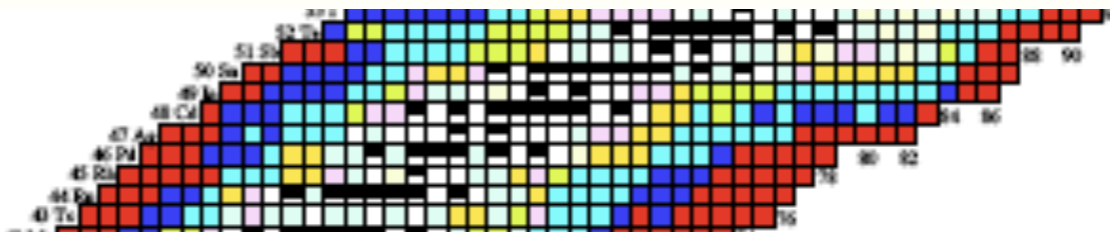


Nuclear Energy Density Functionals

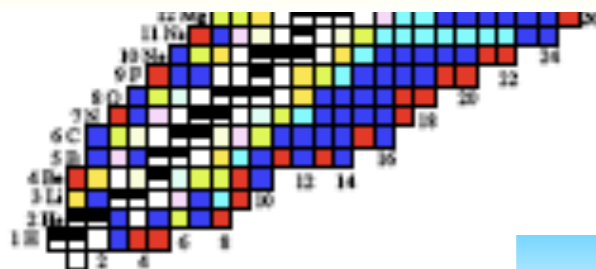
✓ the quantum many-body problem is effectively mapped onto a *one-body problem* without explicitly involving inter-particle interactions!



✓ the exact density functional is approximated with *powers and gradients of ground-state densities and currents*.



✓ *universal density functionals* can be applied to all nuclei throughout the chart of nuclides.



Important for extrapolations to regions far from stability!

... accurate and controlled approximations for the nuclear exchange-correlation energy functional

... microscopic foundation for a universal EDF framework, related to and constrained by low-energy QCD

... correlations related to restoration of broken symmetries and fluctuations of collective coordinates

Kohn-Sham DFT

... uses single-particle orbitals to predict the ground-state density, energy, and related properties → useful compromise between accuracy and computational efficiency.

For any interacting system, there exists a **local single-particle (Kohn-Sham) potential**, such that the exact ground-state density equals the ground-state density of a non-interacting system:

$$n(\mathbf{r}) = n_s(\mathbf{r}) \equiv \sum_i^{occ} |\phi_i(\mathbf{r})|^2$$

The single-particle orbitals are solutions of the Kohn-Sham equations:

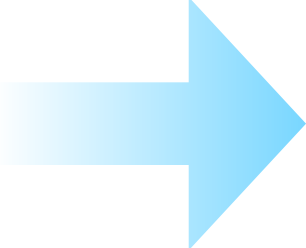
$$\left[-\nabla^2/2 + v_s(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

⇒ Kohn-Sham potential:

$$v_s[n(\mathbf{r})] = v(\mathbf{r}) + \int d^3r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[n(\mathbf{r})]$$

the *exchange-correlation potential* is defined by:

$$v_{xc}[n(\mathbf{r})] = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}$$



self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the Hartree-Fock. It has the advantage of being a *local scheme*.

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found!

