NUCLEAR DFT: SPECIAL PROBLEMS, SOME SOLUTIONS

Back to basics
State potatoes and slices
Hamiltonian
Translation invariance, c.m. trap
Rotation invariance, radial DFT
Intrinsic frame, projector dependence
Particle number, concavity
Constructive DFT, polynomials

Back to basics

- In practice, the nuclear DF and/or EDF calculations which have been published look very much like Hartree-Fock or Hartree-Bogoliubov calculations, where one has to guess a good form for the functional, with efficient parameters for the various energy terms, hence an efficient Kohn-Sham potential.

- This approach has had quite an amount of success for the reproduction of experimental data, but this success pushed several basic problems to be partly forgotten.

- Present DF solutions are always localized, often deformed and often do not have a well defined particle number. The discussion to-day returns to the basic fact that a DFT or EDFT results from an energy minimization under constraint. This gives a new light to the restoration of (E)DF broken nuclear symmetries.
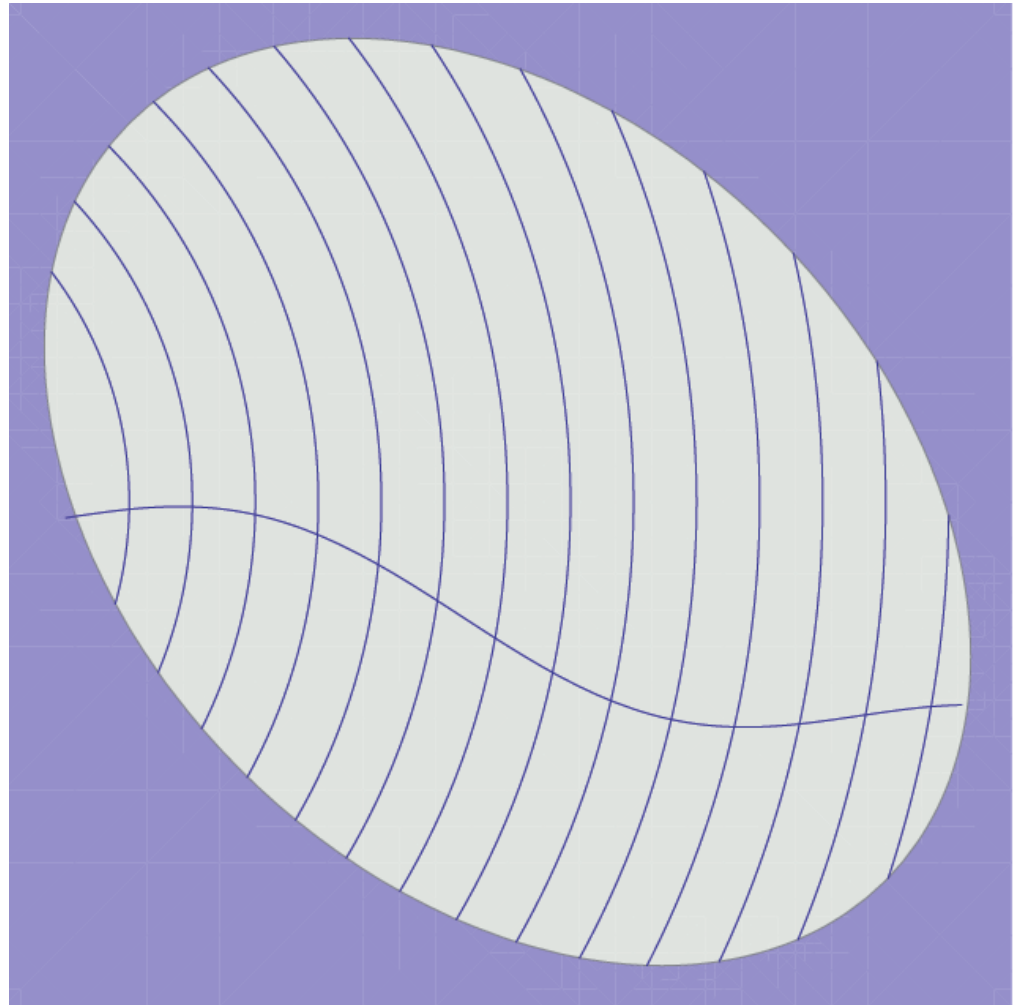
Potato of trial states, slices of density constraint, locus of energy minima

Minima or Infima?

