AN ALTERNATIVE ENERGY DENSITY FUNCTIONAL BASED ON THE HYPERRADIAL DENSITY

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Work In collaboration with

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EXPLORING UNIVERSALITY WITH A MANY-BODY DENSITY FUNCTIONAL

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  consider a very powerful approach: Energy Density Functional
- However, mantain translation/Galileian invariances

  see how to overcome this drawback implicit in usual EDF
- Study systems that are close to the unitary limit and are suited for effective expansion of the interaction

  an example at the end

Summary

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

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

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

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

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

And what is E(**n**) ? It is a particular functional of the one-body density defined as

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

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

The proof of the Theorem (following Levy 1979):

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

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Proof of 2):

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

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⇒ 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** $n_{gs}(r)$ as any given system of **interacting** particles.

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

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

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

$$E^W(n_{gs}) = E\,(n_{gs}) = E_{gs}$$

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

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

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

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

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

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

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

???

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 / Galieian invariance

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

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

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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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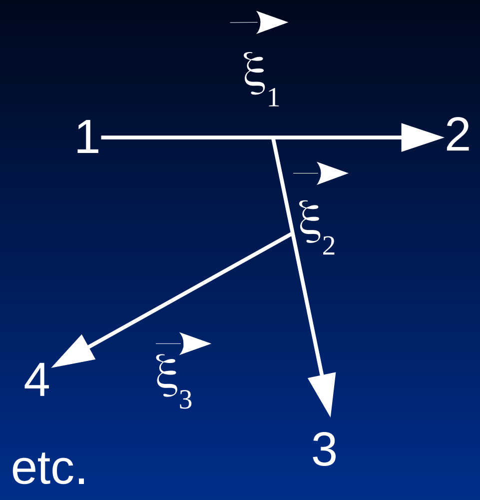
Invariant H_{inv}

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

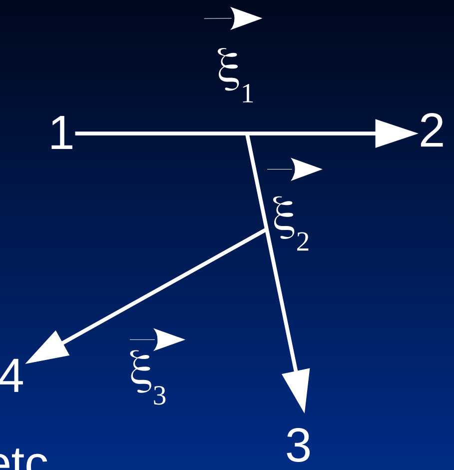
Jacobi coordinates

Jacobi coordinates



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

Jacobi coordinates



etc.

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

$\vec{r}_1 \quad \vec{p}_1$

$\vec{r}_2 \quad \vec{p}_2$

. .

. .

. .

$\vec{r}_N \quad \vec{p}_N$

transformation ⟷

$\vec{\xi}_0 = \vec{R}_{CM} \qquad \vec{\pi}_0 = \vec{P}_{CM}$

$\xi_1 \qquad \pi_1$

. .

. .

. .

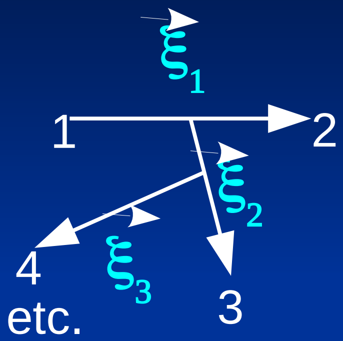
$\xi_{N-1} \qquad \pi_{N-1}$

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



$\lvert\vec{\xi}_1\rvert$		ρ ← hyperradius
θ_1		θ_1
ϕ_1		ϕ_1
$\lvert\vec{\xi}_2\rvert$		α_1
θ_2		θ_2
ϕ_2	transformation →	ϕ_2
.		.
.		.
		.
$\lvert\vec{\xi}_{N-1}\rvert$		α_{N-2}
θ_{N-1}		θ_{N-1}
ϕ_{N-1}		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}

