Ab initio DFT, relation between the energy of a nucleus and the density at its center

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I. SCIENTIFIC ISSUE

Despite its great empirical success, the nuclear density functional theory (NDFT) faces at least four fundamental difficulties. Indeed,

i) Any correct theory of a density functional derives from energy minimization under constraints(s) and it is well known that minimizations under constraint *necessarily* imply strict concavity. However, many irregularities in the table of experimental nuclear ground state energies violate the *average* concavity of the valley of stability. This basic contradiction, namely that a concave theory cannot accurately fit non concave data, demands a cure. Explaining the contradiction and offering a cure make a main motivation for this proposal.

ii) The most obvious constraints to be satisfied for a NDFT solution are proper values of the particle numbers Z and N and a considerable effort has been dedicated to the problem of particle number projection; in particular, "transition density functionals" have received much attention. However, if the projection remains approximate, there are residual fluctuations ΔZ, ΔN, the order of magnitude of which may remain uncontrolled. Such fluctuations may mix energies of neighboring nuclei, and absurd energies might be obtained in the presence of energy convexities. At stake is the empirical claim that there can exist universal parameters for a universal NDF. The proposed workshop will discuss this and propose a solution.

iii) Most present NDF calculations are either two- or three-dimensional, if only to obtain deformed solutions. This raises an angular projection problem, similar to the projection of Z and N, with similar technical costs for "transition densities". It was shown a few years ago, however, that a density functional for a deformed intrinsic state would depend on the angular momentum. This destroys the possibility of "universality". Fortunately, it was also shown that the NDFT can be rigorously reduced to a 1-dimensional theory of radial, scalar density profiles, valid for all nuclei, whether odd, or doubly even, or doubly odd. In that radial theory (RDFT), "universality" becomes again possible and this will be explained.

iv) The distinction between "density functional theory in the laboratory" and "internal density functional theory" is well understood, but there remain difficulties in the latter, because of the implementation of center-of-mass correlations. A comparison between both approaches would be useful and will be part of the discussions.

We therefore propose the organisation of a workshop to i) clarify such basic questions and ii) take advantage of it to create a task group to implement a first, elementary but realistic, fully rigorous calculation.

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For the sake of simplicity at first, this fully rigorous calculation can consist in constraining the density of a light nucleus (the α particle) at its center only, in a spherical formalism. The choice of such a light nucleus obviously implements simplicity, but furthermore allows more "exact" calculations with more "realistic" forces. And it clearly makes an easy case for the radial density theory. Last but not least, it allows an easy verification of the concavity of the energy with respect to the constraint. Hence, as explained just below, a collaboration is being set between colleagues having experience in i) the few body problem, ii) shell model calculations with realistic forces, and iii) the roles of symmetries for the NDFT.

The physics department at the university of Arizona in Tucson has a code which generates an antisymmetrized basis of wave functions, $\phi_i(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3, \sigma_1, \sigma_2, \sigma_3, \sigma_4)$, for the three Jacobi coordinates of an α particle. Here, in an obvious notation, the Jacobi coordinates read, $\vec{\xi}_1 = \vec{r}_2 - \vec{r}_1$, $\vec{\xi}_2 = \vec{r}_3 - (\vec{r}_1 + \vec{r}_2)/2$, $\vec{\xi}_3 = \vec{r}_4 - (\vec{r}_1 + \vec{r}_2 + \vec{r}_3)/3$, and σ_1, ... σ_4 denote the nucleon spins. Isospin labels are understood in the following. It is also understood that this basis induces only real numbers in the following practical calculations.

Realistic interactions are available to us, of which the matrix elements can be expressed in a harmonic oscillator basis. This is the case, in particular, for calculations relating to the *no core shell model* [1].The Hamiltonian matrix elements that we shall use, $H_{ij} = \langle \phi_i | H | \phi_j \rangle$, are real numbers on our basis.

Similar tools are also available at Saclay, if only through the strong experience of J. Carbonell with detailed calculations of three- and four-body systems [2].

If the dimension N of the basis is big enough, the diagonalization of the corresponding matrix, H_N, provides a good description of the α particle. Configuration mixing coefficients, $c_i, i = 1, ..., N$, then define the ground state as, $\psi_0 = \sum_i c_i \, \phi_i$, and one can define a density profile of this nucleus by the integral and sum, $\rho(\vec{\xi}) = 4 \sum_{\sigma_1, ..., \sigma_4} \int d\vec{\xi}_1 d\vec{\xi}_2 \, |\psi_0(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}, \sigma_1, ..., \sigma_4)|^2$. More generally, one can define a "one-body" density matrix in Jacobi and spin space by the integral and sum, $\bar{\rho}(\vec{\xi}, \vec{\xi}', \sigma, \sigma') = 4 \sum_{\sigma_1, \sigma_2, \sigma_3} \int d\vec{\xi}_1 d\vec{\xi}_2 \, \psi_0(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}, \sigma_1, \sigma_2, \sigma_3, \sigma) \, \psi_0(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}', \sigma_1, \sigma_2, \sigma_3, \sigma')$. We recall here that the last Jacobi coordinate also reads, $\vec{\xi}_3 = 4/3 \, (\vec{r}_4 - \vec{R})$, where $\vec{R} = (\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4)/4$ is the center-of-mass coordinate. Hence, except for the scale coefficient 4/3 or its reciprocal 3/4, the degrees of freedom, $\vec{\xi}_3$ and $(\vec{r}_4 - \vec{R})$, refer to the same information, namely the motion of a nucleon with respect to the total center of mass.