Degeneracies?

Analyticity for locus?

Verify concavity of F[\rho]

Slices, constraint calculus

- A proper (E)DFT can consider nuclear states that are pure states, with a many-body density operator $| \psi >< \psi |$. But sets of mixed states, such as $\sum_n w_n | \psi_n >< \psi_n |$, can be most useful to minimize the energy.

- Many states have the same one-body density ρ. Such states with the same ρ make a "slice", labeled by ρ.

- Energy shall be minimized within each slice constrained by its label ρ. The obtained minimum (or infimum) is a function of the slice, hence a functional, $F[\rho]$, of the density.

- This functional is necessarily, mathematically, CONCAVE. Typically, $F[(\rho+\rho')/2] < (F[\rho]+F[\rho'])/2$. This is a major property of minimizations under constraint(s).

Hamiltonian and reduced information

- As will be explained step by step, we advocate completing the usual nuclear Hamiltonian by:

- a center-of-mass harmonic trap: $k\,R^2$, and

- a concavity term, $c\,(N^2+Z^2)$.

- We also advocate a theory with few radial positions for measuring the density. The whole profile is not necessary.

Localizor Hamiltonian

The usual, Galilean invariant Hamiltonian,

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i>j=1}^{A} v_{ij}, \qquad (1)$$

makes impractical the definition of a density: the center of mass (CM) is everywhere.

An elementary modification of H,

$$\mathcal{H} = H + A\omega^2 R^2/2, \quad R = A^{-1} \sum_i r_i, \qquad (2)$$

traps the CM. The ground state of $\mathcal{H}$ now factorizes as a product of a Gaussian for this CM and an "internal" wave function of the $(A-1)$ Jacobi coordinates,

$$\Psi(r_1, r_2, \ldots, r_A) = \Gamma(R)\psi_{\text{int}}(\xi_1, \xi_2, \ldots, \xi_{A-1}),$$

$$\xi_1 = r_2 - r_1, \quad \xi_2 = r_3 - \frac{r_2 + r_1}{2}, \ldots, \qquad (3)$$

$$\xi_{A-1} = r_A - \frac{r_{A-1} + r_{A-2} + \cdots + r_1}{A-1}.$$

Internal density vs Lab density

Calculations in the $\{r_i\}$ representation are much more convenient than those in the $\{R, \xi_j\}$ one, for obvious symmetrization reasons. The laboratory density,

$$\rho(r) = A \int dr_1 dr_2 \ldots dr_{A-1} \, |\Psi(r_1, r_2, \ldots, r_{A-1}, r)|^2, \quad (4)$$

is much easier to calculate than the "internal" density,

$$\sigma(\xi) = A \int d\xi_1 d\xi_2 \ldots d\xi_{A-2} \, |\psi_{\text{int}}(\xi_1, \xi_2, \ldots, \xi_{A-2}, \xi)|^2.$$

Now, because of the FACTORIZATION of the wave functionwith the trapped CM, both densities turn out to be related by a convolution.

$$\rho(r) = \int dR [\Gamma(R)]^2 \sigma \left[\frac{A}{A-1} (r - R) \right].$$

The CM trap does not change the internal physics. It is thus easy to use a DFT in the Lab system and recover the internal density by a deconvolution. Alternate theory: see Messud *et al*, Phys. Rev. C 80 (2009) 054314

Consequence of rotational invariance of H

Let *Z,N,A ≡ Z + N be the proton, neutron, and mass* numbers, respectively. The nuclear Hamiltonian *H is invariant* under rotations. Therefore, besides *Z and N, nuclear g.s.* carry good quantum numbers, *J and M, for the total angular* momentum and its *z-component. Two cases occur: (i) either J = 0, hence a nondegenerate g.s., the density of which is*

ISOTROPIC, or (ii) *J > 0, hence a trivial degeneracy for a* magnetic multiplet of g.s., the densities of which, nonisotropic, contain several multipoles, with the *same monopole part* of the density for all members of the multiplet.

In both cases, the many-body density operator for the (set of) ground state(s) of a given nucleus can read,

$$\mathrm{D} = (2J+1)^{-1} \sum_M |ZNJM\rangle\langle ZNJM|,$$

INVARIANT under rotation, whether the nucleus is odd or even, deformed or spherical. The corresponding one-body density makes an ISOTROPIC profile.

