Optimizing Energy Density Functionals for Nuclear Structure Models



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Energy Density Functionals

the nuclear 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!



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:

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

 \Rightarrow 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!

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



TABLE I. Atomization energies of molecules, in kcal/mol (1 eV = 23.06 kcal/mol). $E_{\rm XC}$ 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	$\Delta E^{ m UHF}$	ΔE^{LSD}	$\Delta E^{ m PW91}$	$\Delta E^{ m PBE}$	$\Delta E^{ m expt}$
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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PHYSICAL REVIEW LETTERS

Mean absolute error of the atomization energies for 20 molecules:

Approximation	Mean abs. error (eV)		
Unrestricted Hartree-Fock	3.1 (underbinding)		
LDA	I.3 (overbinding)		
GGA	0.3 (mostly overbinding)		
Desired "chemical accuracy"	0,05		

 \Rightarrow Multiply by *I0*⁶ and compare with the nuclear case!

Relativistic Energy Density Functionals



✓ natural inclusion of the spin degree of freedom (spin-orbit potential with empirical strength).



✓ unique parameterization of *time-odd components* (currents) of the nuclear mean-field.



✓ the distinction between scalar and vector self-energies leads to a natural saturation mechanism for nuclear matter.



Relativistic energy density functionals:

The elementary building blocks are two-fermion terms of the general type:

 $(\bar{\psi}\mathcal{O}_{\tau}\Gamma\psi) \qquad \mathcal{O}_{\tau}\in\{1,\tau_i\} \qquad \Gamma\in\{1,\gamma_{\mu},\gamma_5,\gamma_5\gamma_{\mu},\sigma_{\mu\nu}\}$

... isoscalar and isovector four-currents and scalar densities:

$$j_{\mu} = \langle \phi_0 | \overline{\psi} \gamma_{\mu} \psi | \phi_0 \rangle = \sum_k \overline{\psi}_k \gamma_{\mu} \psi_k ,$$

$$\vec{j}_{\mu} = \langle \phi_0 | \overline{\psi} \gamma_{\mu} \vec{\tau} \psi | \phi_0 \rangle = \sum_k \overline{\psi}_k \gamma_{\mu} \vec{\tau} \psi_k ,$$

$$\rho_S = \langle \phi_0 | \overline{\psi} \vec{\psi} | \phi_0 \rangle = \sum_k \overline{\psi}_k \psi_k ,$$

$$\vec{\rho}_S = \langle \phi_0 | \overline{\psi} \vec{\tau} \psi | \phi_0 \rangle = \sum_k \overline{\psi}_k \vec{\tau} \psi_k$$

where $|\phi_0
angle$ is the nuclear ground state.

 \Rightarrow build four-fermion (contact) interaction terms in the various isospace-space channels:

isoscalar-scalar: isoscalar-vector: isovector-scalar: isovector-vector:

 $\begin{aligned} &(\bar{\psi}\psi)^2\\ &(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)\\ &(\bar{\psi}\vec{\tau}\psi)\cdot(\bar{\psi}\vec{\tau}\psi)\\ &(\bar{\psi}\vec{\tau}\gamma_\mu\psi)\cdot(\bar{\psi}\vec{\tau}\gamma^\mu\psi) \end{aligned}$

Empirical ground-state properties of finite nuclei can only determine a small set of parameters in the expansion of an effective Lagrangian in powers of fields and their derivatives.

Already at lowest order one finds more parameters than can be uniquely determined from data.

 \Rightarrow effective Lagrangian:

$$\mathcal{L} = \bar{\psi}(i\gamma \cdot \partial - m)\psi -\frac{1}{2}\alpha_{S}(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_{V}(\hat{\rho})(\bar{\psi}\gamma^{\mu}\psi)(\bar{\psi}\gamma_{\mu}\psi) -\frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^{\mu}\psi)(\bar{\psi}\vec{\tau}\gamma_{\mu}\psi) -\frac{1}{2}\delta_{S}(\partial_{\nu}\bar{\psi}\psi)(\partial^{\nu}\bar{\psi}\psi) - e\bar{\psi}\gamma \cdot A\frac{(1-\tau_{3})}{2}\psi$$

Only one isovector term and one gradient term can be constrained by data.