Temporarily, we are only interested in the density at the nuclear center, $\rho_0 = \sum_{ij=1}^{N} c_i \, M_{ij} \, c_j$, where the matrix M is made up of the elements, $M_{ij} = 4 \sum_{\sigma_1, ..., \sigma_4} \int d\vec{\xi}_1 d\vec{\xi}_2 \, \phi_i(\vec{\xi}_1, \vec{\xi}_2, 0, \sigma_1, \sigma_2, \sigma_3, \sigma_4) \, \phi_j(\vec{\xi}_1, \vec{\xi}_2, 0, \sigma_1, \sigma_2, \sigma_3, \sigma_4)$. A clear generalization reads, $\bar{M}_{ij}(\vec{\xi}, \vec{\xi}', \sigma, \sigma') = 4 \sum_{\sigma_1, \sigma_2, \sigma_3} \int d\vec{\xi}_1 d\vec{\xi}_2 \, \phi_i(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}, \sigma_1, \sigma_2, \sigma_3, \sigma) \, \phi_j(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}', \sigma_1, \sigma_2, \sigma_3, \sigma')$, but we will not need it in the context of the present proposal.

The knowledge of both matrices H and M then allows the study of energy minimization under density constraint, using the diagonalization of the matrix, $(H + \lambda M - \varepsilon I)$, where λ is a Lagrange multiplier and I denotes the identity matrix. This leads to a polynomial equation, of total order N in ε and λ,

$$0 = P(\varepsilon, \lambda) \equiv det(H + \lambda M - \varepsilon I). \tag{1}$$

Given λ, the lowest root, $\varepsilon(\lambda)$, defines the constrained ground state, ψ_λ, with its mixing coefficients, $c_i(\lambda)$, its energy, $\eta = \sum_{ij} c_i(\lambda) H_{ij} c_j(\lambda)$, and its center density, $\rho_0 = \sum_{ij} c_i(\lambda) M_{ij} c_j(\lambda)$.

It is well established that the plot of this lowest branch, $\varepsilon(\lambda)$, is convex and that the plot of its Legendre transform, $\eta(\rho_0)$, is concave. It is also trivial that the following properties hold, $\varepsilon = \eta + \lambda \, \rho_0$, $d\varepsilon/d\lambda = \rho_0$, and $d\eta/d\rho_0 = -\lambda$. Obviously, the curvature of the latter plot, $\eta(\rho_0)$, at its minimum with $\lambda = 0$, describes the compressibility.

According to the property, $d\varepsilon/d\lambda = \rho_0$, one takes advantage of Eq. (1) to obtain ρ_0 from,

$$0 = Q(\varepsilon, \lambda, \rho_0) \equiv \frac{\partial P}{\partial \varepsilon} \, \rho_0 + \frac{\partial P}{\partial \lambda}. \tag{2}$$

This creates a second polynomial equation in terms of $\varepsilon, \lambda, \rho_0$, and actually, once ε is replaced by $(\eta + \lambda \rho_0)$, these two equations, $P = 0$, $Q = 0$, become equations in terms of η, λ, ρ_0. A straightforward elimination of λ between P and Q leaves a resolvent polynomial equation,

$$R(\rho_0, \eta) = 0, \tag{3}$$

the order of which turns out to be $N(N-1)$. This result is a most simple, *ab initio* [3] derivation of a relation between density and energy. If the number of constraints is increased for densities along a full mesh, an *ab initio* DFT obtains.

It can be stressed that this first calculation is fully compatible with the four principles, stated above, of rigor for a NDFT and is a first step towards generalizations.

II. GOALS OF THE WORKSHOP

Besides a full day, dedicated to explanations of the problems i) to iv), debates about their solutions and the set up of practical calculations, a goal of this proposal is the constitution of a working group of theorists to

1. calculate H_N and M_N (subscript N introduced here to specify the basis dimension) for various embedded basis subspaces with increasing dimension N,
2. obtain the corresponding polynomials P_N, Q_N, R_N; in case of numerical difficulties, obtain at least the constrained ground state properties $\varepsilon, \rho_0, \eta$, upon letting λ evolve in a neighborhood of the physical value, $\lambda = 0$,
3. attempt for various values N a Taylor or Padé representation of the ground state branch, $\eta(\rho_0)$, and, naturally, compare such representations.

