Correlations

Explicitly included at the mean-field level:

- Statistics (fermions)
- Pairing (BCS or HFB)
- Deformation (can bring up to 20 MeV!)

Absent:

- Symmetry restoration
- Configuration mixing (shape, multi qp excitations, …)

Can all missing correlations be included in the interaction?
("DFT spirit")

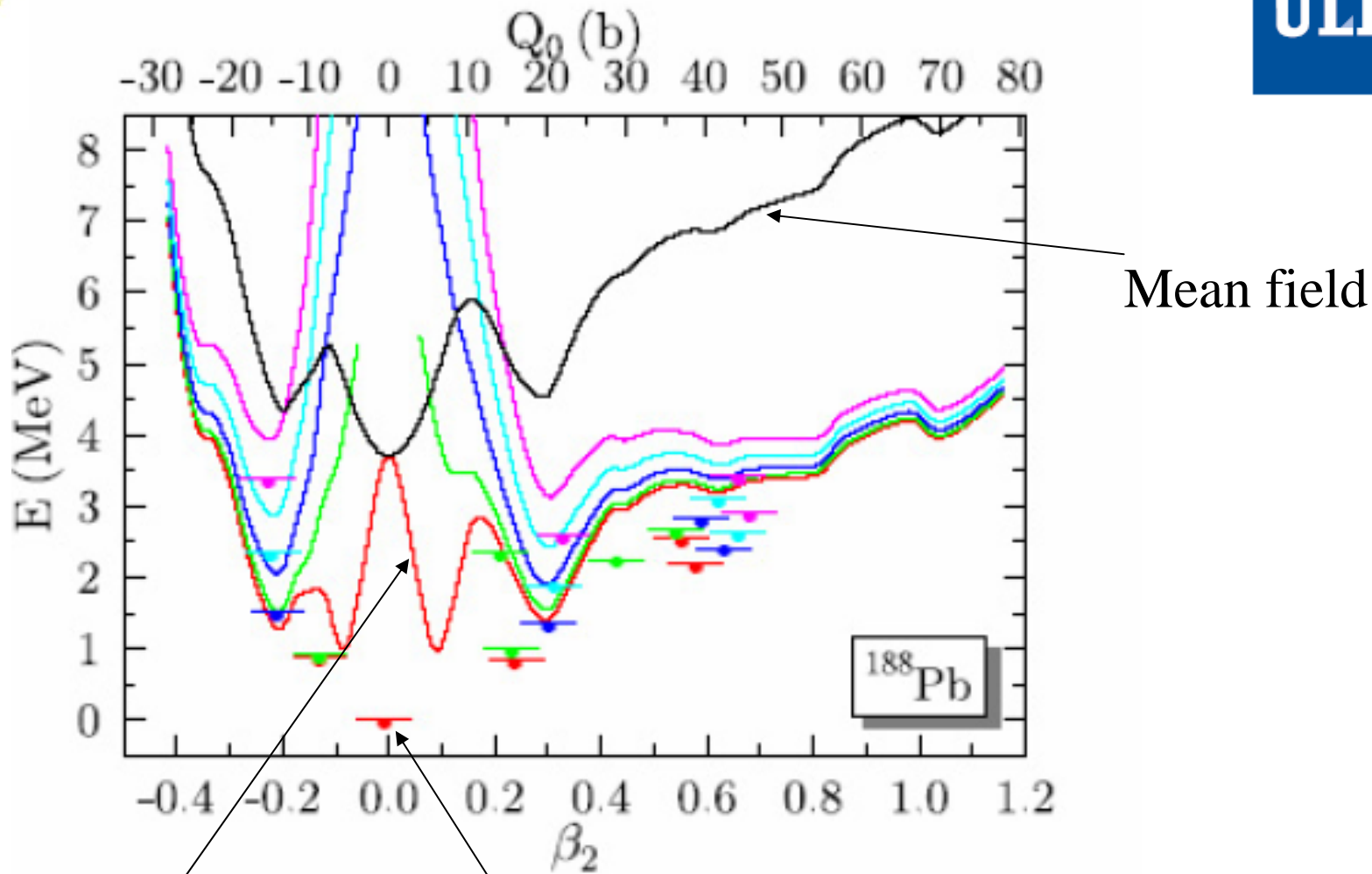Set of mean-field wave functions depending on axial q