Microscopic functionals

... universal exchange-correlation functional $E_{xc}[\rho]$

Ist step: Local Density Approximation

$$E_{xc}^{LDA} \equiv \int \varepsilon^{ChPT} [\rho(\mathbf{r})] \rho(\mathbf{r}) d^3 r$$

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

EFT calculations for inhomogeneous nuclear matter:

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

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.

DD-PCI

... starts from microscopic nucleon self-energies in nuclear matter.

... parameters adjusted in self-consistent mean-field calculations of masses of 64 axially deformed nuclei in the mass regions A ~ 150-180 and A ~ 230-250.

Density dependence of the DD-PCI isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter.

Starting approximation: Hartree-Fock self-energies calculated from the Idaho N³LO NN-potential.



... calculated masses of finite nuclei are primarily sensitive to the three leading terms in the empirical mass formula:

$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

... generate families of effective interactions characterized by different values of a_v , a_s and a_4 , and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

Z	62	64	66	68	70	72	90	92	94	96	98
N_{min}	92	92	92	92	92	72	140	138	138	142	144
N_{max}	96	98	102	104	108	110	144	148	150	152	152

Binding energies used to adjust the parameters of the functional:

Surface energies of semi-infinite nuclear matter that minimize the deviation of the calculated binding energies from data.

Required accuracy $0.05\% \Rightarrow$ absolute error of ±1 MeV for the total binding energy



... 48 parameterizations of the energy density functional:



For each value $\langle S_2 \rangle$ of the symmetry energy, there is a unique combination of volume and surface energies that minimizes χ^2 !

The minimum χ^2 -deviation of the theoretical binding energies from data, as a function of the volume energy coefficient:



Absolute minimum:

 $a_v = -16.06 \text{ MeV} \quad \langle S_2 \rangle = 27.8 \text{ MeV} \quad a_s = 17.498 \text{ MeV}$

Absolute deviations of the calculated binding energies from data for 64 axially deformed nuclei:







Test: calculation of observables not included in the fitting procedure





Test: "double-humped" fission barriers of actinides





Implicitly included in an effective EDF.

...sensitive to shell-effects and strong variations with nucleon number! Cannot be included in a simple Kohn-Sham EDF framework.

Collective correlations



Five-dimensional collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

$$\begin{aligned} H_{\rm coll} &= \mathcal{T}_{\rm vib}(\beta,\gamma) + \mathcal{T}_{\rm rot}(\beta,\gamma,\Omega) + \mathcal{V}_{\rm coll}(\beta,\gamma) \\ \mathcal{T}_{\rm vib} &= \frac{1}{2} B_{\beta\beta} \dot{\beta}^2 + \beta B_{\beta\gamma} \dot{\beta} \dot{\gamma} + \frac{1}{2} \beta^2 B_{\gamma\gamma} \dot{\gamma}^2 \\ \mathcal{T}_{\rm rot} &= \frac{1}{2} \sum_{k=1}^3 \mathcal{I}_k \omega_k^2 \end{aligned}$$

The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ : the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k .

Evolution of triaxial shapes in Pt nuclei:









0.0

 $E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.68$

 $E_{4_1^+}^{exp}/E_{2_1^+}^{exp} = 2.47$





$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.69$$

 $E_{4_1^+}^{exp}$ $E_{2_1^+}^{exp}$ = 2.47





Shape evolution and triaxiality in germanium isotopes









Quadrupole collective Hamiltonian based on the functional DD-PCI



The level of K-mixing is reflected in the staggering in energy between odd- and even-spin states in the γ band:

$$S(J) = \frac{E[J_{\gamma}^{+}] - 2E[(J-1)_{\gamma}^{+}] + E[(J-2)_{\gamma}^{+}]}{E[2_{1}^{+}]}$$

Deformed γ -soft potential \Rightarrow S(J) oscillates between negative values for even-spin states and positive values for odd-spin states.

 γ -rigid triaxial potential \Rightarrow S(J) oscillates between positive values for even-spin states and negative values for odd-spin states.



The mean-field potential of ⁷⁶Ge is γ soft. The inclusion of collective correlations (symmetry restoration and quantum fluctuations) drives the nucleus toward triaxiality, but they are not strong enough to stabilize a $\gamma \approx 30^{\circ}$ triaxial shape.

