Internal density functional theory
and
center-of-mass correlations.

ESNT-CEA workshop
25 November 2014

Jérémie MESSUD (Now geophysical researcher at CGG; formerly CENBG, IRSAMS-LPT)

Introduction

Articles

- Stationary case (first demonstrations of the internal DFT theorem, but approximate Kohn-Sham scheme)

J. Engel, Phys. Rev. C75, 014306 (2007)

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Further speech

1)   Reminder of internal DFT formalism

Translational invariance problematic

Translational invariance: one of the most obvious symmetries of isolated self-bound systems

Implies that center-of mass (c.m.) properties can be separated from "internal properties"

The ones of experimental properties

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If not treated correctly: spurious coupling between the c.m. motion and internal properties
can have non-negligible effects (even for intermediate-sized nuclei…)

"Sacrificed" within Hartree-Fock (HF) ansatz
-HF with effective interaction => addition of a -<$P^2/2mN$ > to "restore" a part of the c.m.
correlations => not sufficient

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A more fundamental way?
-Projection before variation methods to impose Galilean invariance of the wave function
=> large numerical cost, unmanageable in the time-dependent case

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A more fundamental *and* numerically manageable way?
- Internal DFT with a c.m. correlations functional

Separation of internal properties

Translationally invariant N-body Hamiltonian:

$$H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \underbrace{\sum_{\substack{i,j=1 \\ i>j}}^{N} u(\mathbf{r}_i - \mathbf{r}_j)}_{\text{Isolated self-bound Hamiltonian}} + \sum_{i=1}^{N} v^{\text{int}}(\mathbf{r}_i - \mathbf{R})$$

Isolated self-bound Hamiltonian

Corresponding eigenstate $\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ is Galilean invariant

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- "internal" potential, defined in the c.m. frame => acts only on the internal properties.

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-suitable to model the internal effects of a polarization potential, laser potential… used in experiments
-zero in the purely isolated self-bound case
-helps the "internal" DFT theorem demonstration

Separation of internal properties

- c.m. coordinate: $\mathbf{R} = \dfrac{1}{N} \sum_{j=1}^{N} \mathbf{r}_j$

-(N-1) Jacobi coordinates: $\xi_1 = \mathbf{r}_2 - \mathbf{r}_1, \quad \xi_2 = \mathbf{r}_3 - \dfrac{\mathbf{r}_2 + \mathbf{r}_1}{2}, \quad \dots, \quad \xi_{N-1} = \dfrac{N}{N-1}(\mathbf{r}_N - \mathbf{R})$

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Permits to separate the Hamiltonian into:

$$
\begin{aligned}
H_{CM} &= -\frac{\hbar^2}{2mN} \Delta_{\mathbf{R}} \\
H_{int} &= \sum_{\alpha=1}^{N-1} \frac{\tau_\alpha^2}{2\mu_\alpha} + U(\xi_1, \ldots, \xi_{N-1}) + V^{\text{int}}(\xi_1, \ldots, \xi_{N-1})
\end{aligned}
$$

and the wave function into:

$$\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \Gamma(\mathbf{R})\, \psi_{int}(\xi_1, \ldots, \xi_{N-1})$$

with:
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H_{CM}\Gamma &= E_{cm}\Gamma \\
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$\longrightarrow$ (N-1)-body "internal" Hamiltonian describing the internal properties (contains v^{int})

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$\longrightarrow$ Delocalization of R; does not correspond to experimental situations

$$H_{int}\psi_{int} = E_{int}\psi_{int}$$

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Describes "internal" properties, the ones of experimental interest

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Describes "internal" properties, the ones of experimental interest

$\psi_{int}(\xi_1,\ldots,\xi_{N-1})$ can be rewritten $\psi_{int}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ but one coordinate $\mathbf{r}_i$ is then redundant

=> C.M. CORRELATIONS EFFECT WE WANT TO TREAT FUNDAMENTALLY

Internal DFT theorem

1) Define the internal density (i.e. measured in the c.m. frame, the most simple observable, that is always recovered experimentally):

$$\rho_{int}(\mathbf{r}) \;=\; N \int d\mathbf{r}_1 \cdots d\mathbf{r}_N \; \delta(\mathbf{R}) |\psi_{int}(\mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \, \delta\big(\mathbf{r} - (\mathbf{r}_i - \mathbf{R})\big)$$

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2) Existence theorem:

For a non-degenerate ground state (and a given kind of particle), ψ_{int} can be expressed as a unique functional of ρ_{int} $\Rightarrow \psi_{int}[\rho_{int}] \Rightarrow$ every observable can be expressed as a unique functional of ρ_{int}.

In particular: $E_{int}[\rho_{int}] = (\psi_{int}[\rho_{int}]|H_{int}|\psi_{int}[\rho_{int}])$

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HOW?