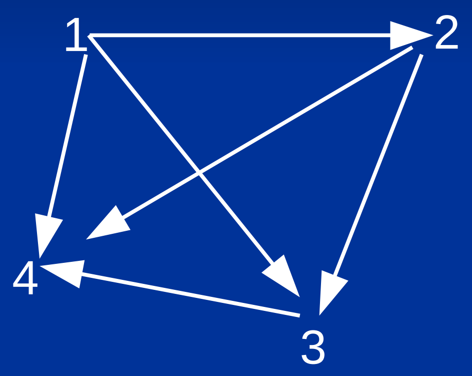
Total: 3N-3 coordinates

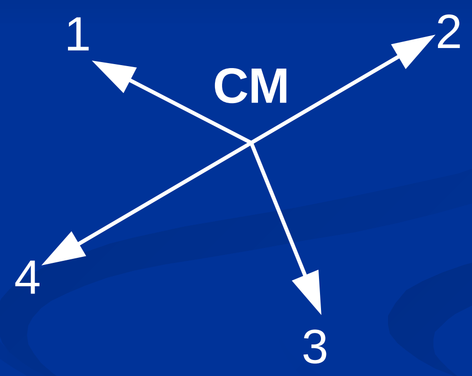
3N-4 angles are indicated with Ω

Total: 3N-3 coordinates: (ρ Ω)

LET'S FOCUS ON THE HYPERRADIUS ρ :

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





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

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

2 body: Kinetic Energy in SPHERICAL coordinates

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

N body: Kinetic Energy in HYPERSPHERICAL coordinates

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

2 body: SPHERICAL HARMONICS

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

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

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

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

In terms of Hyperspherical coordinates the invariant Hamiltonian becomes

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

Kinetic energy

Potential energy

Remember:

- 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

$$n(r) \longrightarrow \nu(\rho)$$

$$r^2 n^{[1]}(r) = \int d\Omega_r\, d\vec{r}_2 ... d\vec{r}_N \Psi^*(\vec{r}, \vec{r}_2, ..., \vec{r}_N) \Psi(\vec{r}, \vec{r}_2, ..., \vec{r}_N) \longrightarrow \rho^{3N-4} \nu(\rho) = \int d\Omega\, \Psi^*(\rho, \Omega) \Psi(\rho, \Omega)$$

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:

$$1)\ E(\nu) \geq E_{gs} \qquad 2)\ E(\nu_{gs}) = E_{gs}$$

The EDF approach for $\nu(\rho)$

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

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

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

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

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

Proof of 2):

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

$$F(\mathbf{n}_{gs}) \equiv \min_{\Psi \to \mathbf{n}_{gs}} \langle \Psi | T + V | \Psi \rangle \leq \langle \Psi_{gs} | T + V | \Psi_{gs} \rangle$$ because it is a minimum

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

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

→ Equal!

Now:

The proof of the Theorem (following Levy 1979):

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

2) $E(\nu_{gs}) = E_{gs}$

Proof of 2):

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

$\mathbf{n} \rightarrow \nu$

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

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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**

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

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

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

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

$$[\,\Delta_\rho + K^2/\rho^2 + W_{AKS}(\rho)\,]\,\Phi_{[\mathbf{K}min]}(\rho) = E_{gs}\;\Phi_{[\mathbf{K}min]}(\rho)$$

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

for KS: $W_{KS}(r)$???

---

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

At $\nu=\nu_{gs}$ E_{gs} is the minimum of $E(\nu)$ namely

$dE^{V}(\nu)/d\nu = 0$ ⇒ $dT^{nV}/dn + dV^{n}/dn = 0$

$dE^{W}(\nu)/d\nu = 0$ ⇒ $dT^{n,W}/d\nu + W(\rho) = 0$

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$$dE^{W}(\nu)/d\nu = 0 \Rightarrow dT^{\nu,W}/d\nu + \boxed{W(\rho)} = 0$$

Simplest guess:

remember

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

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

Sort of "mean field" for the ρ coordinate!

