϕ_3

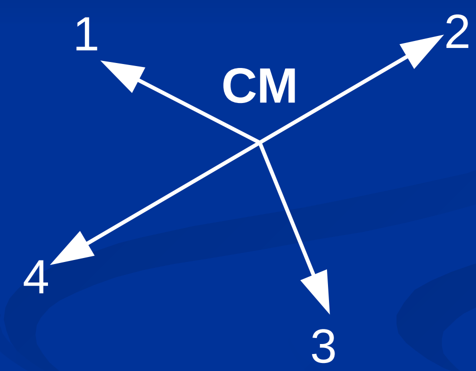


etc.

LET'S FOCUS ON THE HYPERRADIUS ρ :

$$\rho^2 \sim \Sigma_{ij} (\vec{r}_i - \vec{r}_j)^2 \qquad \rho^2 \sim \Sigma_i (r_i - R_{CM})^2$$





ρ can be onsidered 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

$$T = \Delta_r - L^2/r^2 = -1/(2m)\,(\partial^2/\partial r^2 + 2/r\ \partial/\partial r) + L^2/r^2$$

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

N body: Kinetic Energy in HYPERSPHERICAL coordinates

$$T = \Delta_\rho - K^2/\rho^2 = -1/(2m)\,(\partial^2/\partial\rho^2 + (3N-4)/\rho\ \partial/\partial\rho) + K^2/\rho^2$$

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

2 body: Kinetic Energy in SPHERICAL coordinates

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N body: Kinetic Energy in HYPERSPHERICAL coordinates

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

2 body: SPHERICAL HARMONICS

$$T = \Delta_r - L^2/r^2 = -1/(2m)\,(\partial^2/\partial r^2 + 2/r\ \partial/\partial r) + L^2/r^2$$

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

N body: HYPERSPHERICAL HARMONICS

$$T = \Delta_\rho - K^2/\rho^2 = -1/(2m)\,(\partial^2/\partial\rho^2 + (3N-4)/\rho\ \partial/\partial\rho) + K^2/\rho^2$$

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

In terms of Hyperspherical coordinates the invariant Hamiltonian becomes

$$\Omega$$

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

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

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(r) → ν (ρ)

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

→

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

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 $\nu(\rho)$

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

1) $E(\nu) \gtrsim E_0$ 2) $E(\nu_{gs}) = E_0$

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

What is $E(\nu)$?

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

The proof goes along the same line as before

Before:

The proof of the Theorem (following Levy 1979):

1) $E(\mathbf{n}) \geq E_0$ Obvious! because of the Rayleigh–Ritz variational principle

2) $E(\mathbf{n}_{gs}) = E_0$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r}) \geq E_0$$

because of 1)

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

because it is a minimum

by definition

$$E_0 = \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r})$$

therefore

$$E_0 \leq F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n^{[1]}_{gs}(\vec{r})$$

→ Equal!

Now:

The proof of the Theorem (following Levy 1979):

1) $E(\mathbf{n}) \geq E_0$ Obvious! because of the Rayleigh–Ritz variational principle

2) $E(\mathbf{n}_{gs}) = E_0$

Proof of 2):

$$E[\mathbf{n}_{gs}] = F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n_{gs}^{[1]}(\vec{r}) \geq E_0$$

because of 1)

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$$E_0 = \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle + \int d\vec{r}\, v_{ext}(\vec{r})\, n_{gs}^{[1]}(\vec{r})$$

therefore

$$E_0 \leq F(\mathbf{n}_{gs}) + \int d\vec{r}\, v_{ext}(\vec{r})\, n_{gs}^{[1]}(\vec{r})$$

Equal!