Nota: Theorem always valid because ψ_{int} is always normalizable.
Problem in case of standard DFT if applied to self-bound systems, because the laboratory wave function is then not normalizable!

Internal Kohn-Sham (KS) scheme

KS assumption: there exists, in the c.m. frame, a N-body "non-interacting" system (i.e. a local single-particle potential) that reproduces the exact density ρ_{int}.

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$$\rho_{int}(\mathbf{r}) = \sum_{i=1}^{N} \left|\varphi_{int}^i(\mathbf{r})\right|^2$$

We then can rewrite (adding&subtracting the "non-interacting" kinetic energy $\sum_{i=1}^{N}(\varphi_{int}^i|\frac{\mathbf{p}^2}{2m}|\varphi_{int}^i)$)

$$E_{int}[\rho_{int}] = \sum_{i=1}^{N}(\varphi_{int}^i|\frac{\mathbf{p}^2}{2m}|\varphi_{int}^i) + E_{HXC}[\rho_{int}] + \int d\mathbf{r}\, v_{int}(\mathbf{r})\,\rho_{int}(\mathbf{r})$$

with $E_{HXC}[\rho_{int}] = \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\, \gamma_{int}[\rho_{int}](\mathbf{r},\mathbf{r}')\, u(\mathbf{r}-\mathbf{r}') + E_{\Delta kin}[\rho_{int}]$

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Only term of the functional where c.m. correlations appear explicitly (difference with standard DFT)

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We then can rewrite (adding&subtracting the "non-interacting" kinetic energy $\sum_{i=1}^{N} (\varphi_{int}^{i} | \frac{\mathbf{p}^2}{2m} | \varphi_{int}^{i}))$

$$E_{int}[\rho_{int}] = \sum_{i=1}^{N} (\varphi_{int}^{i} | \frac{\mathbf{p}^2}{2m} | \varphi_{int}^{i}) + E_{HXC}[\rho_{int}] + \int d\mathbf{r}\, v_{int}(\mathbf{r})\, \rho_{int}(\mathbf{r})$$

with $E_{HXC}[\rho_{int}] = \frac{1}{2} \int d\mathbf{r}\, d\mathbf{r}'\, \gamma_{int}[\rho_{int}](\mathbf{r}, \mathbf{r}')\, u(\mathbf{r} - \mathbf{r}') + E_{\Delta kin}[\rho_{int}]$ $\longrightarrow$ Hartree + total XC energy (including c.m correlations)

$$E_{\Delta kin}[\rho_{int}] = \int d\mathbf{r}_1 \cdots d\mathbf{r}_N\, \delta(\mathbf{R})\, \psi_{int}^{*}(\mathbf{r}_1, \ldots, \mathbf{r}_N) \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \psi_{int}(\mathbf{r}_1, \ldots, \mathbf{r}_N) - \sum_{i=1}^{N} (\varphi_{int}^{i} | \frac{\mathbf{p}^2}{2m} | \varphi_{int}^{i})$$

Only term of the functional where c.m. correlations appear explicitly (difference with standard DFT)

Nota:

-All functionals are implicitly functionals of ρ_{int} because the KS assumption implies $\varphi_{int}^{i}[\rho_{int}]$
   => permits us to perform KS variation

-Reason for N orbitals: interpretation, explicit antisymetrization, classical limit straightforward; better non-interacting v-representability? => same question in standard DFT

Internal Kohn-Sham (KS) scheme

Minimizing the total energy under orthonormality constraint:

$$\left(-\frac{\hbar^2}{2m}\Delta + U_{HXC}[\rho_{int}] + v_{int} \right)\varphi_{int}^i = \epsilon_i \varphi_{int}^i$$

where all quantum effects (including c.m. correlations) are described by the effective local potential:

$$U_{HXC}[\rho_{int}](\mathbf{r}) = \frac{\delta E_{HXC}[\rho_{int}]}{\delta\rho_{int}(\mathbf{r})}$$

All c.m. correlations effects can ultimately be accounted for by a local functional => question of the parameterization

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Within KS scheme, one-body orbitals φ_{int}^i are simply a mathematical intermediary that allow to compute the physical quantity ρ_{int}

In particular the "non-interacting" kinetic energy does not necessarily give a first order approximation of the true ("interacting") kinetic energy in the case of a self-bound system!

$$E_{\Delta kin}[\rho_{int}] = \underbrace{\int d\mathbf{r}_1 \cdots d\mathbf{r}_N \delta(\mathbf{R})\, \psi_{int}^*(\mathbf{r}_1, \ldots, \mathbf{r}_N) \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} \psi_{int}(\mathbf{r}_1, \ldots, \mathbf{r}_N)}_{\text{True ("interacting") kinetic energy}} - \underbrace{\sum_{i=1}^{N} (\varphi_{int}^i | \frac{\mathbf{p}^2}{2m} | \varphi_{int}^i)}_{\text{"non-interacting" kinetic energy of the KS system}}$$

True ("interacting") kinetic energy = $\underbrace{E_{\Delta kin}[\rho_{int}]}$ + "non-interacting" kinetic energy of the KS system

Not-small even for intermediary sized nuclei, because of c.m. correlations!