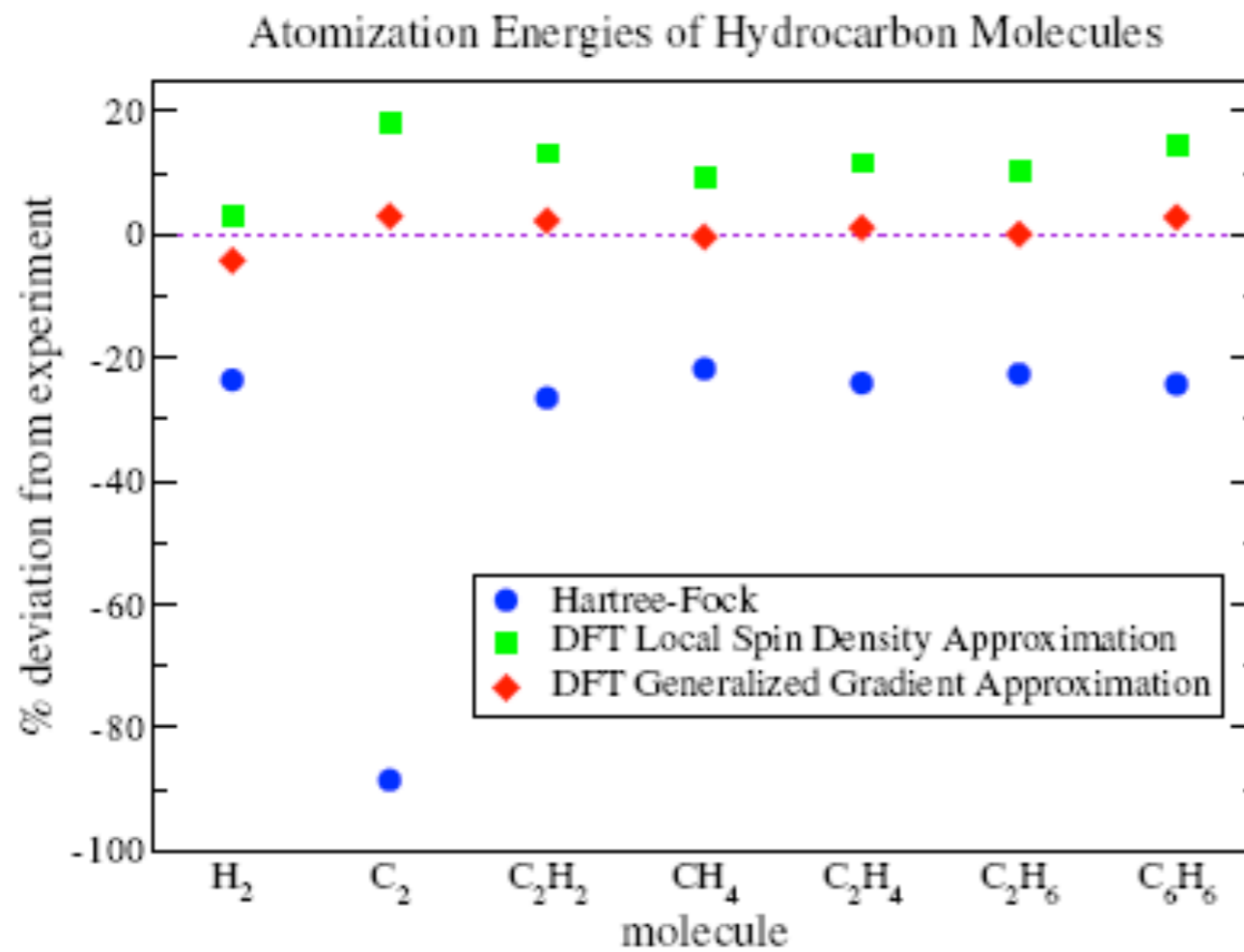
Is there a systematic way to construct density functionals?

Develop E_{xc} from first principles by incorporating known exact constraints.

Empirical approach: a parametric ansatz is optimized by adjusting it to a set of data. Modern approximations for E_{xc} typically combine both strategies.

Exchange-correlation functional \Rightarrow Jacob's ladder of DFT approximations for E_{xc}

Heaven of chemical accuracy



unoccupied $\{\Psi_i\}$

$\{\Psi_i\}$

E_x

\mathcal{T} and/or $\nabla^2 \rho$

$\nabla \rho$

ρ



generalized RPA

hyper-GGA

meta-GGA

GGA

LDA

Hartree world

TABLE I. Atomization energies of molecules, in kcal/mol (1 eV = 23.06 kcal/mol). E_{XC} has been evaluated on self-consistent densities at experimental geometries [33]. Nonspherical densities and Kohn-Sham potentials have been used for open-shell atoms [34]. The calculations are performed with a modified version of the CADPAC program [35]. The experimental values for ΔE (with zero point vibration removed) are taken from Ref. [36]. PBE is the simplified GGA proposed here. UHF is unrestricted Hartree-Fock, for comparison.