- Projection on N, Z, J:

$$|J0q\rangle = \frac{1}{\mathcal{N}_{J0q}} \hat{P}^J_{00} \hat{P}_Z \hat{P}_N |q\rangle,$$

- New wave functions by mixing on q:

$$|J0k\rangle = \sum_q f_{J,k}(q) |J0q\rangle$$

with $f_{J,k}(q)$ determined by minimizing the energy:

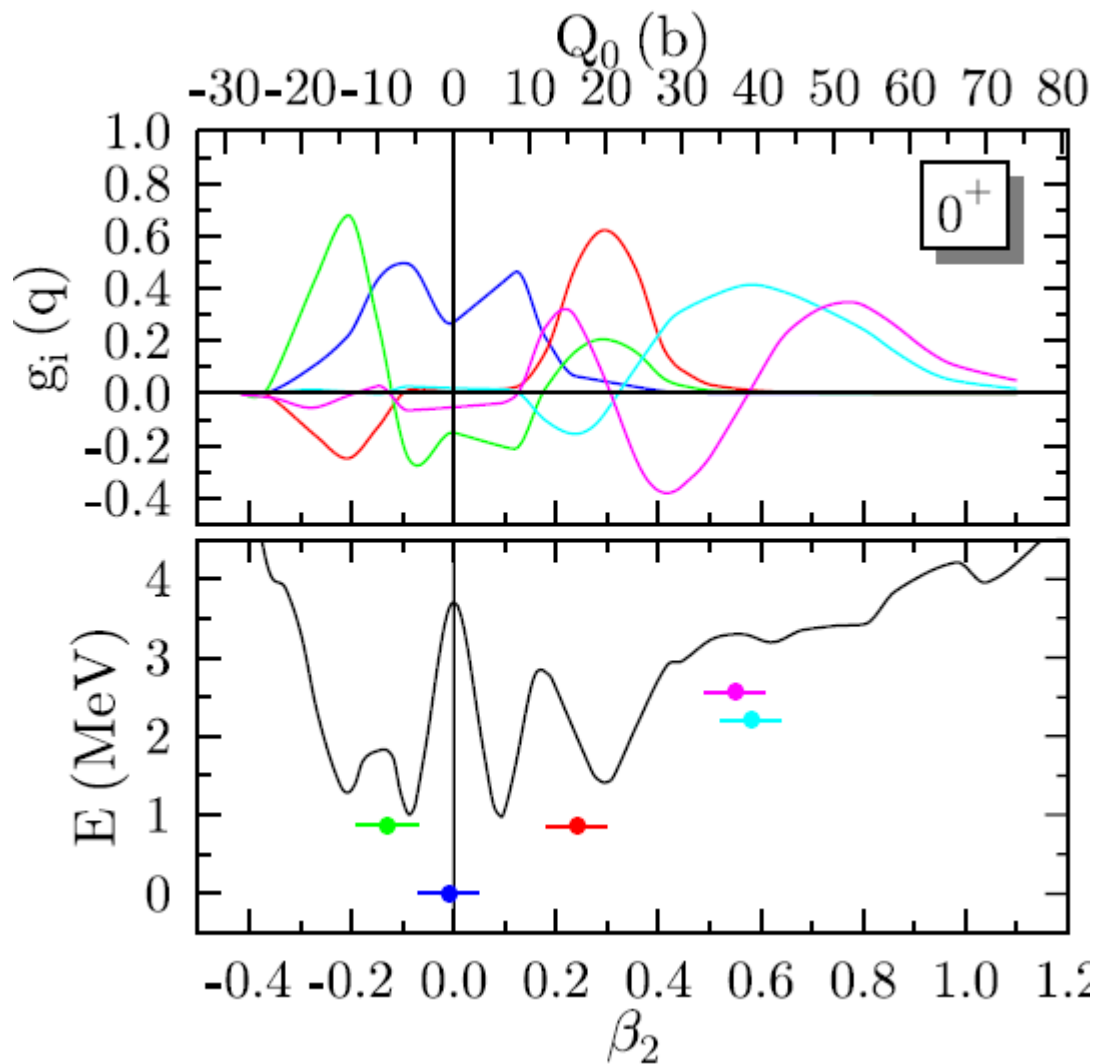$$E_{J,k} = \frac{\langle J0k | \hat{H} | J0k \rangle}{\langle J0k | J0k \rangle}$$