Origin of the quantum c.m. correlations?

In the c.m. frame, only the points of space that satisfy $\delta(\mathbf{R})=0$, i.e. $\sum_{j=1}^{N} \mathbf{r}_j = 0$, are allowed.

Because in quantum mechanics particles have zero-point motion, those motions must be coupled in the c.m. frame so that $\delta(\mathbf{R})=0$ is satisfied.
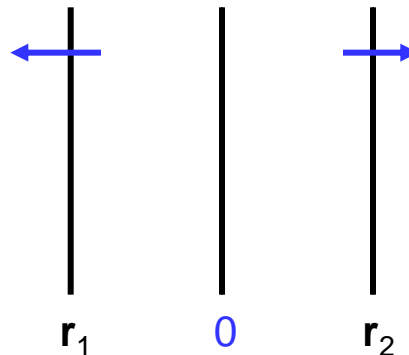
=> Purely quantum contribution to the c.m. correlations.

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$$\mathbf{r}_1 \qquad 0 \qquad \mathbf{r}_2$$

2 particles case, in the c.m. frame: if something tends to move the first particle in one direction, the second particle will tend to move in the opposite direction because of the c.m. correlations.

Existing generalizations of internal DFT / KS

- Bosons systems

- Time-dependent case (fusion, coulomb excitation, laser irradiation…)

- Multi-component systems (proton+neutron, mixtures of ^{3}He and ^{4}He, molecules where nuclei are treated explicitly and quantum mechanically)
    => includes standard DFT

2)   Proposition of a new local c.m. correlations functional

Theory

C.m. correlations parameterization

All c.m. correlations effects can ultimately be accounted for through a local functional => parameterization?

$$E_{HXC}[\rho_{int}] \;=\; \frac{1}{2} \int d\mathbf{r}\, d\mathbf{r}'\, \gamma_{int}[\rho_{int}](\mathbf{r}, \mathbf{r}')\, u(\mathbf{r} - \mathbf{r}') + E_{\Delta kin}[\rho_{int}] \;\longrightarrow$$

Hartree + total XC energy (including c.m correlations)
$\Rightarrow$ Well parameterized by standard effective
  interactions, apart from the c.m. correlations

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Only term of the functional where c.m. correlations appear explicitly
=> It is mostly this term that is not satisfyingly parameterized by standard effective interactions

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We thus have $E_{HXC}[\rho_{int}] = \underbrace{E_{HXC}^{stand}[\rho_{int}]}_{} + \underbrace{E_{cm}[\rho_{int}]}_{}$

Standard effective interactions (Skyrme…)

Approximation of $E_{\Delta kin}[\rho_{int}]$ where only c.m. correlation effects are considered

$\Rightarrow E_{cm}[\rho_{int}]$ can be evaluated from $E_{\Delta kin}[\rho_{int}]$, neglecting the exchange and « standard » correlations terms

An ansatz: $\sqrt{\delta(\mathbf{R})}\psi_{int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \approx \psi^{aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$, where $\psi^{aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N) = \dfrac{1}{\sqrt{N!}}\sum_P (-1)^p \Pi_{i=1}^N \varphi_{int}^{P(i)}(\mathbf{r}_i)$ is the KS Slater

determinant
(Nota: dimension OK.)

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determinant
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We obtain (standard correlations neglected by construction & exchange terms naturally cancel):

$$E_{\Delta kin}[\rho_{int}] \rightarrow E_{cm}^{stand}[\rho_{int}] = -\sum_{i=1}^N (\varphi_{int}^i|\frac{\mathbf{p}^2}{2mN}|\varphi_{int}^i) - \frac{1}{2mN}\sum_{i,j=1}^N (\varphi_{int}^i|\mathbf{p}|\varphi_{int}^i)(\varphi_{int}^j|\mathbf{p}|\varphi_{int}^j)$$

=> standard form for the c.m. correction.

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Limitation of ... the internal DET ... interfacing ? Holds if and only if our approximation holds at least to first order. Cannot be the case in general because

- ψ^{aux} is far from being null when $\sum_{i=1}^N \mathbf{r}_i \neq 0$,

- ψ^{aux} contains a c.m. vibration typical of Slater determinants $((\psi^{aux}|\mathbf{P}^n|\psi^{aux}) \neq 0$ for $n \geq 2)$, whereas $\sqrt{\delta(\mathbf{R})}\psi_{int}$ does not contain such a vibration $((\psi^{int}|\mathbf{P}^n|\psi^{int}) = 0, \forall n)$.