The radial DFT (RDFT)

- For any density matrix D in many-body space, the energy reads, E=Tr (H D), where Tr means the trace in many-body space of such a product of operators.

- The previous slide showed that, for any nucleus, its g.s. energy, degenerate or not, results from a rotation invariant D.

- The density of such a D is therefore a scalar. We need just to study functionals of radial profiles.

- Notice: adding to H a term k J^2, k small and variable, tells the spin.

- Notice that the method is compatible with the CM trap, which is invariant under rotation.

- This reduces (E)DFT to one-dimensional calculations. Partial filling of spherical orbitals will define spherical Kohn-Sham potentials.

About deformed solutions of the usual (E)DFT

- Advantage: they do signal deformations and, when angular momentum projection is available, they give a whole band.
- Defect: 3-dim or 2-dim calculations, while the RDFT means 1-dim.
- Defect: angular momentum projection costly; furthermore, variation after projection costlier.
- Advantage: density \tau in the intrinsic frame.
- Can one define rigorously a DFT in an intrinsic frame? Yes!
- Let D be a many-body density operator, not rotation invariant, and P_J be an angular momentum projector (magnetic label understood). Define a slice of D's having the same one-body density \tau, deformed. Then, within the slice, minimize the ratio,

$$(\text{Tr } H \, P_J \, D) / (\text{Tr } P_J \, D).$$

- This minimum, a function of the slice, defines a functional $F_J(\tau)$.
- Defect: J dependence!