Mean field

Mean field projected on J=0

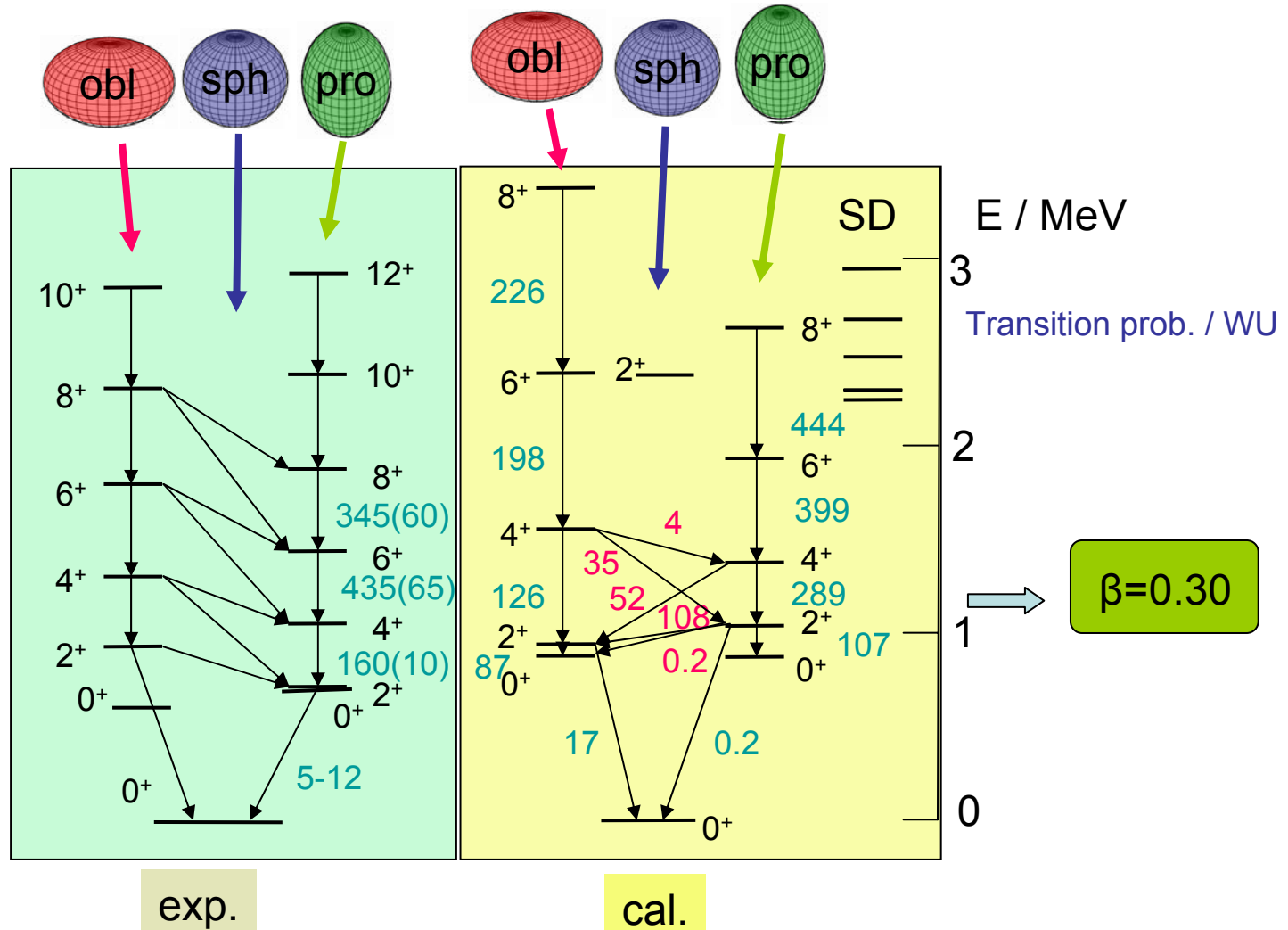Bars in red: 0^+ states obtained after configuration mixing