The real use of the theorem goes via the "Analogous" of the Kohn-Sham equation

The "**Analogous**" of the Kohn- Sham equation is the Schroedinger equation of a fictitious system governed by an **hypercentral potential that generates the same hyperradial density $\nu(\rho)$ as that of the real Hamiltonian, namely one has**

$$H_{AKS} = T + W_{AKS}(\rho) \quad \text{where } W_{AKS} \text{ is such that } E(\nu) = E(\nu_W)$$

Again, by *reductio ad absurdum* one can show that $W_{AKS}(\rho)$ **is unique!**

Therefore finding the minimum of $E(\nu)$ is equivalent to solve a one-dimensional Schr .Eq.

$$\Delta_\rho$$

$$\left[-\frac{1}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{(3N-4)}{\rho}\frac{\partial}{\partial\rho}\right) + \frac{K^2}{\rho^2} + W_{AKS}(\rho)\right]\Phi_{K_{min}}(\rho) = E_0\,\Phi_{K_{min}}(\rho)$$

$$\rho^{(3N-4)}\,\nu_W(\rho_{gs}) = |\Phi_{K_{min}}(\rho)|^2$$

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

Remember: **for KS:**

Since the $\mathbf{n}_{gs}$ is the **minimum** of the density functional **E(n),** the KS potential is defined by

$$\left.\frac{\delta E(\mathbf{n})}{\delta \mathbf{n}}\right|_{\mathbf{n}=\mathbf{n}_{gs}} = 0 \Longleftrightarrow W_{KS}(\vec{r}) = \frac{\delta V(\mathbf{n})}{\delta \mathbf{n}} + v_{ext}(\vec{r})$$

Therefore it is crucial to guess **V(n)**

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

???

for AKS: $W_{AKS}(\rho)$???

Simplest guess:

remember

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

$$= V^{[2]}(\rho, \Omega) + V^{[3]}(\rho, \Omega) + \ldots$$

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

Sort of "mean field" for the ρ coordinate!

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

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

Helium clusters

Observations:

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

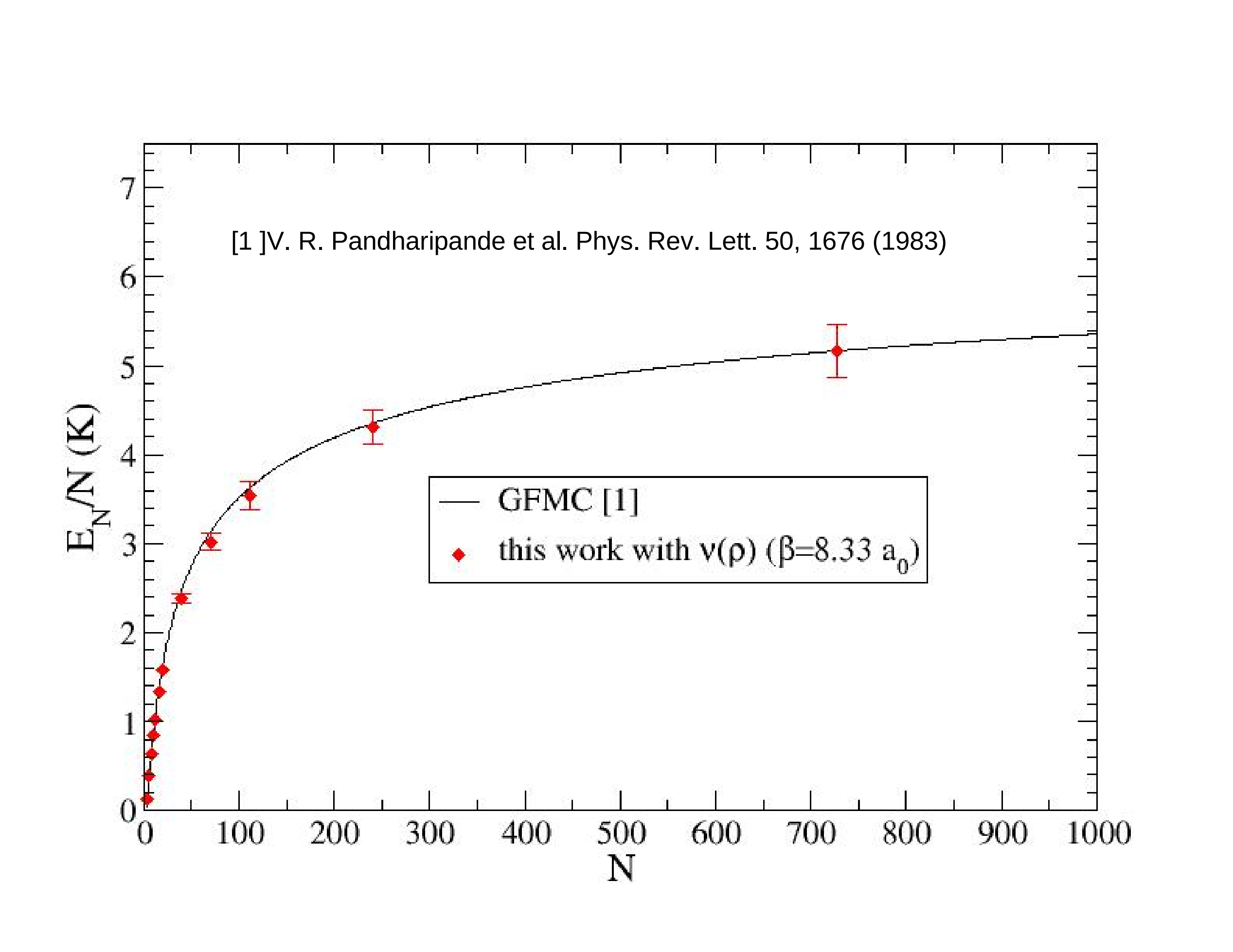
Moreover, the two-body scattering length has been estimated to be **$a \approx 190\, a_0$** , twenty times larger than **r_{vdW} =5.08 a_0** .In the limiting case, **$a \to \infty$**, the system is located at the **unitary limit** well suited for an **effective expansion** of the interaction

