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Results on a 1D model.

Some numerical results

- A self-bound system with two particles of different kinds => the c.m. correlations are the most demanding for small systems

- A 1D model: more sensible to c.m. correlations effects

- A harmonic oscillator interaction (models proton + neutron):

$$H = \frac{p^{(1)^2}}{2m} + \frac{p^{(1)^2}}{2m} + \frac{1}{4}m\omega^2(r^{(1)} - r^{(2)})^2$$

$$H_{int} = \frac{\tau^2}{2\mu} + \frac{1}{2}\mu\omega^2\,\xi^{\,2}$$

- A benchmark:

Energy: $E_{int} = \frac{1}{2}\hbar\omega$

C.m. frame 1-body density:

$$\rho^{(l)}_{int}(r) = \int dr^{(1)}dr^{(2)}\delta(R)|\psi_{int}(r^{(1)} - r^{(2)})|^2\delta\big(r - (r^{(l)} - R)\big)$$

$$= \sqrt{\frac{2m\omega}{\pi\hbar}}\exp\Big\{-\frac{2m\omega}{\hbar}r^2\Big\}$$

Some numerical results

- The internal DFT energy:

$$E_{int}[\rho^{(1)}_{int},\rho^{(2)}_{int}] = (\varphi^{(1)}_{int}|\frac{p^2}{2m}|\varphi^{(1)}_{int}) + (\varphi^{(2)}_{int}|\frac{p^2}{2m}|\varphi^{(2)}_{int})$$
$$+E^{(12)}_{H}[\rho^{(1)}_{int},\rho^{(2)}_{int}] \longrightarrow \text{Hartree}$$
$$+E^{(12)}_{C}[\rho^{(1)}_{int},\rho^{(2)}_{int}] \longrightarrow \text{« Standard » correlations}$$
$$+E^{(12)}_{\Delta kin}[\rho^{(1)}_{int},\rho^{(2)}_{int}] \longrightarrow \text{« Standard » correlations + c.m. correlations}$$

- The exact density functionals (valid only for this system):

$$E^{(12)}_{H}[\rho^{(1)}_{int},\rho^{(2)}_{int}] = \int dr dr' \rho^{(1)}_{int}(r)\rho^{(2)}_{int}(r')\frac{1}{4}m\omega^2(r-r')^2$$

$$E^{(12)}_{C}[\rho^{(1)}_{int},\rho^{(2)}_{int}] = \int dr\, dr' \left[\gamma^{(12)}_{int}(r,r') - \rho^{(1)}_{int}(r)\rho^{(2)}_{int}(r')\right]\frac{1}{4}m\omega^2(r-r')^2$$
$$= \int dr \frac{1}{2}\Big(\rho^{(1)}_{int}(r)+\rho^{(2)}_{int}(r)\Big)m\omega^2 r^2 - \int dr\, dr' \rho^{(1)}_{int}(r)\rho^{(2)}_{int}(r')\frac{1}{4}m\omega^2(r-r')^2$$

$$E^{(12)}_{\Delta kin}[\rho^{(1)}_{int},\rho^{(2)}_{int}] = \sum_{l=1}^{2}\Big[\int dr^{(1)}dr^{(2)}\delta(R)\psi^{*}_{int}(r^{(1)}-r^{(2)})\frac{p^{(l)2}}{2m}\psi_{int}(r^{(1)}-r^{(2)}) - (\varphi^{(1)}_{int}|\frac{p^2}{2m}|\varphi^{(1)}_{int})\Big]$$
$$= -\frac{3}{2}\hbar\omega + \frac{3}{2}\int dr\Big(\rho^{(1)}_{int}(r)+\rho^{(2)}_{int}(r)\Big)m\omega^2 r^2$$

Some numerical results

- A proposition for the c.m. correlation functional:

