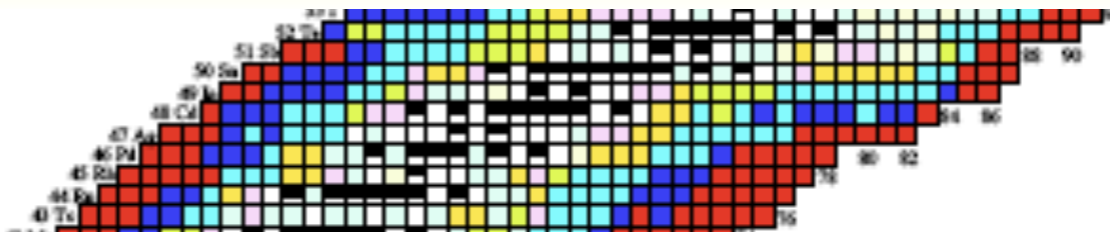# Nuclear Energy Density Functionals
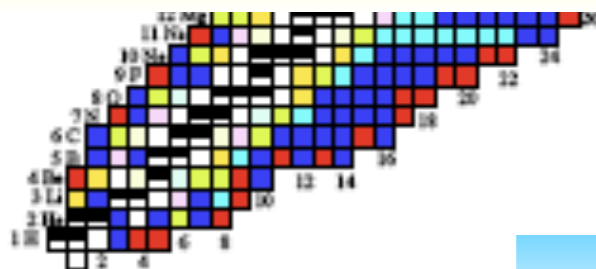
✔ the quantum many-body problem is effectively mapped onto a *one-body problem* without explicitly involving inter-particle interactions!

✔ 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!

Open questions

... 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:

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

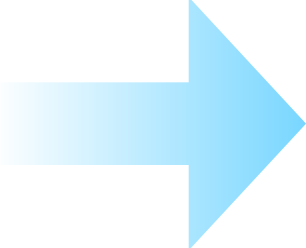The single-particle orbitals are solutions of the Kohn-Sham equations:

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

⇒ Kohn-Sham potential:

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

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!
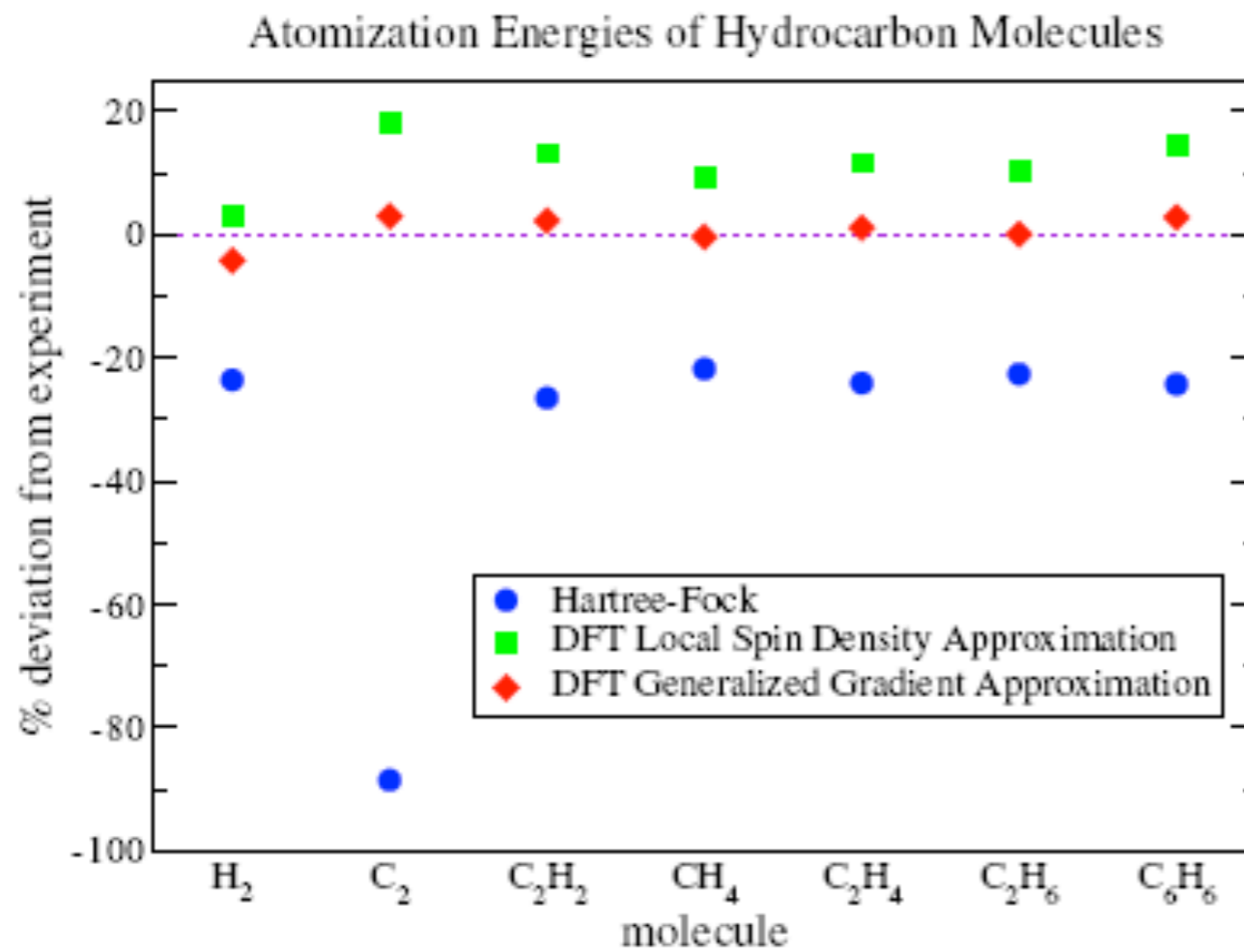
Is there a systematic way to construct density functionals?