The leading order (LO) of this effective theory has two terms, a **two-body term** and a **three-body term**, associated with two constants, named low-energy constants (LECs), needed to determine their strengths, usually fixed by the 2 and 3-body binding energies .

RESULTS FOR BINDING ENERGIES

FOR ANY NUMBER N OF PARTICLES

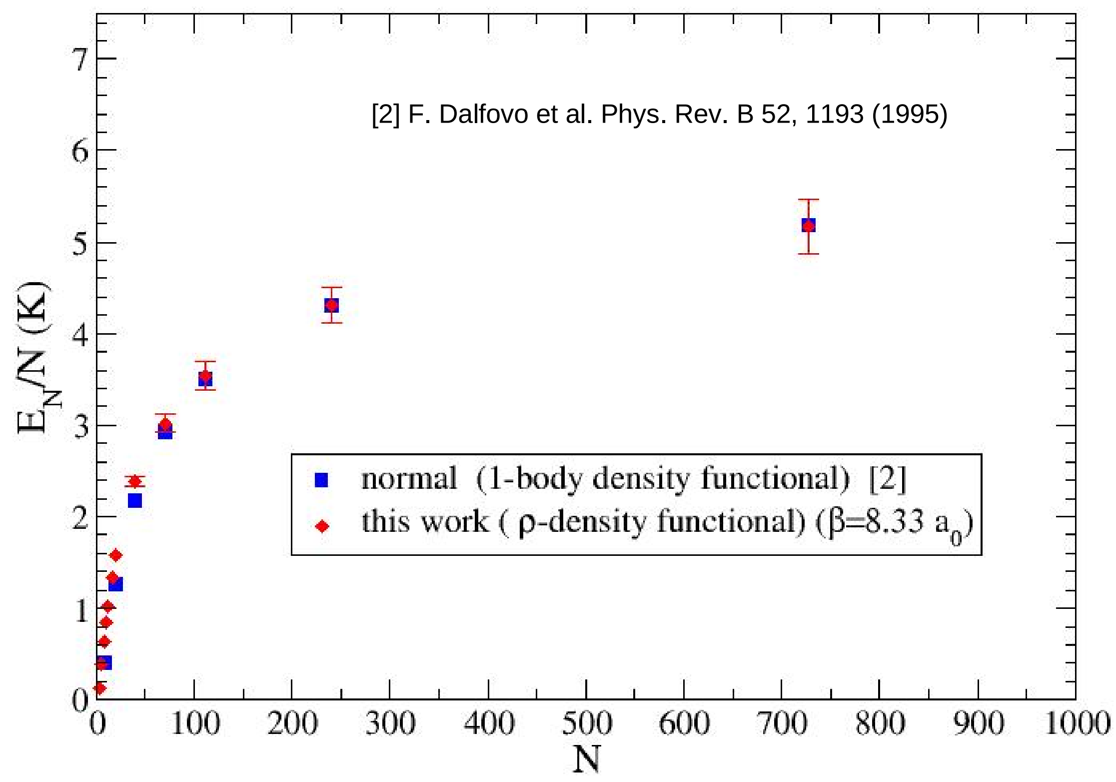
Phys. Rev. A 104, 030801 (2021) BE/N FOR ANY N