Nature is not concave

- Experimental binding energies show a valley of stability, hence at least an approximate amount of concavity. But second differences, $E_{A-1}-2E_A+E_{A+1}$, can be negative, because of, among other causes, pairing and/or shell effects. See, for instance, the sequence of tin isotopes:
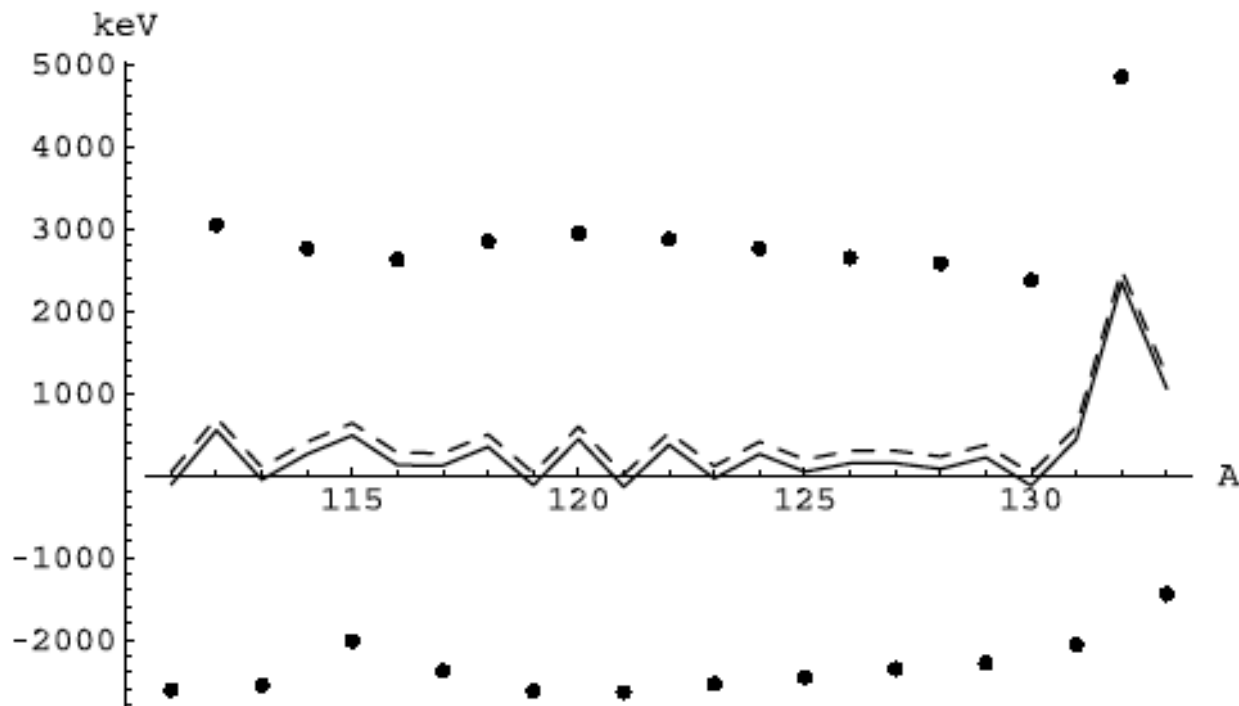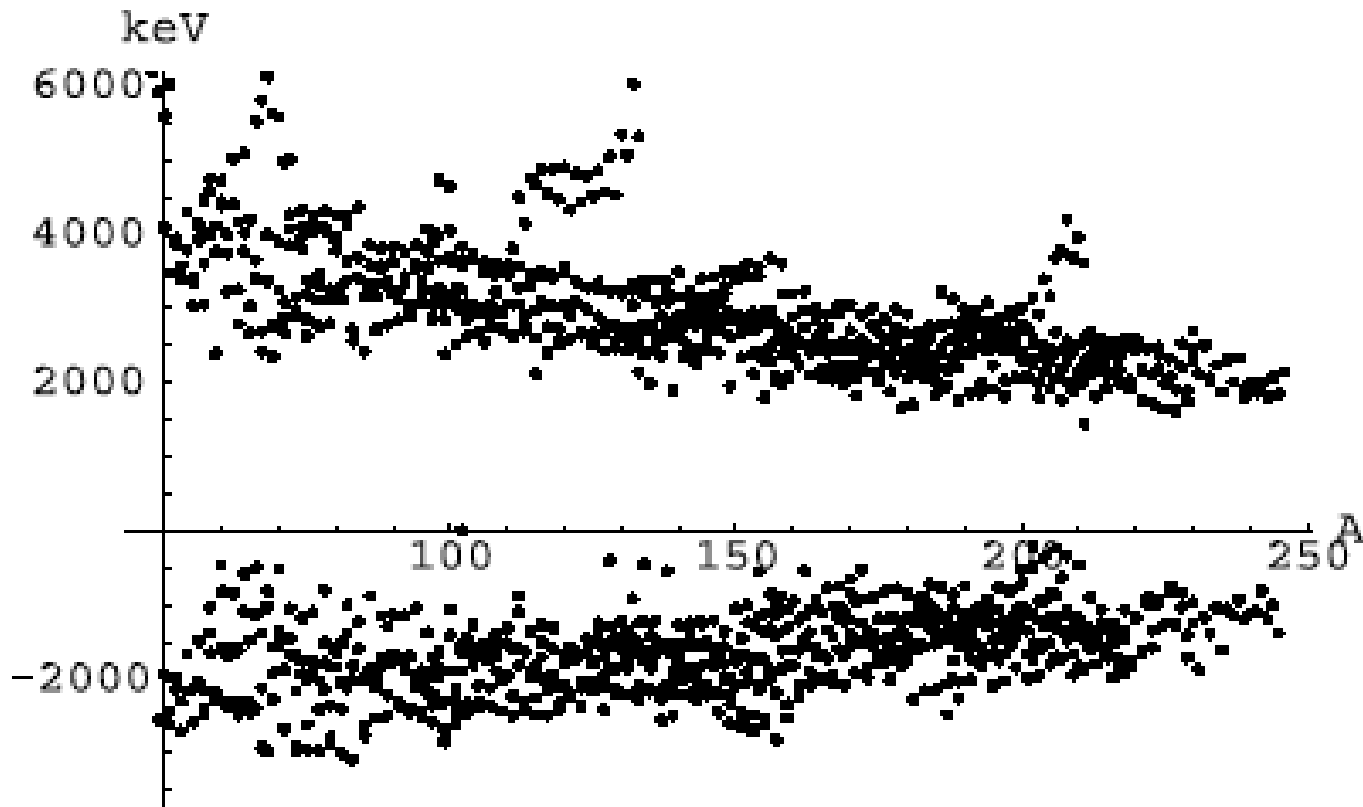
Nature is not concave