Coexisting shapes in N=28 isotones





Neutron N=28 spherical energy gaps



⁴⁶Ar: single-particle levels



⁴⁴S: single-particle levels



⁴²Si: single-particle levels









Energy Density Functionals - Covariance Analysis

Quality measure:

$$\chi^{2}(\mathbf{p}) = \sum_{n=1}^{N} \left(\frac{\mathcal{O}_{n}^{(\text{th})}(\mathbf{p}) - \mathcal{O}_{n}^{(\text{exp})}}{\Delta \mathcal{O}_{n}} \right)^{2}$$

"Best model"
$$\mathbf{p}_0 \Rightarrow \qquad \frac{\partial \chi^2(\mathbf{p})}{\partial p_i}\Big|_{\mathbf{p}=\mathbf{p}_0} \equiv \partial_i \chi^2(\mathbf{p}_0) = 0 \quad (\text{for } i = 1, \dots, F)$$

Expand the quality measure around the optimal model $p_0 \Rightarrow$

$$\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}_0) + \frac{1}{2} \sum_{i,j=1}^F (\mathbf{p} - \mathbf{p}_0)_i (\mathbf{p} - \mathbf{p}_0)_j \partial_i \partial_j \chi^2(\mathbf{p}_0) + \dots$$

dimensionless variables:

$$x_i \equiv \frac{(\mathbf{p} - \mathbf{p}_0)_i}{(\mathbf{p}_0)_i}$$

 \rightarrow the quadratic deviations of χ^2 from its minimum value: $\chi^2(\mathbf{p}) - \chi^2(\mathbf{p}_0) \equiv \Delta \chi^2(\mathbf{x}) = \mathbf{x}^T \hat{\mathcal{M}} \mathbf{x}$

The symmetric F×F matrix of second derivatives:

$$\mathcal{M}_{ij} = \frac{1}{2} \left(\frac{\partial \chi^2}{\partial x_i \partial x_j} \right)_{\mathbf{x}=0} = \frac{1}{2} (\mathbf{p}_0)_i (\mathbf{p}_0)_j \partial_i \partial_j \chi^2 (\mathbf{p}_0)$$

Diagonalization \Rightarrow

$$\Delta \chi^2(\mathbf{x}) = \mathbf{x}^T \left(\hat{\mathcal{A}} \hat{\mathcal{D}} \hat{\mathcal{A}}^T \right) \mathbf{x} = \xi^T \hat{\mathcal{D}} \xi = \sum_{i=1}^F \lambda_i \xi_i^2$$

The deviations of the χ^2 from its minimum value are parameterized in terms of F uncoupled harmonic oscillators \rightarrow the eigenvalues play the role of the spring constants.

Soft direction \Rightarrow small eigenvalue λ , little deterioration in χ^2 . The corresponding eigenvector ξ involves a particular linear combination of model parameters that is not constrained by the observables included in the fit.

Stiff direction \Rightarrow large eigenvalue λ , χ^2 rapidly worsens away from minimum, the fit provides a stringent constraint on this particular linear combination of parameters.

... covariance between two observables A and B:

$$\operatorname{cov}(A,B) = \frac{1}{M} \sum_{m=1}^{M} \left[\left(A^{(m)} - \langle A \rangle \right) \left(B^{(m)} - \langle B \rangle \right) \right] = \langle AB \rangle - \langle A \rangle \langle B \rangle$$

Pearson product-moment correlation coefficient:

$$\rho(A, B) = \frac{\operatorname{cov}(A, B)}{\sqrt{\operatorname{var}(A)\operatorname{var}(B)}}$$

$$\operatorname{cov}(A,B) = \sum_{i,j=1}^{F} \frac{\partial A}{\partial x_i} \left[\frac{1}{M} \sum_{m=1}^{M} x_i^{(m)} x_j^{(m)} \right] \frac{\partial B}{\partial x_j} \equiv \sum_{i,j=1}^{F} \frac{\partial A}{\partial x_i} C_{ij} \frac{\partial B}{\partial x_j}$$

$$\operatorname{cov}(A,B) = \sum_{i,j=1}^{F} \frac{\partial A}{\partial x_i} (\hat{\mathcal{M}}^{-1})_{ij} \frac{\partial B}{\partial x_j} = \sum_{i=1}^{F} \frac{\partial A}{\partial \xi_i} \lambda_i^{-1} \frac{\partial B}{\partial \xi_i}$$

... relativistic energy density functional DD-PC1 \Rightarrow is it "predictive" ? Agreement with experiment?