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

W(ρ) must entail a very complex **kinetic and potential** dynamics, in fact:

- With **H=T+V** the true solution is obtained via **a set of coupled HH equations** in principle for an infinite number of **K** (diagionalization of the Hamiltonian represented on HH up to convergence)

- With **H=T+ W** the true solution is obtained only with **one single equation at K_{min}!**

- **…. "universal" character ? ….**

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

Helium clusters

Remarks:

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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,

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

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

a) *fit to* ***trimer*** *and* ***tetramer*** *binding energies*

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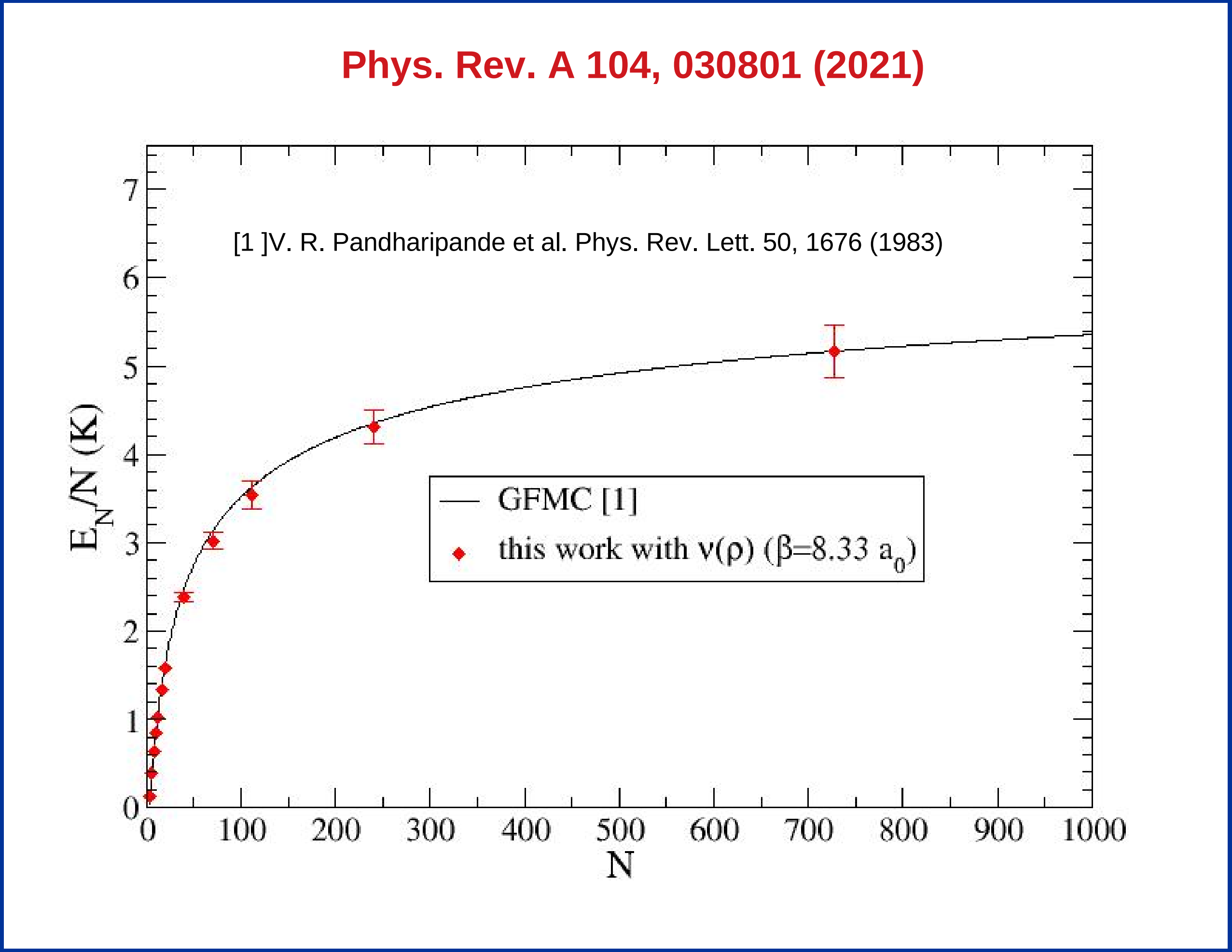
RESULTS FOR BINDING ENERGIES