Scatter plot of second differences with respect to N
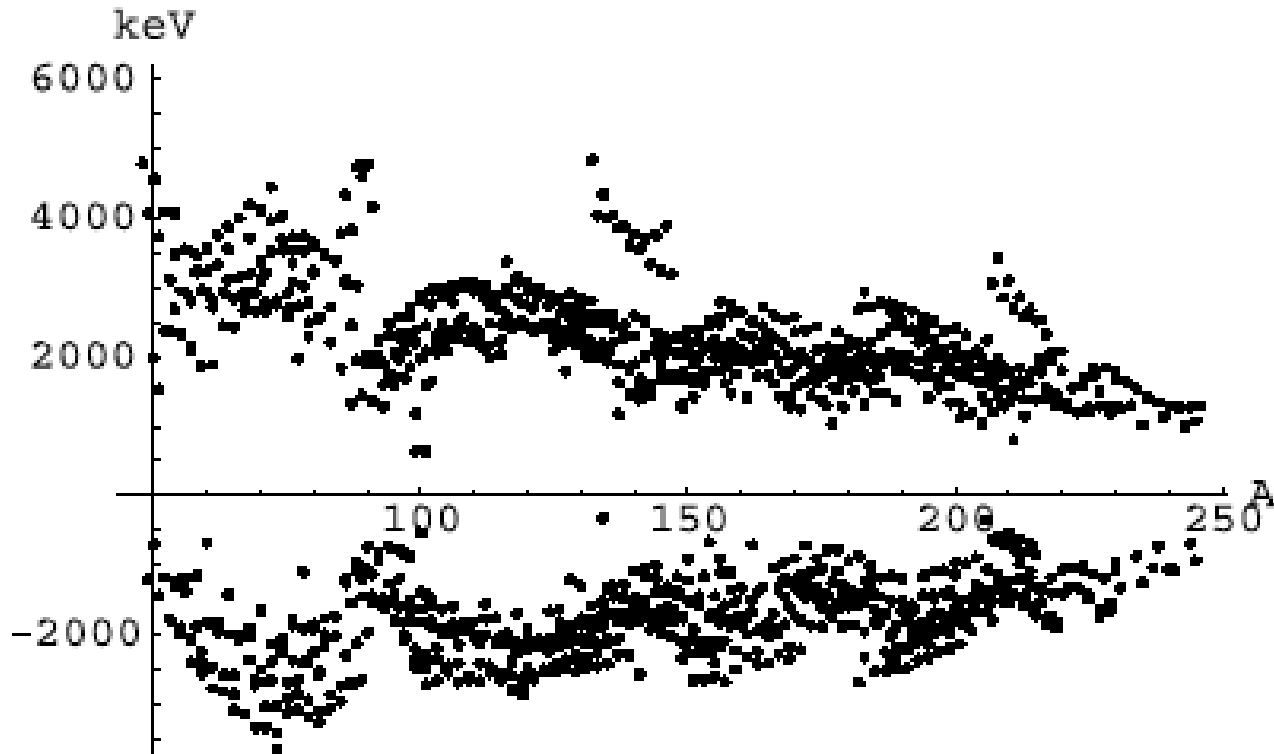
Nature is not concave

Scatter plot of second differences with respect to Z

Forcing Nature to be concave

If the set of trial states carries good quantum numbers N and Z, one obtains a functional $F_{N,Z}[\rho]$. But there is no reason to expect that, after changing N and Z, there will be concavity with respect to either N or Z. For instance, given the three g.s. densities $\rho_{N,Z-1}$, $\rho_{N,Z}$, $\rho_{N,Z+1}$, it can happen that

$F_{N,Z}[\rho_{N,Z}] > (F_{N,Z-1}[\rho_{N,Z-1}]+F_{N,Z+1}[\rho_{N,Z+1}])/2$. Namely, interpolations can overestimate the binding!

One would prefer a universal functional $F(\rho)$, valid for all values of N and Z as defined by integrating ρ. This is specially useful for Hartree-Bogoliubov cases, where N and Z are treated as constrained average values of operators **N** and **Z**, within trial states that do not have such good quantum numbers.

As already stated, constrained minimizations make necessarily concave function(al)s. Let -c be the worst negative second difference observed experimentally. Then a term, $c(\mathbf{N}^2+\mathbf{Z}^2)/2$, added to H, increases every second differences by c. Physics is not changed, since the added term commutes with H. But, this way, "Nature has been made concave" and, now, it can be accounted for by a "universal" DF.