 \Rightarrow is it "unique" ? A model is unique if all the eigenvalues

 λ_i of \mathcal{M} are large.

$$\alpha_s(\rho) = a_s + (b_s + c_s x)e^{-d_s x}$$
$$\alpha_v(\rho) = a_v + b_v e^{-d_v x}$$
$$\alpha_{tv}(\rho) = b_{tv} e^{-d_{tv} x}$$

PARAMETER	
$a_s \ (\mathrm{fm}^2)$	-10.0462
$b_s ~({\rm fm^2})$	-9.1504
$c_s ~({\rm fm^2})$	-6.4273
d_s	1.3724
$a_v \ (\mathrm{fm}^2)$	5.9195
$b_v ~({ m fm}^2)$	8.8637
d_v	0.6584
$b_{tv} \ (\mathrm{fm}^2)$	1.8360
d_{tv}	0.6403
$\delta_s \; ({\rm fm}^4)$	-0.8149

Correlations between the lowest-order terms in a Taylor expansion of the density-dependent coupling functions around the saturation point:

$$c_{s} = -\frac{\rho_{\text{sat}}}{d_{s}} e^{d_{s}} \left[d_{s} \alpha_{s}'(\rho_{\text{sat}}) + \rho_{\text{sat}} \alpha_{s}''(\rho_{\text{sat}}) \right],$$

$$b_{s} = c_{s} \left(\frac{1}{d_{s}} - 1 \right) - \alpha_{s}'(\rho_{\text{sat}}) \rho_{\text{sat}} \frac{e^{d_{s}}}{d_{s}},$$

$$a_{s} = \alpha_{s}(\rho_{\text{sat}}) - (b_{s} + c_{s})e^{-d_{s}}$$

$$d_{v} = -\frac{\alpha_{v}''(\rho_{\text{sat}})}{\alpha_{v}'(\rho_{\text{sat}})}\rho_{\text{sat}},$$

$$b_{v} = -\alpha_{v}'(\rho_{\text{sat}})\frac{e^{d_{v}}}{d_{v}},$$

$$a_{v} = \alpha_{v}(\rho_{\text{sat}}) - b_{v}e^{-d_{v}}$$

$$d_{tv} = -\rho_{\text{sat}} \frac{\alpha'_{tv}(\rho_{\text{sub}})}{\alpha_{tv}(\rho_{\text{sub}})},$$
$$b_{tv} = \alpha_{tv}(\rho_{\text{sub}})e^{d_{tv}(\rho_{\text{sub}}/\rho_{\text{sat}})}$$
$$\rho_{\text{sub}} = 0.12 \text{ fm}^{-3}$$

Nuclear matter pseudo-observables

OBSERVABLE	DD-PC1
ρ_0	0.152 fm^{-3}
$\epsilon(ho_0)$	$-16.06 \mathrm{MeV}$
$\epsilon(ho_{low})$	$-6.48 \mathrm{MeV}$
$\epsilon(ho_{high})$	$34.38 { m ~MeV}$
K_0	$230 { m MeV}$
m_D	0.58
m^*	0.66
$S_2(ho_{ m sub})$	$27.8 \mathrm{MeV}$
$L(ho_{ m sub})$	$57.2 { m ~MeV}$
a_4	$33 { m MeV}$



Eigenvalues and eigenvectors of the 9 × 9 matrix of second derivatives M of $\chi^2(p)$ for the functional DD-PC1





Uncertainties σ_i of model parameters for the functional DD-PCI.

36 independent correlation coefficients between 9 model parameters that contribute to infinite nuclear matter calculations .







Uncertainties σ_i of model parameters for the functional DD-PCI.

45 independent correlation coefficients between 10 model parameters that contribute to semi-infinite nuclear matter calculations .

Finite nuclei



Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives \mathcal{M} to the variances of the binding energy of tin isotopes.



Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives \mathcal{M} to the variances of the binding energy of rare-earth nuclei.



Relative contributions in percentage of the ten linear combinations of model parameters that correspond to the eigenvectors of the matrix of second derivatives \mathcal{M} to the variances of the binding energy of actinide nuclei.

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