Collective wave functions

Hartree-Fock + BCS (Skyrme SLy6 interaction + density dependent zero-range pairing force) ⇒configuration mixing of angular-momentum and particle-number projected self-consistent mean field states
(M. Bender, P. Bonche, T. Duguet, and P.H. Heenen, PRC 69, 2004, 064303)
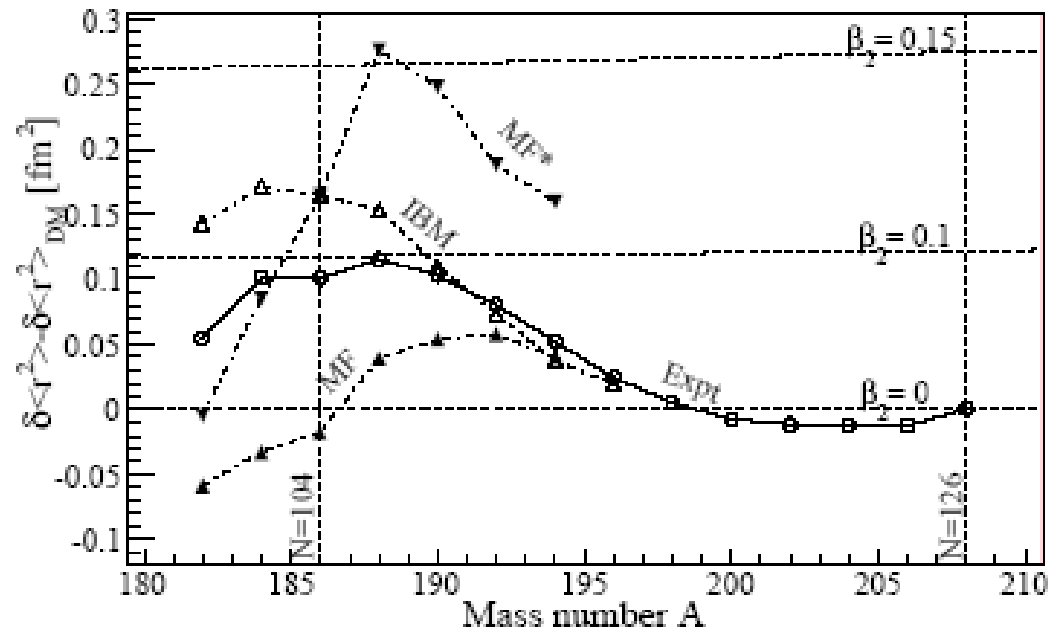
Pb isotopic shifts

FIG. 3: Difference from the experimental mean square charge radii (*Expt*), the beyond mean field calculations with normal [4] (*MF*) and decreased pairing [18] (*MF**) and the IBM calculations (*IBM*) to the droplet model calculations for a spherical nucleus. Isodeformation lines from the droplet model at $\beta_2 = 0.1$ and 0.15 are shown.

BriX

Global calculations
Projection + Configuration mixing for all e-e nuclei

ULB

Correlations due to - symmetry restorations
                     - configuration mixing