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.

Heaven of chemical accuracy

unoccupied $\left\{\Psi_i\right\}$ generalized RPA

$\mathcal{E}_x$ hyper-GGA

τ and/or $\nabla^2\rho$ meta-GGA

$\nabla\rho$ GGA

ρ LDA

Hartree world

Atomization Energies of Hydrocarbon Molecules

% deviation from experiment vs molecule (H_2, C_2, C_2H_2, CH_4, C_2H_4, C_2H_6, C_6H_6)

Legend:
- Hartree-Fock
- DFT Local Spin Density Approximation
- DFT Generalized Gradient Approximation

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_2O	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_2H_2	294	460	415	415	405
C_2H_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	⋯

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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

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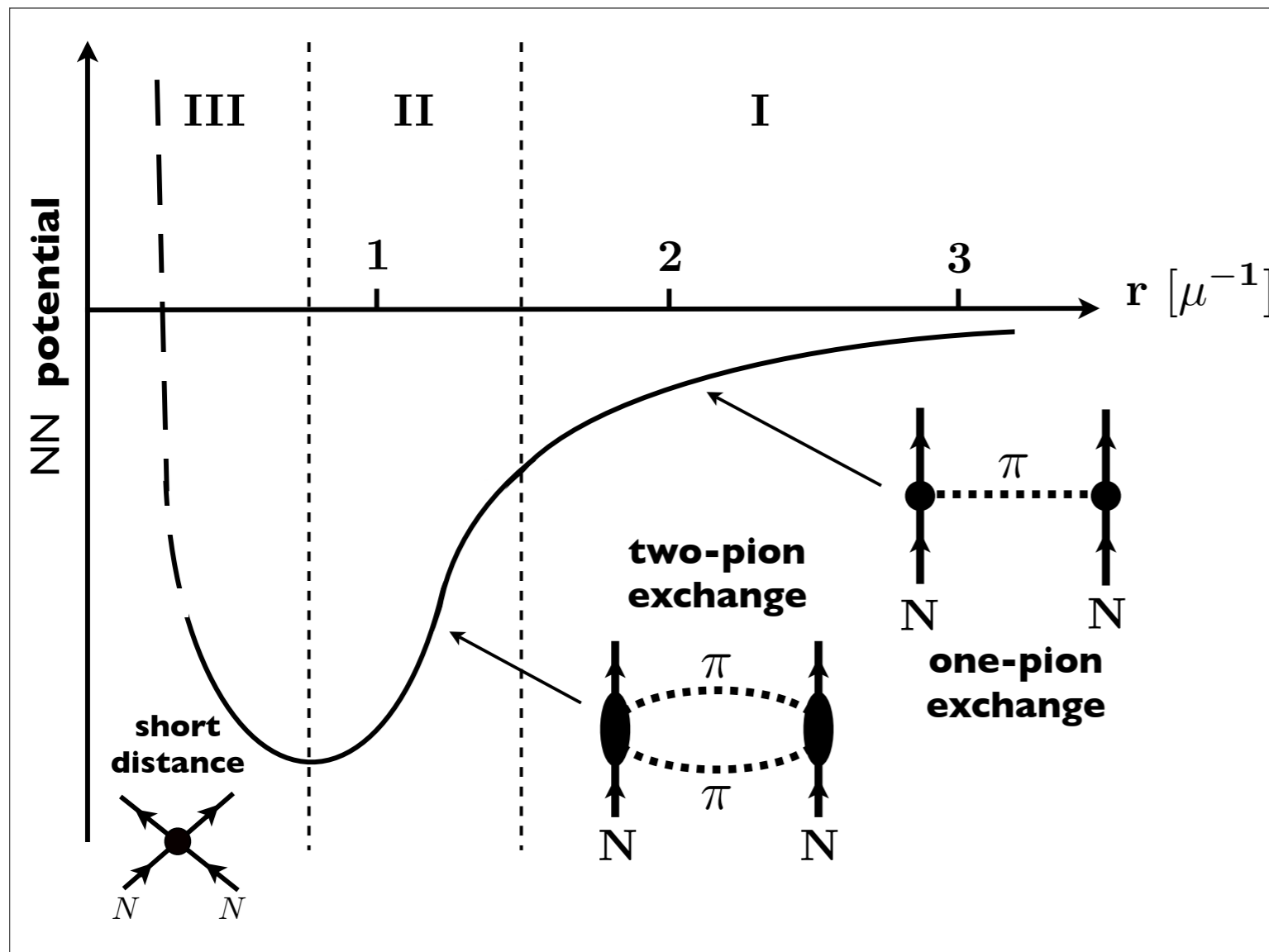
An *effective field theory* of low-energy in-medium NN interactions can be used to construct approximations to *the exact exchange-correlation functional.*

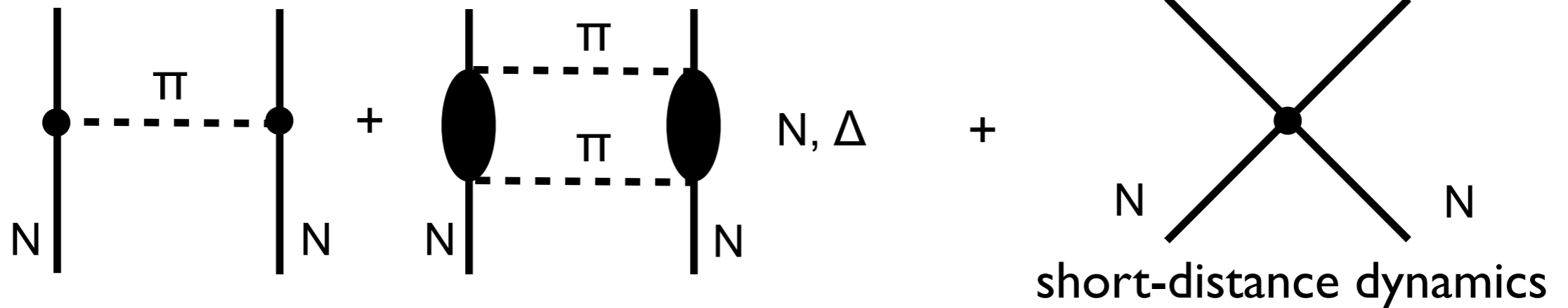In the nuclear medium:

➡ the relevant scale:
Fermi momentum

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

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

short-distance dynamics

The density functional involves an expansion in *powers of the Fermi momentum.*

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:

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

⇒ 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?