Why? In the ansatz, the c.m. correlations δ(**R**) are implicitly considered as included in the KS Slater determinant.

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Limitation of our method in the standard DFT point of view ?

Holds if and only if our approximation holds at least to first order. Cannot be the case in general because

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Why? In the ansatz, the c.m. correlations δ(**R**) are implicitly considered as included in the KS Slater determinant.

=> Find a better ansatz where the c.m. correlations, i.e. the δ(**R**), remains explicit.

Proposition of a better ansatz: $\sqrt{\delta(\mathbf{R})}\psi_{int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \quad \approx \quad \sqrt{\delta(\mathbf{R})}\dfrac{1}{\Gamma^{aux}(\mathbf{R})}\psi^{aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$

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We obtain (the pertinence of the ansatz will be explained further)

$$
\begin{aligned}
E_{\Delta kin}[\rho_{int}] \quad \rightarrow \quad E_{cm}[\rho_{int}] &= -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int d\mathbf{r}\,\Re e\Big\{\varphi_{int}^{i*}(\mathbf{r})\Delta_{\mathbf{r}}\varphi_{int}^{i}(\mathbf{r})\Big\}\Big[A\int d\mathbf{r}'\,|\varphi_{int}^{l\neq i}(\mathbf{r}')|^2 \times f_{i,l\neq i}(\mathbf{r}+\mathbf{r}') - 1\Big] \\
&\quad -\frac{\hbar^2}{2mN}B\int d\mathbf{r}\,|\varphi_{int}^{i}(\mathbf{r})|^2\int d\mathbf{r}'\,|\varphi_{int}^{l\neq i}(\mathbf{r}')|^2 \times f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')
\end{aligned}
$$

where A and B are 2 free-parameters (to be fit) defined by:

$$A = \frac{1}{|\Gamma^{aux}(\mathbf{0})|^2}$$

$$B = \Re e\Big\{\frac{1}{\Gamma^{aux*}(\mathbf{0})}\Delta_{\mathbf{R}}\frac{1}{\Gamma^{aux}(\mathbf{R})}\Big|_{\mathbf{R}=\mathbf{0}}\Big\}$$

and $f_{i,l\neq i}(\mathbf{r}) = \quad N^3\int \Pi_{\substack{j=1\\j\neq i,l}}^{N} d\mathbf{r}_j\,\delta\Big(\sum_{\substack{k=1\\k\neq i,l}}^{N}\mathbf{r}_k + \mathbf{r}\Big)\Pi_{\substack{j=1\\j\neq i,l}}^{N}|\varphi_{int}^{j}(\mathbf{r}_j)|^2$

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- real and has the dimension of a density
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- "multiconvolution" of all single densities, unless these are associated to orbitals i and l
- $\frac{1}{N^3}f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')$: is the probability that particle $l\neq i$ has position $\mathbf{r}'$, given that particle i has position $\mathbf{r}$ (because of the c.m. correlations the positions of those particles are not independent; every single orbital φ_{int}^{i} is coupled to every single orbital $\varphi_{int}^{l\neq i}$ through $f_{i,l\neq i}$)

Proposition of a better ansatz: $\sqrt{\delta(\mathbf{R})}\psi_{int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \approx \sqrt{\delta(\mathbf{R})}\frac{1}{\Gamma^{aux}(\mathbf{R})}\psi^{aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$

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C.m correlations now appear explicitly in the functional:

$$f_{i,l\neq i}(\mathbf{r}) = 2^3\delta(\mathbf{r}) \qquad\qquad\qquad\qquad\qquad\qquad\qquad if \quad N=2$$

$$3^3|\varphi_{int}^{k\neq i,l}(-\mathbf{r})|^2 \qquad\qquad\qquad\qquad\qquad if \quad N=3$$

$$N^3\int \Pi_{\substack{j=1\\j\neq i,l,m}}^N d\mathbf{r}_j\,\Pi_{\substack{j=1\\j\neq i,l,m}}^N |\varphi_{int}^j(\mathbf{r}_j)|^2|\varphi_{int}^m\big(-\sum_{\substack{k=1\\k\neq i,l,m}}^N \mathbf{r}_k - \mathbf{r}\big)|^2 \qquad if \quad N\geq 4$$

$$\ldots$$

$$Constant \qquad\qquad\qquad\qquad\qquad for\ very\ large\ N\ (limit\ of\ a\ Fermi\ gas)$$

$$E_{\Delta kin}[\rho_{int}] \quad \rightarrow \quad E_{cm}[\rho_{int}] = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \int d\mathbf{r} \, \Re e\Big\{\varphi_{int}^{i*}(\mathbf{r})\Delta_\mathbf{r}\varphi_{int}^i(\mathbf{r})\Big\}\Big[A \int d\mathbf{r}' \, |\varphi_{int}^{l\neq i}(\mathbf{r}')|^2 \times f_{i,l\neq i}(\mathbf{r}+\mathbf{r}') - 1\Big]$$