BriX
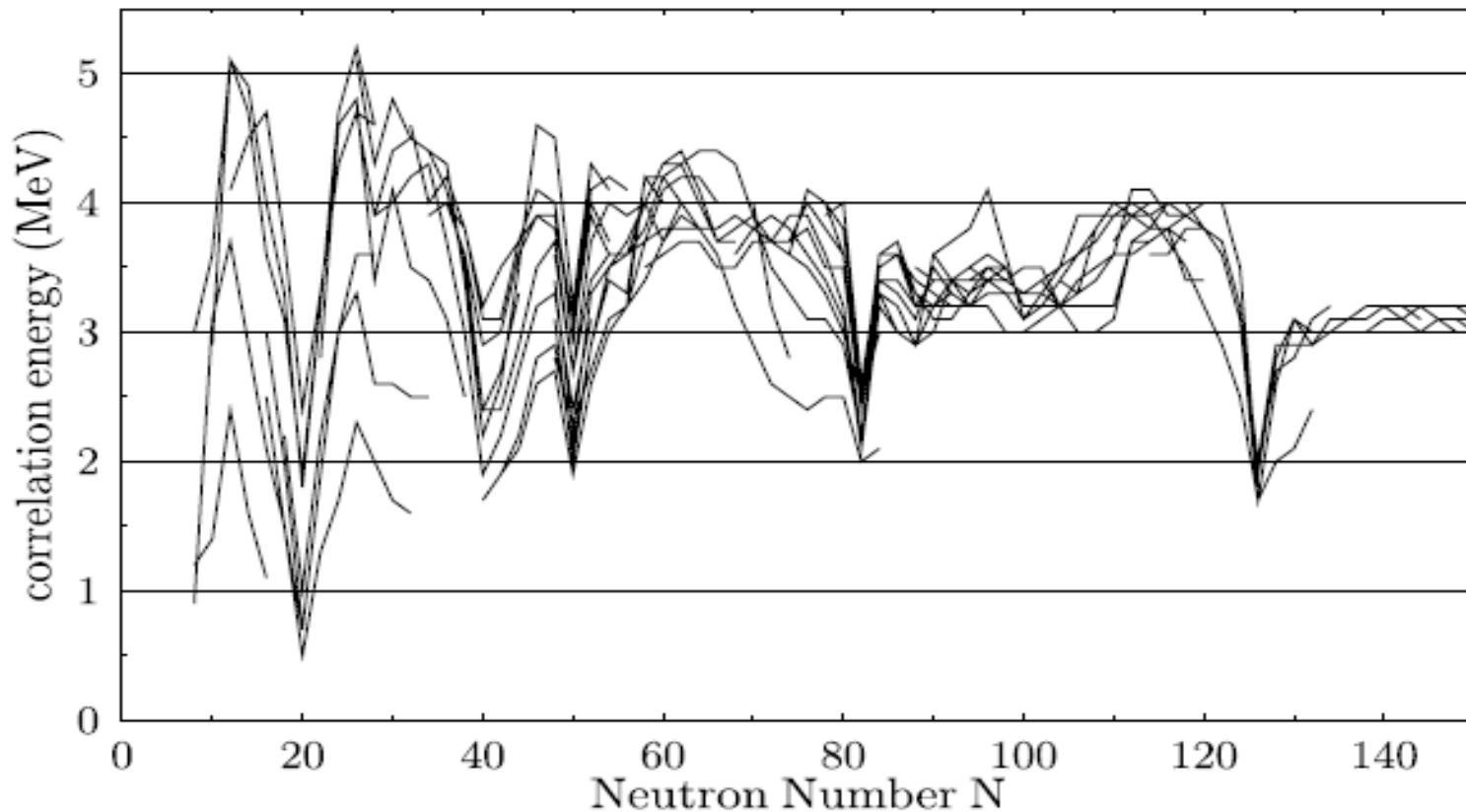
Density functional method

- Beyond mean-field: correlations introduced explicitly
- Why not implicitly in the interaction?
- How to fit an interaction?
- Existing tool: the density functional theory

- What do we want to be able to calculate:
    ground state properties only?
    spectra, transition probabilities, … also?

J. Perdew and S. Kurth, LNP 620, 1 (2003), Springer Verlag

Starting point of the DFT ideas:
analysis of the Hartree-Fock method

(clarifying case: atoms and Coulomb interaction)

HF equations written as a function of the one-body diagonal
and non diagonal densities:

$$n(\mathbf{r}) = \sum_{\mathbf{j}} |\phi_{\mathbf{j}}(\mathbf{r})|^2$$

$$n^{(1)}(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{j}} \phi_{\mathbf{j}}^*(\mathbf{r}') \phi_{\mathbf{j}}(\mathbf{r})$$

The HF equation:

$$\epsilon_k \phi_k(\mathbf{r}) = \left(- \frac{\hbar^2}{2m}\Delta + v_{ext}(\mathbf{r})\right)\phi_k(\mathbf{r}) + u(\mathbf{r})\phi_k(\mathbf{r})$$

$$- \int d^3\mathbf{r}' n^{(1)}(\mathbf{r}, \mathbf{r}')v(\mathbf{r}' - \mathbf{r})\phi_k(\mathbf{r}')$$

where $\quad u(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r}' - \mathbf{r})n(\mathbf{r}')$

The first line is easy: problem in a potential.
The second line is complicate: non local exchange term.
Moreover, correlations beyond a Slater determinant are missing.