Constructive DFT, via polynomials, from configuration mixing

Let $\mathcal{H}$ be the matrix representing the Hamiltonian on an orthonormal basis for a suitable subspace of wave functions, and, similarly, let, for instance, $\mathcal{D}_1, \mathcal{D}_2$ be the matrices representing two constraints selected to parametrize the density, such as, for instance,

the density at the origin and the density at the mid-surface or in the tail. Then the free energy and the Lagrange multipliers are related by polynomial equations,

$$P(\varepsilon, \lambda_1, \lambda_2) \equiv \det(\mathcal{H} - \lambda_1 \mathcal{D}_1 - \lambda_2 \mathcal{D}_2 - \varepsilon) = 0. \tag{5}$$

Here ε is the free energy, lowest eigenvalue of $(\mathcal{H} - \lambda_1 \mathcal{D}_1 - \lambda_2 \mathcal{D}_2)$, and the λ's are Lagrange multipliers. It is well known that $\partial\varepsilon/\partial\lambda_i = -D_i$, $i = 1, 2$, where $D_i \equiv \langle \mathcal{D}_i \rangle$ is the expectation value of the corresponding constraint. From Eq. (5) such partial derivatives read, $\partial\varepsilon/\partial\lambda_i = -(\partial P/\partial\lambda_i)/(\partial P/\partial\varepsilon)$, $i = 1, 2$, hence two more polynomial relations are obtained,

$$Q_i(D_i, \varepsilon, \lambda_1, \lambda_2) \equiv (\partial P/\partial\varepsilon)D_i - (\partial P/\partial\lambda_i) = 0. \tag{6}$$

Constructive DFT, via polynomials, from configuration mixing

Replace in Eqs. (5), (6) the free energy by its value, $\varepsilon = \eta - \lambda_1 D_1 - \lambda_2 D_2$, in terms of the energy, $\eta \equiv \langle \mathcal{H} \rangle$ and the constraints, D_1, D_2. This creates three polynomials in terms of $\eta, D_1, D_2, \lambda_1, \lambda_2$, out of which λ_1, λ_2 can be eliminated, for a final polynomial equation, $\mathcal{E}(\eta, D_1, D_2) = 0$. This easy Legendre transform generates our "algebraic DF". A generalization to any number of quadratic constraints is trivial. Such algebraic DFs are not open formulae of the form, $\eta = F(D_1, \ldots, D_{\mathcal{N}'})$, but they provide roots for η at any realistic degree of numerical accuracy. Incidentally, they may also give excited energies and/or spurious ones, a well-known property [17] of DFs.

Constructive DFT, toy model, 1 constraint, subspace dimension 4

$$\mathcal{H} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 7/4 & 3\sqrt{3}/4 & 0 \\ 0 & 3\sqrt{3}/4 & 13/4 & 0 \\ 0 & 0 & 0 & 45/8 \end{bmatrix} \qquad \mathcal{D} = \begin{bmatrix} 2 & \sqrt{3/2} & \sqrt{1/2} & 0 \\ \sqrt{3/2} & 4 & 0 & \sqrt{1/2} \\ \sqrt{1/2} & 0 & 4 & \sqrt{3/2} \\ 0 & \sqrt{1/2} & \sqrt{3/2} & 6 \end{bmatrix}.$$

The equations which correspond to Eqs. (5), (6) read

$$P_{\text{toy}}(\varepsilon, \lambda) = -360 + 154\varepsilon + 344\varepsilon^2 - 154\varepsilon^3 + 16\varepsilon^4 + 1464\lambda$$
$$+ 1692\varepsilon\lambda - 1636\varepsilon^2\lambda + 256\varepsilon^3\lambda + 725\lambda^2 - 5140\varepsilon\lambda^2$$
$$+ 1408\varepsilon^2\lambda^2 - 4192\lambda^3 + 3072\varepsilon\lambda^3 + 2064\lambda^4 = 0,$$

$$Q_{\text{toy}}(D, \varepsilon, \lambda) = -1464 - 1692\varepsilon + 1636\varepsilon^2 - 256\varepsilon^3 - 1450\lambda$$
$$+ 10\,280\varepsilon\lambda - 2816\varepsilon^2\lambda + 12\,576\lambda^2 - 9216\varepsilon\lambda^2$$
$$- 8256\lambda^3 + \big(154 + 688\varepsilon - 462\varepsilon^2 + 64\varepsilon^3$$
$$+ 1692\lambda - 3272\varepsilon\lambda + 768\varepsilon^2\lambda - 5140\lambda^2$$
$$+ 2816\varepsilon\lambda^2 + 3072\lambda^3\big)D = 0. \tag{10}$$

Finally, the substitution, $\varepsilon = \eta - \lambda D$, followed by the elimination of λ, generates the desired polynomial equation, $\mathcal{E}_{\text{toy}}(\eta, D) = 0$.