FOR ANY NUMBER N OF PARTICLES

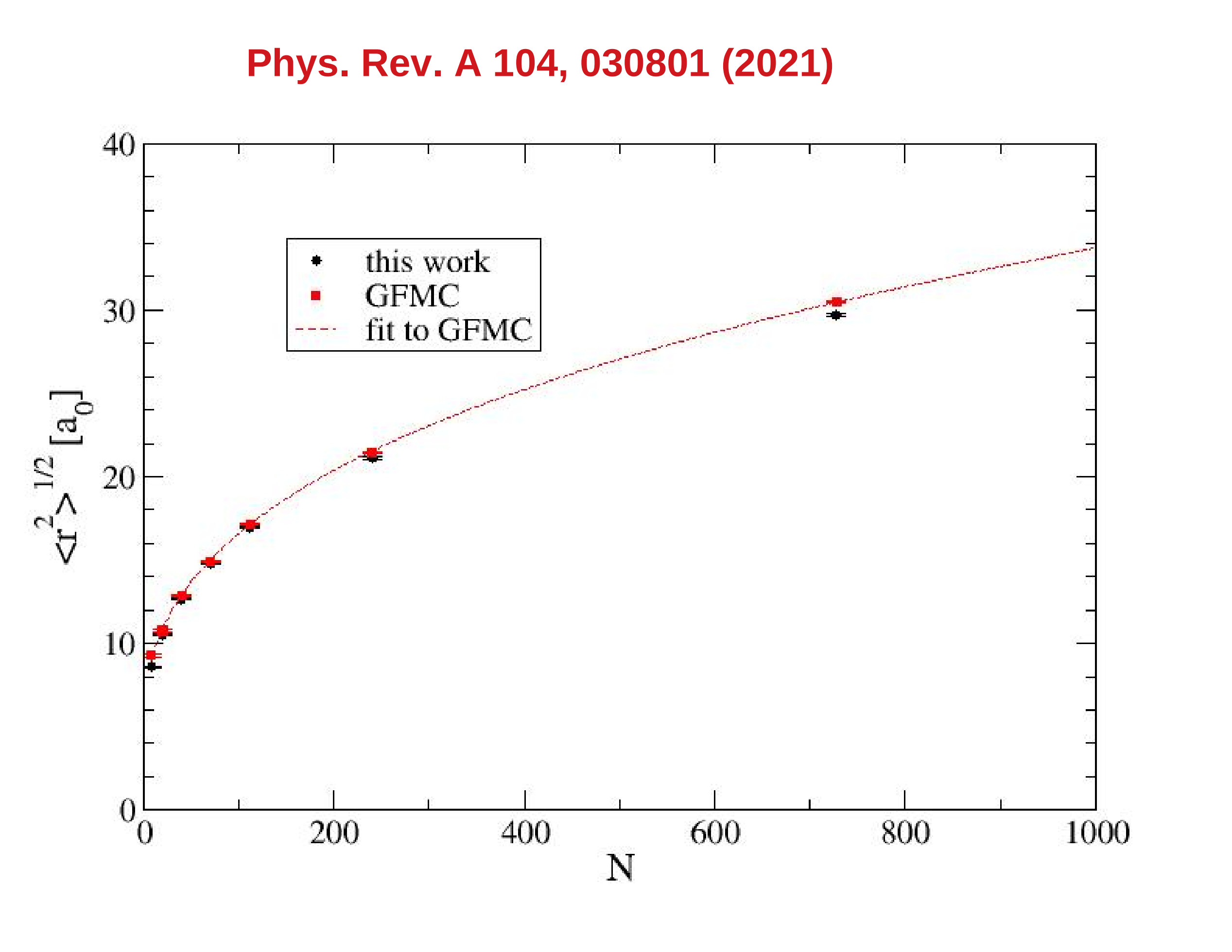
Binding energy per particle for any N

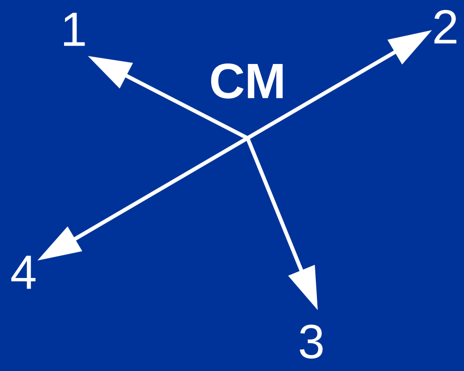


GFMC results are obtained with the “phenomenological” HFDHe2 Aziz potential (two-body only!!)