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Numerical considerations:

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Numerical considerations:

-Fit A & B simultaneously with Skyrme (…) force parameters

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$$-\frac{\hbar^2}{2mN} B \int d\mathbf{r}\ |\varphi_{int}^{i}(\mathbf{r})|^2 \int d\mathbf{r}'\ |\varphi_{int}^{l\neq i}(\mathbf{r}')|^2 \times f_{i,l\neq i}(\mathbf{r}+\mathbf{r}')$$

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-Other solution: A is given by a normalization condition (see article);
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Numerical cost of the scheme = cost of computation of the multi-convolution $f_{i,l\neq i}(\mathbf{r})$
= (N+1) FFT when N≥4

Pertinence of the new ansatz $\sqrt{\delta(\mathbf{R})}\psi_{int}(\mathbf{r}_1,\ldots,\mathbf{r}_N) \approx \sqrt{\delta(\mathbf{R})}\frac{1}{\Gamma^{aux}(\mathbf{R})}\psi^{aux}(\mathbf{r}_1,\ldots,\mathbf{r}_N)$?

-$\delta(\mathbf{R})$ remains explicit

-$\Gamma^{aux}(\mathbf{R})$ allows to recover good dimensions

is coherent with a well known analytical solution (harmonic oscillator case)

is coherent with anti-symmetrization

is considered as an additional "degree of liberty" that allows effective subtraction

of c.m. vibration from $\cdot\psi^{aux}$

leads to a result that has clear a physical meaning (see below)

Numerical results

Two different particles with a strong interaction (1D)

1D & 2 different particles => maximizes c.m. correlations effects

Strong (parabolic) interaction:
may model a deuterium nuclei

$$
\begin{aligned}
H &= \frac{p^{(1)^2}}{2m} + \frac{p^{(1)^2}}{2m} + \frac{1}{4}m\omega^2(r^{(1)} - r^{(2)})^2 \\
H_{int} &= \frac{\tau^2}{2\mu} + \frac{1}{2}\mu\omega^2\xi^2
\end{aligned}
$$

A benchmark (analytical) solution ($l=1,2$):

$$
\begin{aligned}
E_{int} &= \tfrac{1}{2}\hbar\omega \\
\rho_{int}^{(l)}(r) &= \int dr^{(1)}dr^{(2)}\delta(R)|\psi_{int}(r^{(1)} - r^{(2)})|^2\delta\big(r - (r^{(l)} - R)\big) \\
&= \sqrt{\frac{2m\omega}{\pi\hbar}}\exp\left\{-\frac{2m\omega}{\hbar}r^2\right\}
\end{aligned}
$$

Two different particles with a strong interaction (1D)

-Hartree part (no exchange): $E_H[\rho_{int}^{(1)}, \rho_{int}^{(2)}]$

- Exact internal DFT (very simple form valid only in the considered case):

$$E_{HXC}[\rho_{int}^{(1)}, \rho_{int}^{(2)}] = \int dr \frac{1}{2}\Big(\rho_{int}^{(1)}(r) + \rho_{int}^{(2)}(r)\Big)m\omega^2 r^2$$

$$E_{\Delta kin}[\rho_{int}^{(1)}, \rho_{int}^{(2)}] = -\frac{3}{2}\hbar\omega + \frac{3}{2}\int dr\Big(\rho_{int}^{(1)}(r) + \rho_{int}^{(2)}(r)\Big)m\omega^2 r^2$$

- Our proposed approximation + "Gaussian set" ($\Gamma^{aux}(R) = \left(\frac{K}{\pi}\right)^{1/4}\exp\left\{-\frac{K}{2}R^2\right\}$)

$$E_{cm}[\varphi_{int}^{(1)}, \varphi_{int}^{(2)}] = -\frac{\hbar^2}{2m}\int dr\left[\varphi_{int}^{(1)*}(r)\Delta_r\varphi_{int}^{(1)}(r)\Big(2\sqrt{\frac{\pi}{K}}|\varphi_{int}^{(2)}(-r)|^2 - 1\Big) + \varphi_{int}^{(2)*}(r)\Delta_r\varphi_{int}^{(2)}(r)\Big(2\sqrt{\frac{\pi}{K}}|\varphi_{int}^{(1)}(-r)|^2 - 1\Big)\right]$$
$$-\frac{\hbar^2}{2m}\sqrt{K\pi}\int dr|\varphi_{int}^{(1)}(r)|^2|\varphi_{int}^{(2)}(-r)|^2$$

-Standard approximation:

$$E_{cm}^{stand}[\varphi_{int}^{(1)}, \varphi_{int}^{(2)}] \rightarrow -\sum_{i=1}^{\cdot\cdot}(\varphi_{int}^i|\frac{\mathbf{P}^2}{2mN}|\varphi_{int}^i)$$