Constructive DFT, toy model, 1 constraint, subspace dimension 4

This final polynomial has order d x (d-1), with d the number of mixed states. It can be unwieldy. But it ensures analyticity, and the lowest root makes a concave branch.
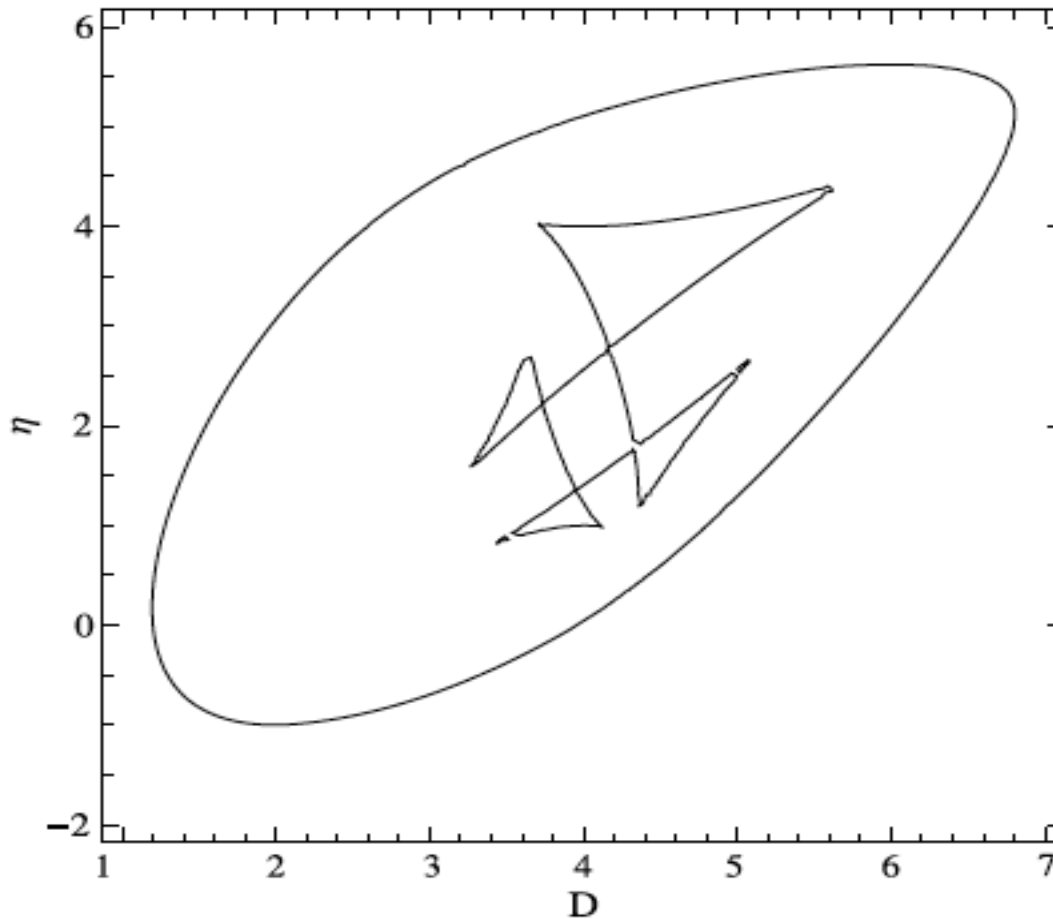
Summary of results

- CM problem solved; modest cost 1- and 2-body operator trap.

- Rotation problem solved; RDFT brings 1-d simplification.

- Existence of DFT for deformations in intrinsic frame, but complicated projection and J-dependence.

- Compatibility between Hamiltonian and concavity; modest cost N^2+Z^2 term.

- Constructive theory; cost big polynomials.

References and Thanks

- Translation: Phys. Rev. C 77, 014311 (2008)

- Rotation: Phys. Rev. C 78, 014307 (2008)

- Deformed intrinsic: B.G. G., B.K. Jennings, B.R. Barrett, Phys. Rev. A 78, 032507 (2008)

- Concavity: B.R. Barrett, B.G. G., B.K. Jennings, N. Toberg, Nucl. Phys. A 828, 267 (2009)

- Constructive DFT: B.G.G., S. Karataglidis, Phys. Lett. B 703, 88 (2011)