Mean square radius

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





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

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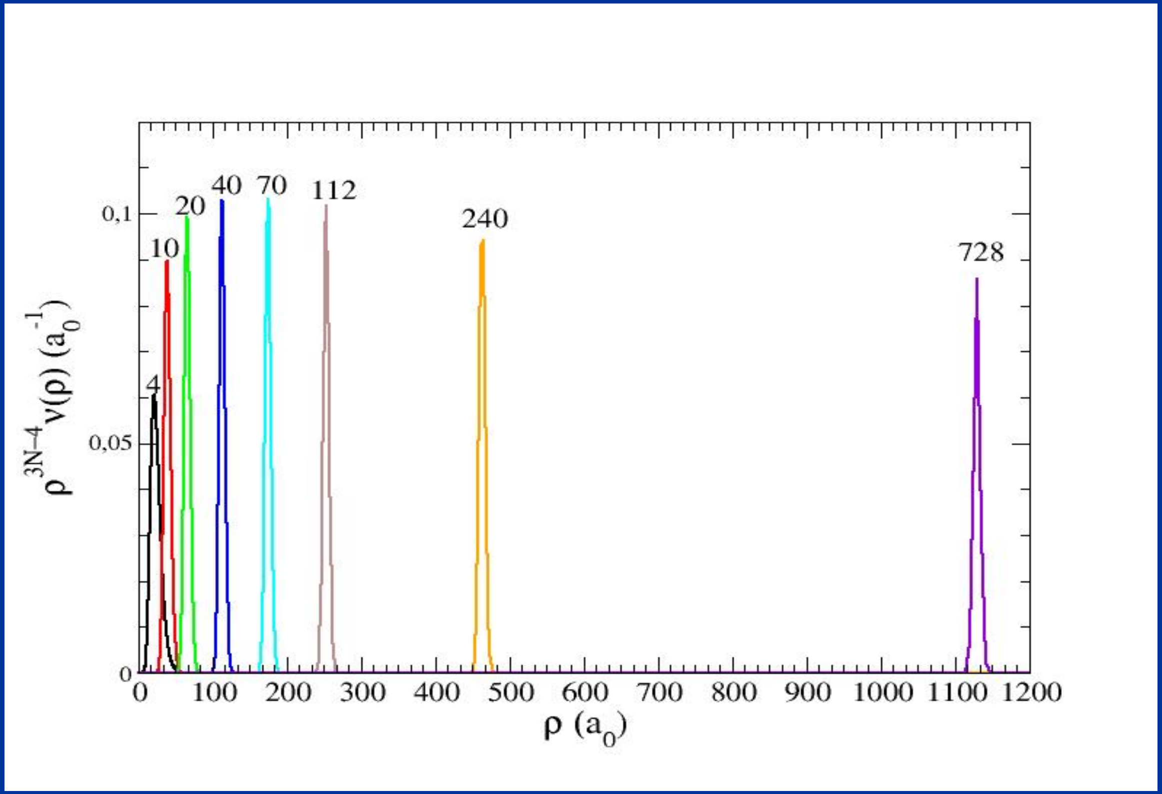


Extremely **localized density** around a value almost **linear with N** .

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

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 **^{4}He clusters**.
- The guess for **$W(\rho)$** has been **inspired by the effective theory** approach together with a **generalization of the mean field** concept.

OUTLOOK

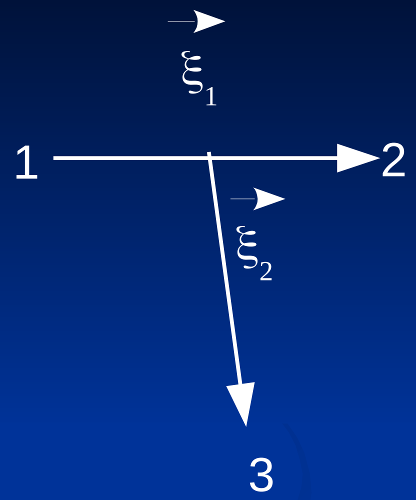
- Extension to **trapped systems**
- Extension to **Fermions.** In Nuclear Physics: **W (ρ)** ??? EFT ???