Next figures:

- "H only": E_H
- "H + standard correlations": E_{HXC}
- "H + standard correlations + standard c.m. correction": $E_{HXC} - <\frac{\mathbf{P}^2}{2mN}>$
- "internal DFT with c.m. correlations functional": $E_{HXC} + E_{cm}$
- "exact internal DFT": $E_{HXC} + E_{\Delta kin}$
- benchmark

Two different particles with a strong interaction (1D)

The internal densities $\rho_{int}^{(1)}$ and $\rho_{int}^{(2)}$ of the various formalisms (x-axis: position in units where $\hbar = m = 1$).
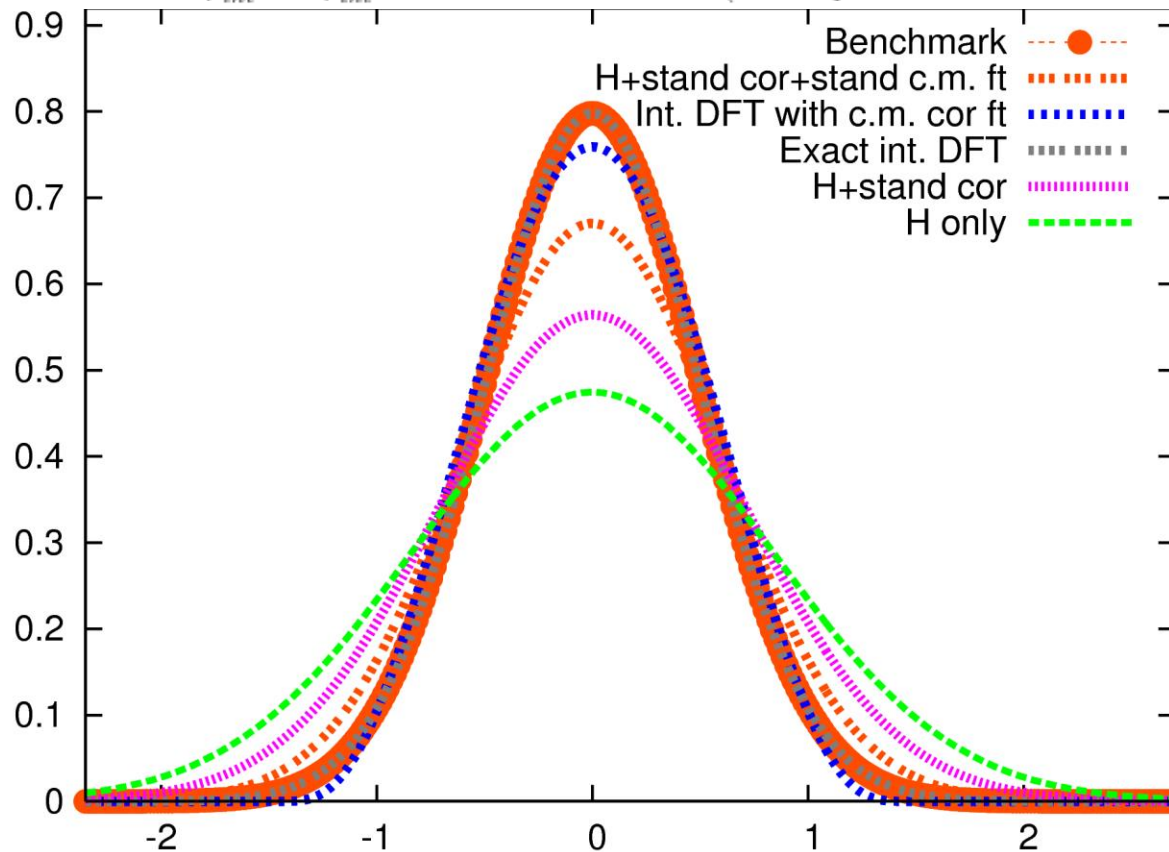
Int. DFT with c.m. cor. ft.:

-represents a great improvement

-cannot be exact in this case because we did not model the standard correlations part of $E_{\Delta kin}\left[\rho_{int}^{(1)}, \rho_{int}^{(2)}\right]$

=> Result even more close when use effective interactions

Two different particles with a strong interaction (1D)

True ("interacting") kinetic energy = $\underbrace{E_{\Delta kin}[\rho_{int}]}$ + "non-interacting" kinetic energy of the KS system

Not-small even for intermediary sized nuclei, because of c.m. correlations!

Energies of the various formalisms

(in units where $\hbar = m = 1$; benchmark: total energy = 0.50; and interacting kinetic energy $(\psi_{int}|\frac{\tau^2}{2\mu}|\psi_{int}) = 0.25$).