System	ΔE^{UHF}	ΔE^{LSD}	ΔE^{PW91}	ΔE^{PBE}	ΔE^{expt}
H ₂	84	113	105	105	109
LiH	33	60	53	52	58
CH ₄	328	462	421	420	419
NH ₃	201	337	303	302	297
OH	68	124	110	110	107
H ₂ O	155	267	235	234	232
HF	97	162	143	142	141
Li ₂	3	23	20	19	24
LiF	89	153	137	136	139
Be ₂	-7	13	10	10	3
C ₂ H ₂	294	460	415	415	405
C ₂ H ₄	428	633	573	571	563
HCN	199	361	326	326	312
CO	174	299	269	269	259
N ₂	115	267	242	243	229
NO	53	199	171	172	153
O ₂	33	175	143	144	121
F ₂	-37	78	54	53	39
P ₂	36	142	120	120	117
Cl ₂	17	81	64	63	58
Mean abs. error	71.2	31.4	8.0	7.9	...

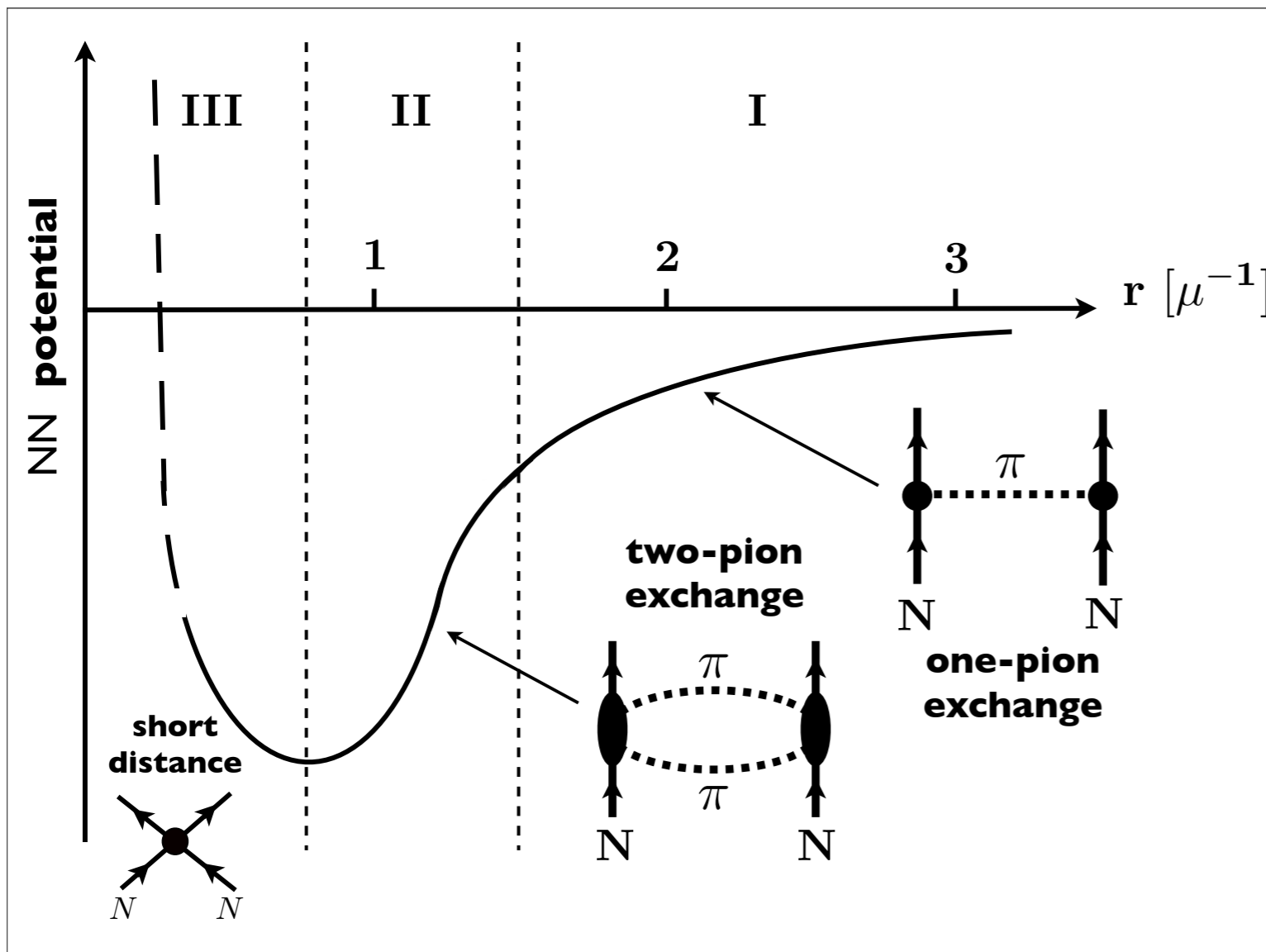
Mean absolute error of the atomization energies for 20 molecules:

