TWO RESULTS ABOUT THE NUCLEAR DENSITY FUNCTIONAL

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I- SCALAR FORM OF THE NUCLEAR DENSITY FUNCTIONAL

Nuclear eigenstates carry good quantum numbers J and M. In particular, all doubly even nuclei have $J = 0$ for their ground states. The corresponding ground state energies, $E = \langle 0|H|0\rangle = \mathrm{Tr}\, H\, |0\rangle\langle 0|$, live in a world of spherically symmetric densities, $\rho(r) = \langle 0|a_r^\dagger a_r|0\rangle = \mathrm{Tr}\, a_r^\dagger a_r\, |0\rangle\langle 0|$.

For odd nuclei, or those few doubly odd nuclei with $J \neq 0$ in their magnetic multiplet of ground states, *there exists also a spherically invariant representation.* Indeed, the density operator in many-body space, $\mathcal{D} = \sum_M |JM\rangle\langle JM|/(2J+1)$, rotates as a scalar. Concomitantly, the energy, $E = \mathrm{Tr}\, H\, \mathcal{D}$, corresponds to a spherical density, $\rho(r) = \mathrm{Tr}\, a_r^\dagger a_r\, \mathcal{D}$.

CONCLUSION: *The nuclear density functional theory can be, universally, a one-dimensional theory, using just radial profiles.*

II- FLUCTUATIONS AND ERROR BARS FOR COLLECTIVE COORDINATES

Energy surfaces $e(b)$ occur in many nuclear models. Here, b means the expectation value(s), $b \equiv \langle B \rangle$, of one (or several) collective coordinate operator(s) B. Often, $e(b) \equiv \langle H \rangle$ results from a constrained mean field calculation, where the "free energy", $\varepsilon(\lambda) \equiv \langle H \rangle - \lambda \langle B \rangle$, is made minimal, or at least stationary, as a function of the Lagrange multiplier(s) λ. An elimination of λ(s) between $\langle H \rangle$ and $\langle B \rangle$ returns $e(b)$.

Because of the Kohn-Sham theorem, density functional calculations amount to mean-field calculations, and energy surfaces now often result from constrained density functionals.

This talk wants to draw attention upon the difference between $\langle B \rangle^2$ and $\langle B^2 \rangle$. Error bars, $\Delta b \equiv \sqrt{\langle B^2 \rangle - \langle B \rangle^2}$, can corrupt $e(b)$, even if one introduces, as usually in the literature, a $\langle B \rangle^2$ stabilization in the form, $\langle H \rangle - \lambda \langle B \rangle + \mu \langle B \rangle^2$.

Toy model showing BIMODAL solutions making $\langle B \rangle$ misleading

Consider $H = -d^2/dr^2 + (r^4 - 18r^2 - 2r + 93)/120$, a 1-D Hamiltonian, and the constrained ground state wave function ψ and eigenvalue ε of $(H - \lambda r)$,

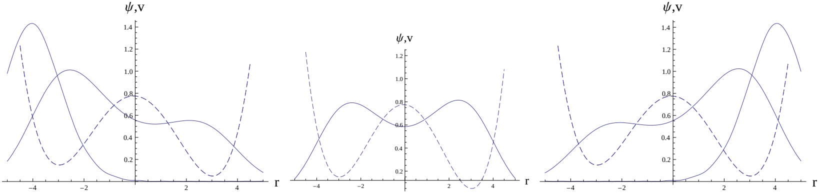

Figure: Dashes, toy potential. Full lines, five cases of ψ. From left to right, $\lambda = -1, -.04, -.016, 0, 1$, and $\langle r \rangle = -3.84, -1.61, .06, 1.28, 3.86$.

When $\langle r \rangle$ sits in a valley, ψ shows one peak only, at the correct spot. However, when $\langle r \rangle$ sits on top or near a mountain, tunnel effects delocalize ψ. Bimodal shapes occur. An increase of Δr is a signature that ψ has become a bad probe of the energy landscape.

Such tunnel effects and fluctuations of the constraint have a dire consequence: one can prove a *theorem* that, for any Hamiltonian H and any constraint operator B, the strict minimization of the constrained energy returns $\varepsilon(\lambda)$ as a *concave* function. Hence, its Legendre transform, $e(b) \equiv \langle H \rangle (\langle B \rangle)$, is *convex*. Poor landscape!