	Non-interacting kin. energy	E_H	E_C	$-<\frac{\mathbf{P}^2}{2mN}>$ or $E_{\Delta kin}$ or E_{cm}	Total energy
H only	0.353	0.353	0	0	0.71
H + stand. corr.	0.5	0.25	0.25	0	1.00
H + stand. corr. + stand. c.m. correct.	0.706	0.177	0.177	-0.353	0.71
Internal DFT with c.m. corr. ft	1.225	0.120	0.120	-0.918	0.55
Exact internal DFT	1.000	0.125	0.125	-0.750	0.50

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Our c.m. correlations functional allows us to recover confidently the interacting (true) kinetic energy.

Many identical bosons with a smooth interaction (1D)

Smooth attractive interaction:
$$u(r - r') = -\frac{1}{\sqrt{(r - r')^2 + e}}$$

$$E_{int}[\rho_{int}] = N(\varphi_{int}|\frac{p^2}{2m}|\varphi_{int}) + E_{HXC}[\rho_{int}] + E_{\Delta kin}[\rho_{int}]$$

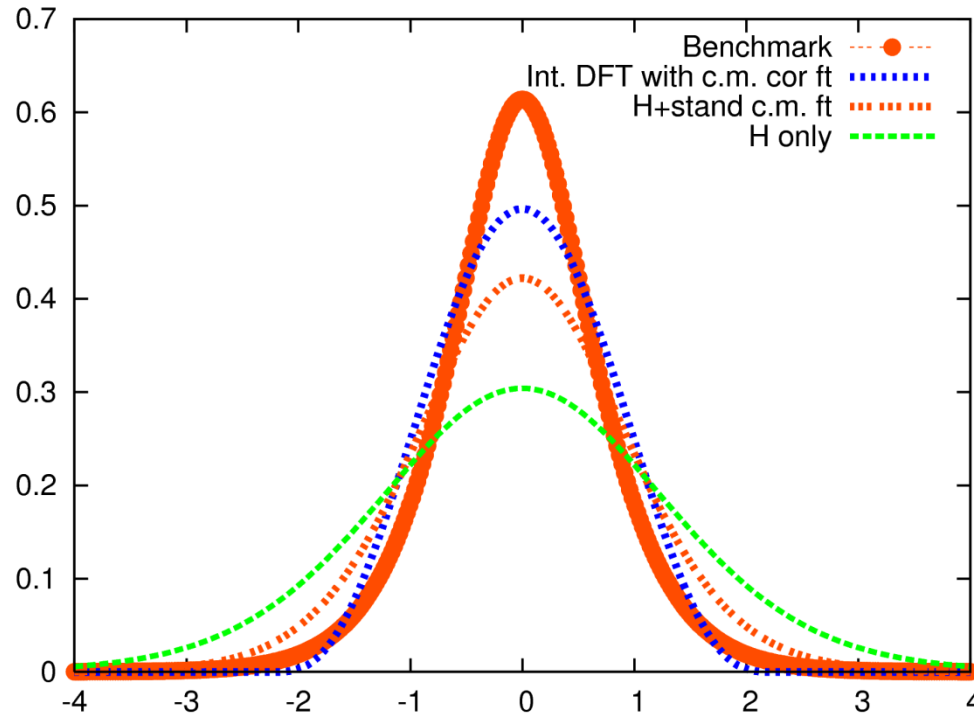$$E_{HXC}[\rho_{int}] = E_H[\rho_{int}] \times (1 - \frac{1}{N}) + E_C[\rho_{int}]$$

$$E_{cm}[\rho_{int}] = -\frac{\hbar^2}{2m} \int dr \ \sqrt{\rho_{int}(r)} \Delta_{\mathbf{r}} \sqrt{\rho_{int}(r)} \times \left(\sqrt{\frac{\pi}{K(N)}} \int dr' \ \frac{1}{N}\rho_{int}(r')f(r + r') - 1 \right)$$

$$- \frac{\hbar^2}{2mN} \sqrt{\pi K(N)} \int dr \ \frac{1}{N}\rho_{int}(r) \int dr' \ \frac{1}{N}\rho_{int}(r')f(r + r')$$

Next results:
- "H only": $E_H \times (1 - \frac{1}{N})$
- "H + standard c.m. correction": $E_H \times (1 - \frac{1}{N}) - < \frac{\mathbf{p}^2}{2mN} >$, called
- "internal DFT with c.m. correlations functional": $E_H \times (1 - \frac{1}{N}) + E_{cm}$
- benchmark (for the $N = 2$ case only)

2 bosons:

Internal density $\rho_{int}/2$ of the various formalisms in the $N = 2$ case (x-axis: position in units where $\hbar = m = 1$).

We here have neglected all standard correlations
$\Rightarrow$Result much closer when use effective interactions

Nevertheless same conclusions than previously.