This work for a nucleus as light as the α particle is a first step towards more ambitious ones for heavier nuclei. But it already helps in evaluating serious questions, such as,
- the nature of the constraint ; while it is obviously a positive definite operator, it can be unbounded from above, maybe creating difficulties if $\lambda < 0$,
- the slow or fast numerical convergence of the plot of $\eta(\rho_0)$, as a function of the dimension N, towards a limit plot,
- the mathematical relation between a polynomial R_N and a polynomial R_{N+1}; this would illustrate convergence better than just numerical evidence.

If only for such preliminary results, the next step of this constructive theory, for a heavier nucleus, demanding a shell model representation with center-of-mass trapping rather than Jacobi coordinates hence large values of matrix dimension N, would be easier attempted and more realistic estimates of the compressibilty could be trusted.

Another extension constrains the energy by more than one value of the density : for instance one can add a constraint in the surface region ; the question of surface energy is very sensitive, see for instance the gradient terms used in EDFT.

An ultimate goal of the theory is, naturally, to verify how results for light nuclei extrapolate and/or generalize for heavier ones, namely whether universality with respect to particle number can be obtained. The concavity [4] property of the present constructive theory is an essential ally for an attempt at universality.

III. USEFUL REFERENCES

1 P. Navrátil, J.P. Vary, and B.R. Barrett, Phys. Rev. Lett. **84** 5728 (2000) ; Phys. Rev. **C 62** 054311 (2000) ; P. Navrátil, S. Quaglioni, I. Stetcu, and B.R. Barrett, J. Phys.**G 36** 083101 (2009)

2 R. Lazauskas, J. Carbonell, Phys. Rev C70 (2004) 044002 ; nucl-th/04080

3 B.G. Giraud and S. Karataglidis, Phys.Lett.**B 703** 88 (2011)

4 B.R. Barrett, B.G. Giraud, B.K. Jennings and N. Toberg, Nucl. Phys. **A 828** 267 (2009)

IV. LIST OF POTENTIAL SPEAKERS

At present, the working group motivated by this subject, with a possible participation in numerical calculations, involves : B.R. Barrett (U-Ariz), R. Carbonell (IRFU-Saclay), B.G. Giraud (IPhT-Saclay), S. Karataglidis (U-Johanesburg), M. Kruse (U-Ariz) and J. Messud. First meetings of the group are planned for the period between about March 23 and April 13 in the framework of ENST at Saclay. The presence of B.B., J.C., B.G. is sure. The presence of M. Kruse is much less sure, because of the possibility of a position opening at that time, but a short visit is not excluded. Finally, because of other duties, the presence of S. Karataglidis and J. Messud will be about one week.

Besides private discussions, about six talks, one hour each, with 15 additional minutes for discussion, are planned :

– B. Barrett (bbarrett@physics.arizona.edu) *title : The no core interaction*
– J. Carbonell (jaume.carbonell@cea.fr) *title : How to calculate the nuclear wave-function of helium 4*
– B. Giraud (bertrand.giraud@cea.fr) *title : Impact on the DFT of the symmetries of the Hamiltonian, universality, Kohn-Sham potentials, special polynomials, all that*
– S. Karataglidis (stevenka@uj.ac.za) *title : Polynomial method to relate energy to constraint(s)*
– J. Messud (jeremie.messud@aquitaine.fr) *title : Implementing center-of-mass correlations in a DF*
– G. Ripka (georges.ripka@@cea.fr) *title : Rigorous diagrammatic formulation of a DF*

V. SHORT-TERM VISITORS

Barrett will stay at the ESNT for three weeks, starting March 26 after a first week (March 19-23) for a FUSTIPEN collaboration at GANIL. Kruse most likely will not come this time. Karataglidis and Messud will come one week.

VI. PROGRAM

Technical discussions start on Friday March 23. Every interested outsider is welcome. Contact either B. G. (bggiraud@yahood.fr) or J. C. (jaume.carbonell@cea.fr). Official talks on Wednesday April 11.

09h00-09h15 Welcome

09h15-10h15 Barrett ; 10h15-10h30 Discussion

10h30-10h45 Break

10h45-11h45 Carbonell ; 11h45-12h00 Discussion

12h00-12h45 Giraud ; 12h45-13h00 Discussion

13h00-14h00 Lunch

14h00-15h00 Karataglidis ; 15h00-15h15 Discussion

15h15-16h15 Messud ; 16h15-16h30 Discussion

16h30-16h45 Break

16h45-17h45 Ripka ; 17h45-18h Discussion

18h00 End