Approximation	Mean abs. error (eV)
Unrestricted Hartree-Fock	3.1 (underbinding)
LDA	1.3 (overbinding)
GGA	0.3 (mostly overbinding)
Desired “chemical accuracy”	0,05

⇒ Multiply by 10^6 and compare with the nuclear case!

The description of **nuclear many-body systems** must be related to and constrained by **low-energy QCD**.

A **microscopic nuclear energy density functional** must include the **exchange-correlation part**, starting from the relevant active degrees of freedom at low energy:
PIONS & NUCLEONS



An **effective field theory** of low-energy in-medium NN interactions can be used to construct approximations to **the exact exchange-correlation functional**.

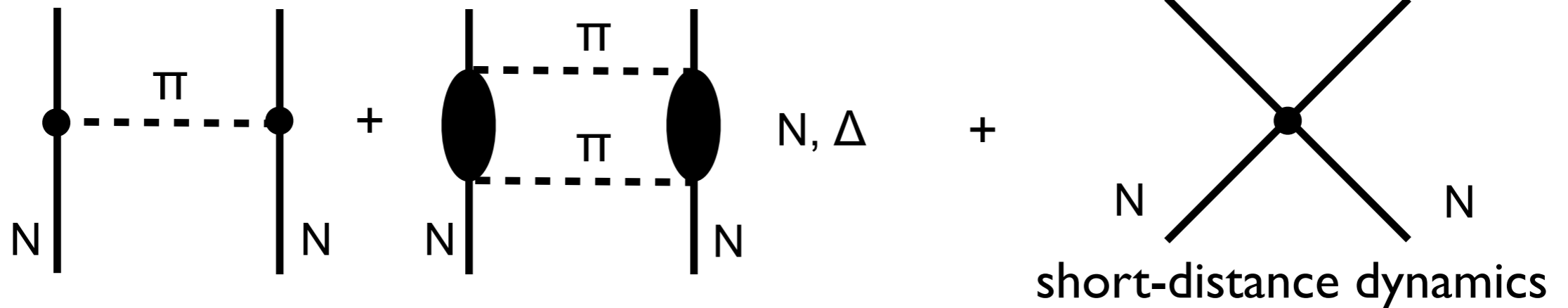
In the nuclear medium:



relevant scale:
Fermi momentum

$$k_f \approx 2m_\pi \ll 4\pi f_\pi$$

pion-exchange processes in the presence of a filled Fermi sea:



The density functional involves an expansion of nucleon self-energies in **powers of the Fermi momentum.**

Chiral (pionic) fluctuations in combination with three-nucleon (3N) interactions determine **nuclear binding and saturation.**

...exchange-correlation functional $E_{xc}[\rho] \Rightarrow$ universal functional of the density:

1st step: Local Density Approximation

$$E_{xc}^{LDA}[n] = \int d^3r n(\mathbf{r}) e_{xc}^{unif}[n(\mathbf{r})]$$

2nd step: second-order gradient correction to the LDA

Calculations for inhomogeneous nuclear matter:

$$\mathcal{E}(\rho, \nabla\rho) = \rho \bar{E}(k_f) + (\nabla\rho)^2 F_{\nabla}(k_f) + \dots$$

\Rightarrow generalized gradient approximations (GGAs):

$$E_{xc}^{GGA}[n] = \int d^3r f[n(\mathbf{r}), \nabla n(\mathbf{r})]$$

The function f is not unique and, depending on the method of constructing f , very different GGAs can be obtained.

etc.

Infinite nuclear matter cannot determine the density functional on the level of accuracy that is needed for a quantitative description of structure phenomena in finite nuclei.

... start from a favorite microscopic nuclear matter EOS.

... the parameters of the functional are fine-tuned to data of finite nuclei.

Which nuclei?

Which data?

Correlations between parameters?

Accuracy of the fit?