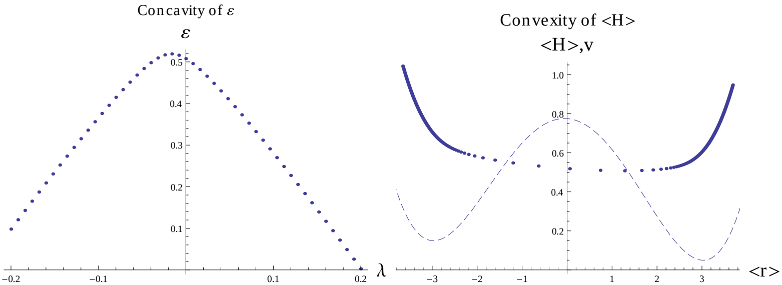

Figure: Same toy model. Left: concavity of $\langle (H - \lambda r) \rangle$ as a function of λ. Right: convexity of $e(\langle r \rangle)$ and mismatch between shapes of e and v.

Introducing B^2

To obtain a *unimodal* ψ as a good quality probe of the landscape, one must keep track of both $\langle B \rangle$ and its error bar, Δb. A second constraint operator, μB^2, must be added to the first one, $-\lambda B$.

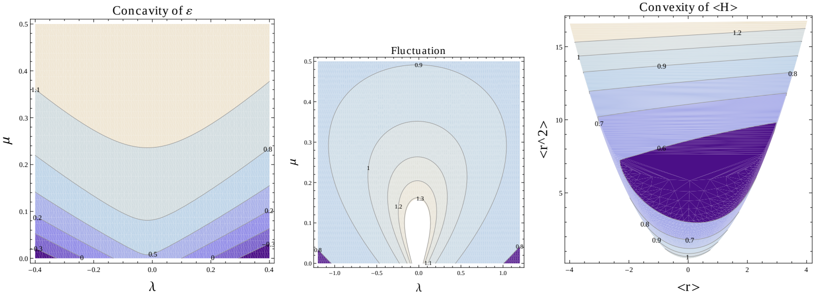

Figure: Same model. Left: concavity of $\langle (H - \lambda r + \mu r^2) \rangle$ as a function of λ and μ. Center: contours of $\Delta r(\lambda, \mu)$. Right: convexity of $e(\langle r \rangle, \langle r^2 \rangle)$.

Representation $\{b, \Delta b\}$

Replace the plot of $\langle H \rangle$ in terms of $\langle B \rangle$ and $\langle B^2 \rangle$ by a plot in terms of $\langle B \rangle$ and Δb. *Now, ride a line where Δb is constant.* This keeps constant, and under control, the quality of the probe ψ.

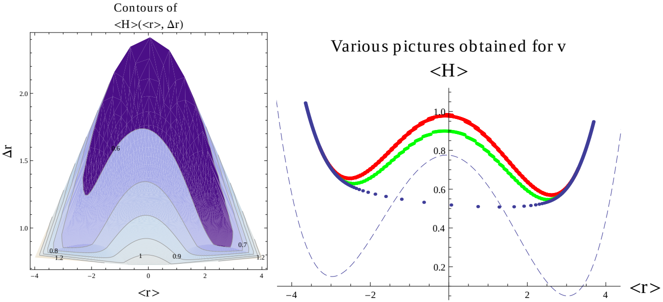

Figure: Still same model. Left: $\langle H \rangle(\langle r \rangle, \Delta r)$. Right: red, $\langle H \rangle(\langle r \rangle)$ along $\Delta r = .9$; green, same if $\Delta r = 1$; blue, $\langle H \rangle(\langle r \rangle)$ if $\mu = 0$; dashes, true v.

CONCLUSION: *Energy surfaces demand a verification of the fluctuations of their collective coordinates.*

THE THEOREM

Let Q be the projector out of the ground state (g.s.) ψ of the constrained operator $\mathcal{H} = H - \lambda B$.
We know that the derivative of the g.s.eigenvalue ε is,

$$d\varepsilon/d\lambda = -\langle\psi|B|\psi\rangle.$$

The Brillouin-Wigner theorem also states that

$$d|\psi\rangle/d\lambda = -\frac{Q}{\varepsilon - Q\mathcal{H}Q} B|\psi\rangle.$$

Consequently, the second derivative reads,

$$d^2\varepsilon/d\lambda^2 = 2\langle\psi|B\frac{Q}{\varepsilon - Q\mathcal{H}Q} B|\psi\rangle,$$

a negative number since the operator, $\varepsilon - Q\mathcal{H}Q$, is negative definite. This makes ε a concave function and its Legendre transform, the energy $\langle H\rangle$, a convex function.

No way to obtain maxima or saddle points.