But do we need all the information of the true gs wave function?

DFT: take full benefit of the form of the energy as a function of densities
    simplify the exchange term
    introduce what is missing from a mean-field model

Hohenberg Kohn theorem

Hamiltonian separated in two parts: H_0 (electron coordinates)
(kinetic + 2-body)

V_{ext} (external field, nucleus-electron)

Ground state wave function Ψ gives the gs energy:

$$E = <\Psi|H_0 + V_{ext}|\Psi>$$

and the density n(**r**)

density $\longleftrightarrow$ energy $\longleftrightarrow$ ground state wave function

(non degenerate)

Ground state wf minimizes *H* over all antisymmetrised N-particle wf's.

$$E = \min_{\Psi} \langle \Psi | \hat{H} | \Psi \rangle$$

Two steps:

1. minimizing with respect to all the Ψ giving the same density n(**r**)

$$\min_{\Psi \to n} \langle \Psi | \hat{H} | \Psi \rangle = \min_{\Psi \to n} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle + \int d^3r \, v(\mathbf{r}) n(\mathbf{r})$$

All wave functions corresponding to the same density give the same matrix element for v(**r**)!

One defines the universal functional of the density:

$$F[n] = \min_{\Psi \to n} \langle \Psi | \hat{T} + \hat{V}_{ee} | \Psi \rangle = \langle \Psi_n^{\min} | \hat{T} + \hat{V}_{ee} | \Psi_n^{\min} \rangle$$

$\Psi^{\min}$ is the wave function corresponding to the minimum for a given n

2. Minimization of the energy with respect to all N-electron densities

$$E = \min_n E_v[n]$$

$$= \min_n \left\{ F[n] + \int \mathrm{d}^3 r \, v(\mathbf{r}) n(\mathbf{r}) \right\}$$

Constraint on the number of particles N by a Lagrange multiplier μ

$$\delta \left\{ F[n] + \int \mathrm{d}^3 r \, v(\mathbf{r}) n(\mathbf{r}) - \mu \int \mathrm{d}^3 r \, n(\mathbf{r}) \right\} = 0$$

equivalent to:

$$\frac{\delta F}{\delta n(\mathbf{r})} + v(\mathbf{r}) = \mu$$

Definition:

the exchange-correlation energy $E_{xc}[n]$ is defined by

$$F[n] = T_s[n] + U[n] + E_{xc}[n]$$

$$U[n] = \frac{1}{2} \int d^3r \int d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}$$

The energy is given by:

$$E = T_s[n] + \int v(\vec{r})n(\vec{r})d\vec{r} + U[n] + E_{xc}[n]$$

The density is determined through the Kohn Sham equation:

$$\left(-\frac{\hbar^2}{2m}\Delta + u([n];\vec{r}) + v_{xc}([n];\vec{r})\right)\psi_\alpha(\vec{r}) = \epsilon_\alpha\psi_\alpha(\vec{r})$$

which is a fictitious one-electron Shrödinger equation.

- The kinetic energy is treated exactly: large term
  responsible for density oscillations

 The exchange correlation energy is approximated

- Two terms:

$$E_{xc}[n] = E_x[n] + E_c[n]$$

where: $E_x[n] = <\phi_n^{min}|V_{ee}|\phi_n^{min}> - U[n]$

If Φ_n^{min} is a Slater, E_x is the Fock term of the KS orbital
Not HF term because Φ_n^{min} differs from the true HF orbital of the system

The correlation energy is well defined:

$$E_c[n] = F[n] - \{T_s[n] + U[n] + E_x[n]\}$$

Prescriptions to design a DFT

• Construction by "constraint satisfaction": DFT must satisfy as many known exact constraints as possible

• Correct in the uniform density limit

• Scaling properties

• Correct long range part

• Avoid divergences caused by the approximation of the exchange energy (should the exchange be calculated exactly?)

• Self interaction problem

• No need that KS determinant display all symmetries of the true wave function.