$$E_{\Delta kin} = E_{\Delta kinXC} + E_{cm}$$

« Standard » correlations

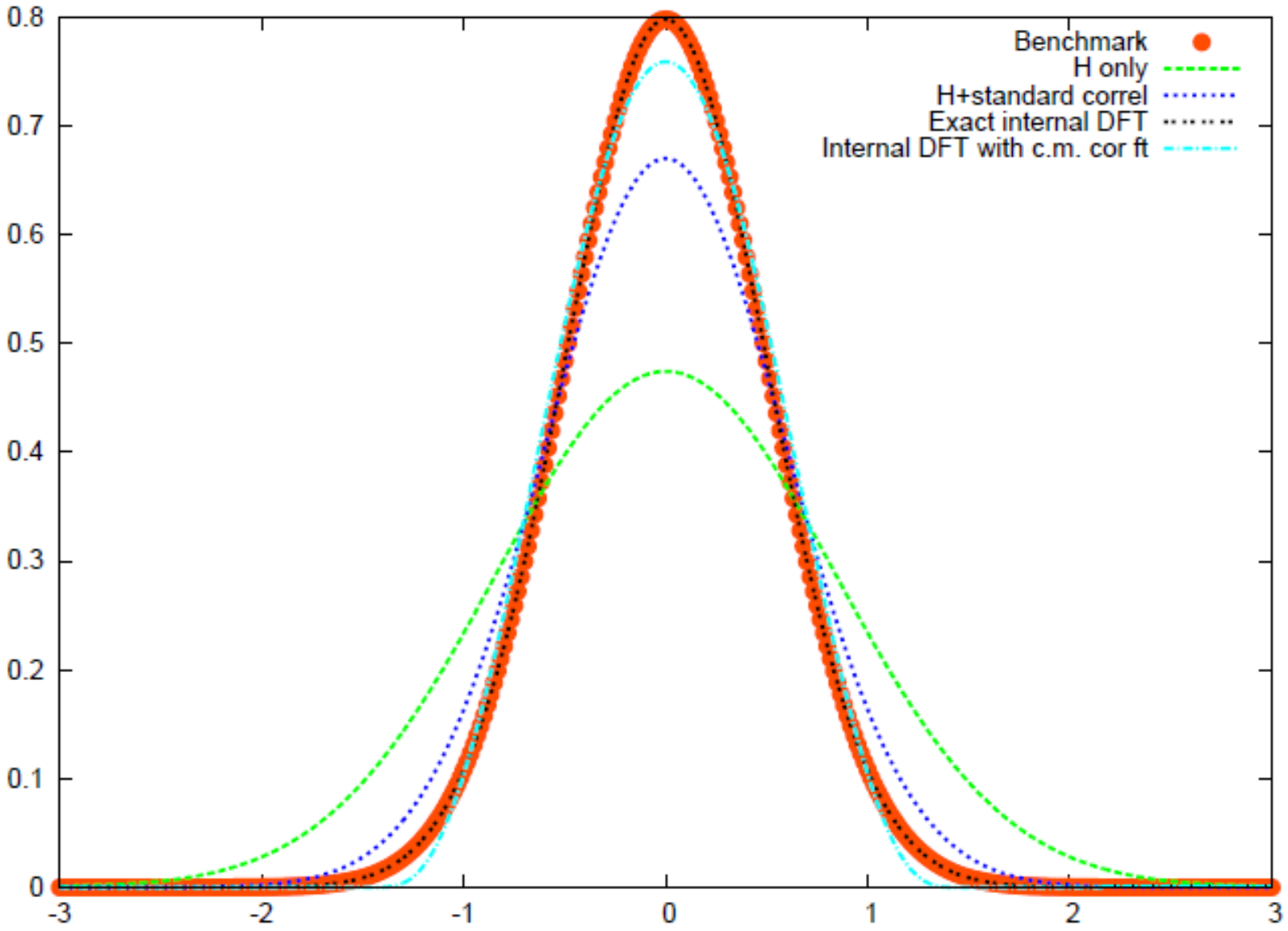
Mostly included in actual realistic parametrized functionals

C.m. correlations

The proposed functional (in progress):

$$E_{cm}^{(12)} = -\frac{\hbar^2}{2m}\int dr\left[\varphi_{int}^{(1)*}(r)\Delta_r\varphi_{int}^{(1)}(r)\left(2\sqrt{\frac{\pi}{K}}|\varphi_{int}^{(2)}(-r)|^2 - 1\right) + \varphi_{int}^{(2)*}(r)\Delta_r\varphi_{int}^{(2)}(r)\left(2\sqrt{\frac{\pi}{K}}|\varphi_{int}^{(1)}(-r)|^2 - 1\right)\right]$$
$$-\frac{\hbar^2}{2m}\sqrt{K\pi}\int dr|\varphi_{int}^{(1)}(r)|^2|\varphi_{int}^{(2)}(-r)|^2$$

Some numerical results



Some numerical results

Formalism	Non-interacting kin. energy	$E_H^{(12)}$	$E_C^{(12)}$	$E_{\Delta kin}^{(12)}$ or E_{cm}	Total energy
H only	0.353	0.353	0	0	0.71
H + standard corr.	0.706	0.177	0.177	0	1.06
Exact internal DFT	1.000	0.125	0.125	-0.750	0.50
Internal DFT with c.m. corr. ft	1.275	0.115	0.115	-1.001	0.50

TABLE I: The energies of the various formalisms (in units where $\hbar = m = 1$;total energy of the benchmark = 0.50, with $(\psi_{int}|\frac{\tau^2}{2\mu}|\psi_{int}) = (\psi_{int}|\frac{1}{2}\mu\omega^2\xi^2|\psi_{int}) = 0.25$).

Interacting kinetic energy = non-interacting kinetic energy + $E_{cm}^{(12)}$ ~ 0.25

=> One has to be cautious with the meaning that is given to the non-interacting kinetic energy in mean-field like calculations: it cannot be interpreted as a first order approximation of the kinetic energy of the interacting system, at least for small self-bound systems.

Prospects

- Local c.m. correlations potential

- To be published soon; tests on 1D models in progress
- Tests on fully realistic 3D nuclear codes ? You're very welcome

- Non-interacting v-representability related questions

- Adaptation of the Lieb constrained search formalism and other funny mathematical but fundamental stuff to answer some open questions

- Generalization to any symmetry group ?

- Study under which conditions there is a decoupling for the kinetic energy term
- Should shed some light on the symmetry breaking question

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

Thank you for your attention

- Stationary internal DFT: J. Messud, M. Bender, E. Suraud, Phys. Rev. C **80**, 054314 (2009)
- Time-dependent internal DFT: J. Messud, Phys. Rev. C **80**, 054614 (2009)
- Multicomponent internal DFT: J. Messud, Phys. Rev. A **84**, 052113 (2011)
- Local c.m. correlations potential: J. Messud, to be submitted soon