Energies of the various formalisms in the $N = 2$ case
(in units where $\hbar = m = 1$; benchmark: total energy $= -0.59$; and interacting kinetic energy $(\psi_{int}|\frac{\tau^2}{2\mu}|\psi_{int}) = 0.12$).

	Non-interacting kin. energy	$E_H \times (1 - \frac{1}{N})$	$- < \frac{\mathbf{P}^2}{2mN} >$ or E_{cm}	Total energy
H only	0.133	-0.626	0	-0.49
H + stand. c.m. correct.	0.260	-0.712	-0.065	-0.52
Internal DFT with c.m. corr. ft	0.535	-0.776	-0.418	-0.66

# Many identical bosons with a smooth interaction (1D)

Many bosons:

"Internal DFT with c.m. corr. ft." energies for various N (in units where $\hbar = m = 1$).

N	Non-interacting kin. energy	E_{cm}	Total energy	K	Interacting kin. energy
2	0.535	-0.418	-0.66	1.94	0.117
3	0.463	-0.185	-1.90	1.74	0.278
4	0.702	-0.196	-3.97	2.74	0.507
5	1.014	-0.217	-6.84	4.01	0.799
6	1.390	-0.239	-10.56	4.54	1.151

Non-interacting kinetic energy tends to become closer to interacting (true) kinetic energy

Internal density $\rho_{int}/6$ of the various formalisms in the $N = 6$ case (x-axis: position in units where $\hbar = m = 1$).
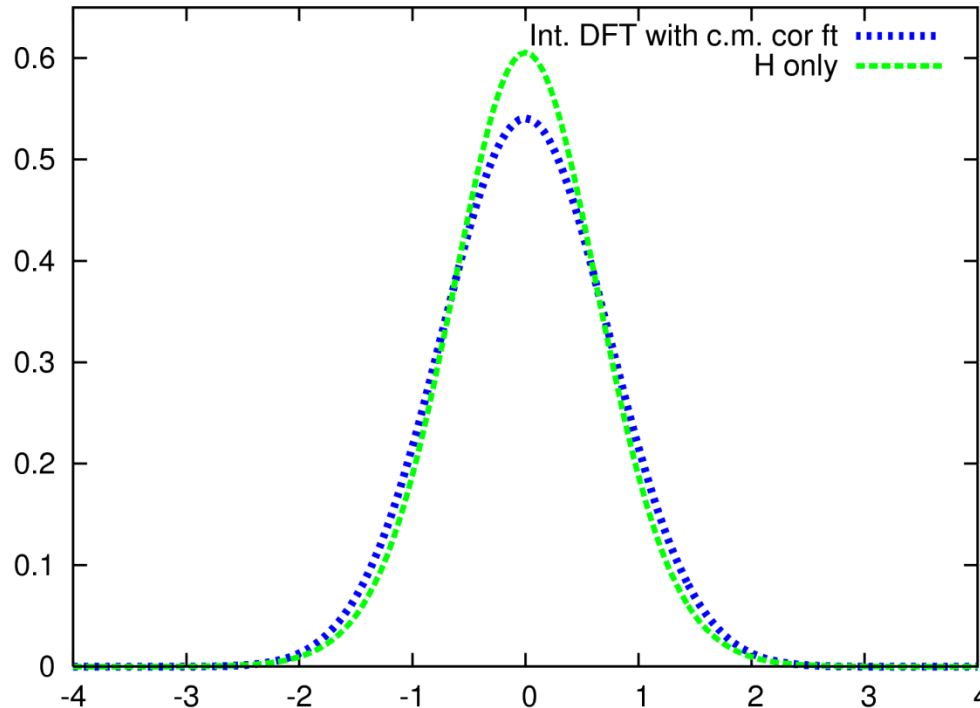
Our c.m correlations functional acts less and less (on average) when N increases.

Conclusion

- Well-founded alternative to projection techniques to treat the c.m. correlations.

- Numerically manageable scheme, even for time-dependent situations.

- The new functional can directly be added to actual energy functionals although a simultaneous fitting of them would be necessary.

- Permits us to recover the precise value of the interacting (true) kinetic energy.

Next step: include the proposed functional in realistic 3D calculations, for instance in mean-field-like calculations of nuclei with Skyrme interaction.
    => You are very welcome.

3)   On exactness of Kohn-Sham scheme (non-interacting v-representability?)

A problem inherent to standard DFT / KS

Using Levi-Lieb formulation applied to self-bound systems, we can show that the set of non-interacting densities is dense in the set of interacting densities.

Open question: Is non-interacting v-representability better achieved with a certain number of orbitals?

Prospects

Prospects

- **Local c.m. correlations potential**

Tests with realistic 3D nuclear codes. You're very welcome

Method adaptable to other symetries

- **Non-interacting v-representability related questions**

- **Generalization to any symmetry group**

=> T. Lesinski

… and certainly other suprises that do all the charms of Physics.

Thank you for your attention.

jeremie.messud@cgg.com