And much more to explore with the AKS equation and

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

Thank You!

HOW ARE HYPERRADIUS ρ AND HYPERANGLES α_ι DEFINED ???

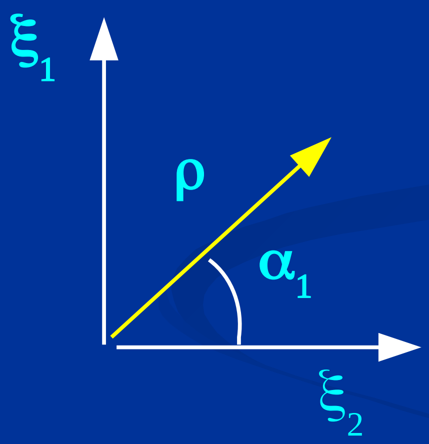


e.g. for **3** particles

ξ_1
θ_1
ϕ_1
ξ_2
θ_2
ϕ_2

transform $\longrightarrow$

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



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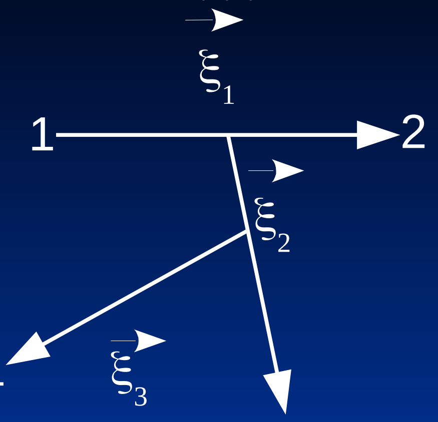
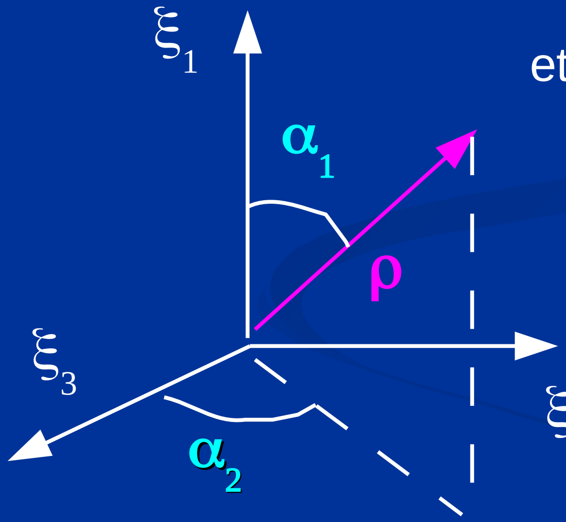


etc.

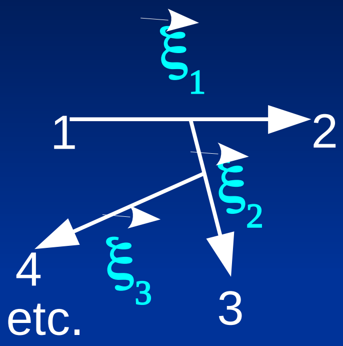
e.g. for **4** particles

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



etc.

HYPERSPHERICAL COORDINATES



$|\vec{\xi}_1|$
θ_1
ϕ_1
$|\vec{\xi}_2|$
θ_2
ϕ_2
.
.
$|\vec{\xi}_{N-1}|$
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}

hyperangles ($\alpha_1 \ldots \alpha_{N-2}$)

Total: 3N-3 coordinates

By *reductio ad absurdum* one can show that

W_{KS} is unique!

[redacted] 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 $\nu(\rho)$. 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:

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

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

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

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

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 $\nu(\rho)$ uniquely determines the hyper-radial potential $W(\rho)$ that generates it. [redacted]