Table 1.1. Typical errors for atoms, molecules, and solids from selfconsistent Kohn-Sham calculations within the LSD and GGA approximations of (1.11) and (1.12). Note that there is typically some cancellation of errors between the exchange (E_x) and correlation (E_c) contributions to E_{xc}. The "energy barrier" is the barrier to a chemical reaction that arises at a highly-bonded intermediate state

Property	LSD	GGA
E_x	5% (not negative enough)	0.5%
E_c	100% (too negative)	5%
bond length	1% (too short)	1% (too long)
structure	overly favors close packing	more correct
energy barrier	100% (too low)	30% (too low)

Table 1.2. Mean absolute error of the atomization energies for 20 molecules, evaluated by various approximations. (1 hartree $= 27.21$ eV) (From [20])

Approximation	Mean absolute error (eV)
Unrestricted Hartree-Fock	3.1 (underbinding)
LSD	1.3 (overbinding)
GGA	0.3 (mostly overbinding)
Desired "chemical accuracy"	0.05

Table 1.3. Exchange-correlation energies of atoms, in hartree

Atom	LSD	GGA	Exact
H	-0.29	-0.31	-0.31
He	-1.00	-1.06	-1.09
Li	-1.69	-1.81	-1.83
Be	-2.54	-2.72	-2.76
N	-6.32	-6.73	-6.78
Ne	-11.78	-12.42	-12.50

Table 1.4. Atomization energies of molecules, in eV. ($1\,$hartree $= 27.21\,$eV). From [20]

Molecule	LSD	GGA	Exact
H_2	4.9	4.6	4.7
CH_4	20.0	18.2	18.2
NH_3	14.6	13.1	12.9
H_2O	11.6	10.1	10.1
CO	13.0	11.7	11.2
O_2	7.6	6.2	5.2

The Lyon interactions: how were they constrained?

- a good reproduction of the saturation point of the symmetric infinite nuclear matter, i.e. $\rho_0 \simeq 0.16 \text{ fm}^{-3}$, $E/A \simeq -16 \text{ MeV}$,
- a compression modulus of the symmetric nuclear matter $K_\infty \simeq 230 \text{ MeV}$,
- a symmetry energy $a_S \simeq 32 \text{ MeV}$,
- an enhancement factor of the Thomas–Reiche–Kuhn sum rule $\kappa = 0.25$ (energy weighted sum rule occurring in the E1; $T = 1$ giant dipole resonance),
- a reasonable reproduction of the Wiringa et al. [8] equation of state for pure neutron matter,
- a good reproduction (see Table 5 in part I) of the binding energies of doubly magic nuclei – ^{16}O, ^{40,48}Ca, ^{56}Ni, ^{132}Sn and ^{208}Pb – as well as their r.m.s. radii when experimentally known,
- no constraint on the surface properties.

Large importance of nuclear matter and of neutron matter
(as the electron gas for usual DFT)

Consensus on the need of a larger set of data (UNEDF)

Spherical Nuclei

- Masses, r.m.s. radii, diffraction radii and surface thickness
- Giant monopole and dipole resonance in ^{90}Zr, ^{116}Sn and ^{208}Pb
- Experimental energy of the first 2+ state and B(E2) value in Ca, Ni, Sn and Pb isotopes

Axially-deformed Nuclei

- Binding energy of well-deformed even-even nuclei.
- Super-deformed bandheads and fission isomers

Symmetry-unrestricted

- Ground-state spin and parity for odd-mass nuclei (odd-even, even-odd and odd-odd)
- High-K terminating states in f-p shell nuclei
- 1q.p. excited states of odd-mass heaviest elements

All correlations in the interaction?

- There should be according to the DFT!
- BUT: form of the functional is unknown
- Double counting problem if correlations are added
   to a density functional

- It is better to avoid in the density functional correlations which vary rapidly with A
- Physical interpretations could be more obvious if beyond mean-field correlations are explicitly treated

   (rotational and vibrational correlations)
- Spectra, transition probabilities?

Example: shell effects far from stability

- How do shell effects evolve with N and Z far from stability
- Quenching of shell effects?
- Coupling between the continuum and the bound sp states?

- M. Bender, G. Bertsch, P.-H. Heenen:

  Calculation of the ground state of all e-e nuclei including correlations due to   symmetry restorations

                        configuration mixing