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 < β < 9.0 a $_0$**

the central value is **β = 8.33 a $_0$** with corresponding **B = 7.211 K**

Phys. Rev. A 104, 030801 (2021) **BE/N FOR ANY N**



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 < β < 9.0 a_0**

the central value is **β = 8.33 a_0** with corresponding **B = 7.211 K**

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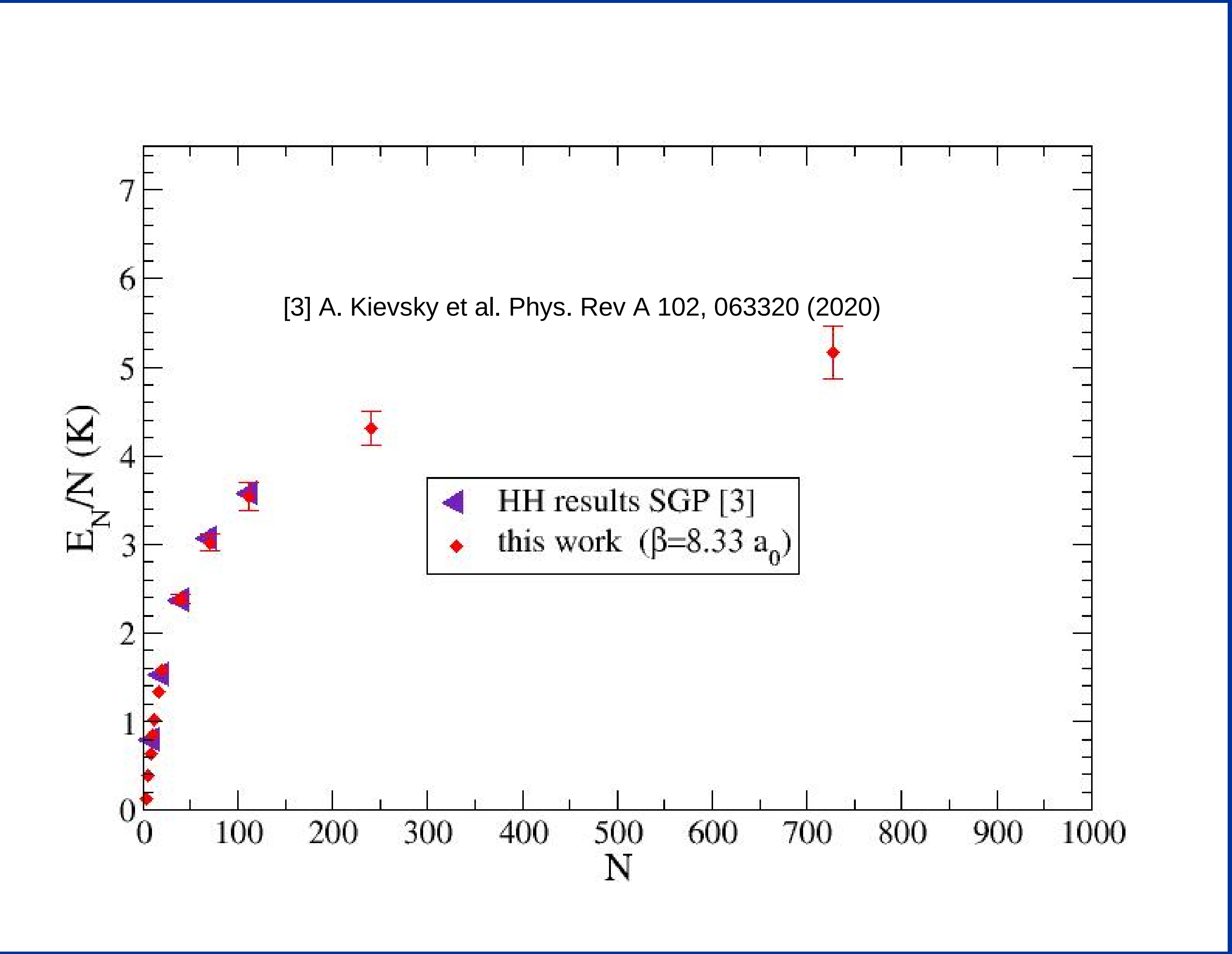

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(reduced) many-body density **ν(ρ)** for selected number of particles

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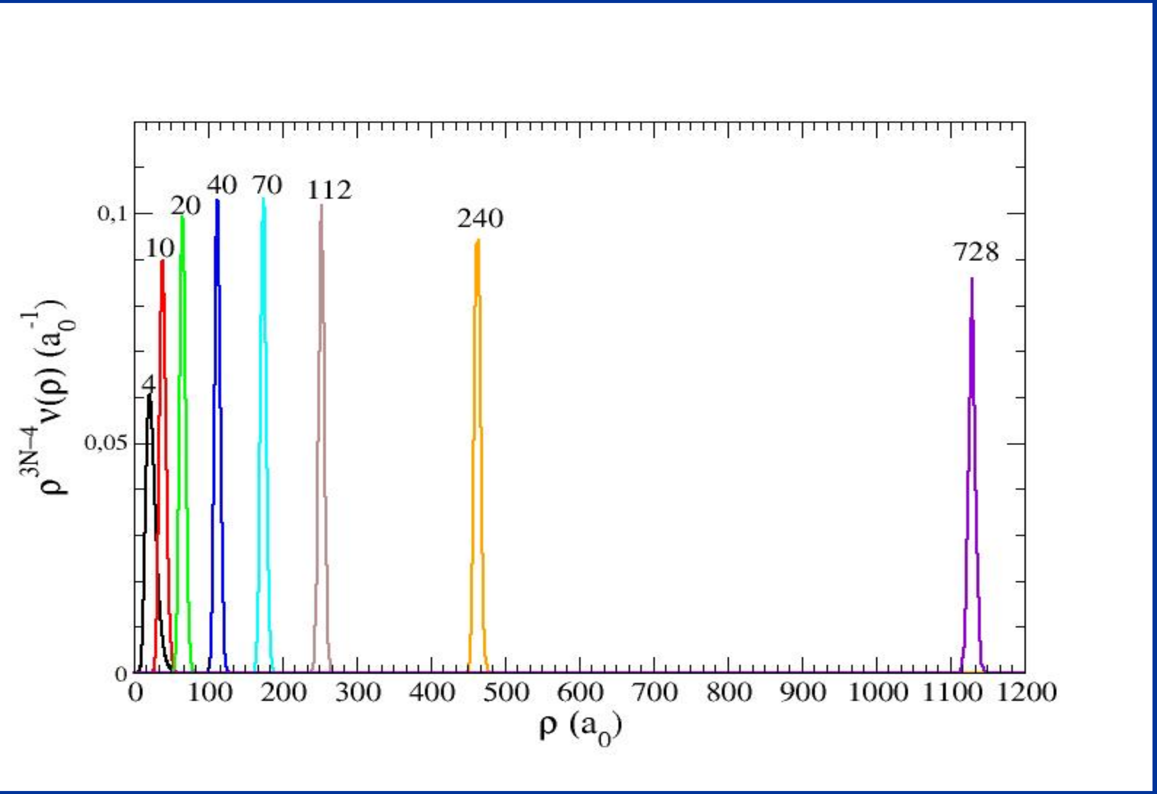

Extremely **localized density** around a value almost **linear with N** .

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

Mean square radius $\rho^2 \sim \Sigma_i (r_i - R_{CM})^2$

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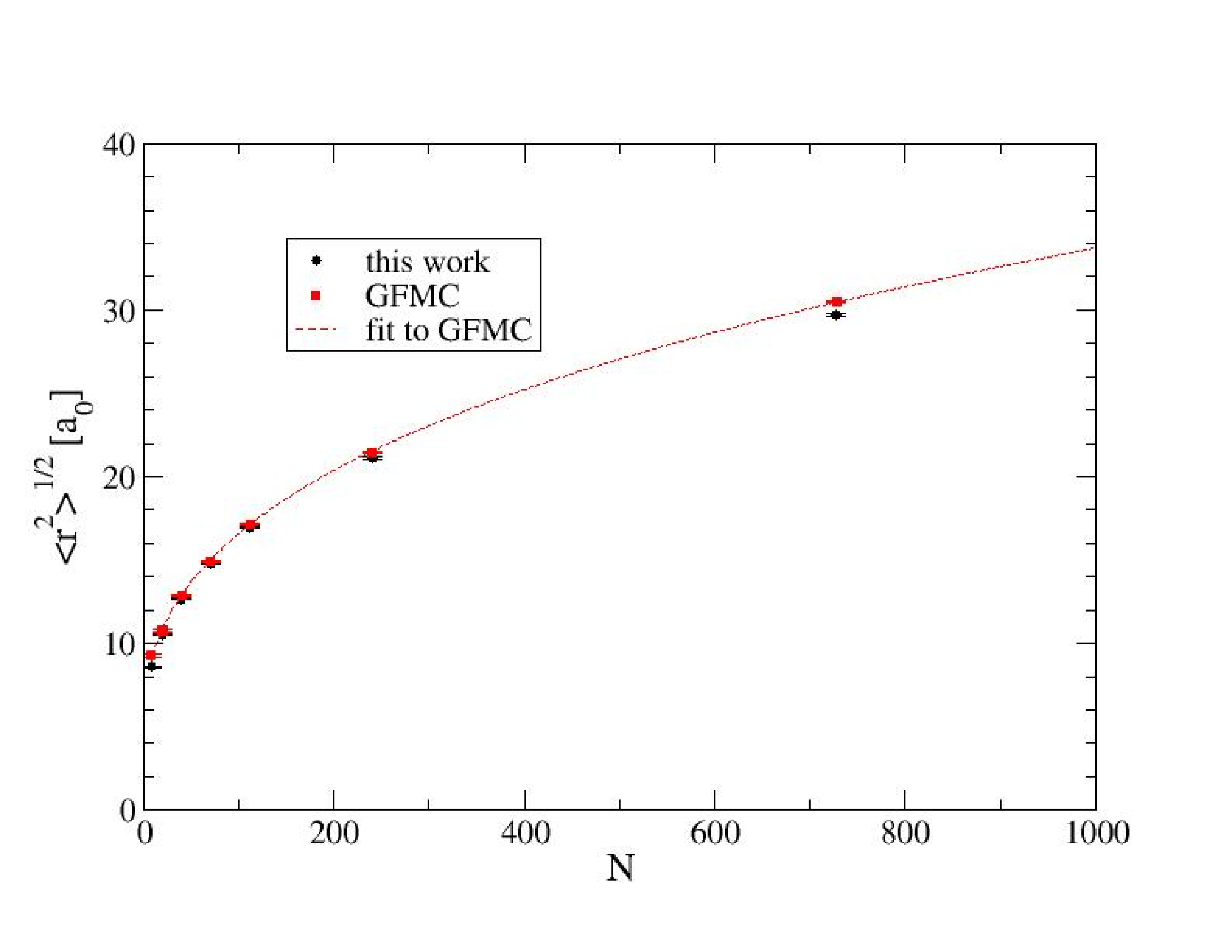

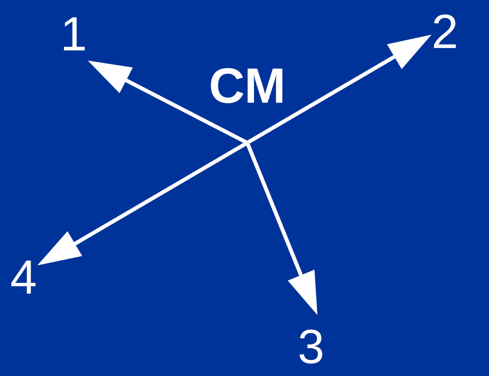

CONCLUSIONS

- An energy density functional approach has been formulated in terms of the density **ν(ρ)** where **ρ** is a translation invariant variable of collective nature
- It has been shown that the functional **E[ν]** is governed by a **unique** (unknown) **hyperradial potential W (ρ)**.
- 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 **^{4}He clusters**.
- The guess for **W (ρ)** 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 (ρ)**.

OUTLOOK

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

And much more to explore with the AKS equation and

the Many-Body Density Functional $E(\nu(\rho))$!!!