Analytic density functionals

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Abstract. A systematic strategy for the calculation of density functionals (DFs) consists in coding informations about the density and the energy into polynomials of the degrees of freedom of wave functions. DFs and Kohn-Sham potentials (KSPs) are then obtained by standard elimination procedures of such degrees of freedom between the polynomials. Numerical examples illustrate the formalism.

Existence theorems [1] for DFs do not provide directly constructive algorithms. Fortunately, the Kohn-Sham (KS) method [2] spares the construction of a "kinetic functional" and reduces energy and density calculations to the tuning of a local potential, $v_{KS}(r)$. Hence, a considerable amount of work has been dedicated to detailed estimates of electronic correlation energies and the corresponding KSPs, see for instance [3, 4, 5]. Many authors were also concerned with representability and stability questions, see for instance [6] and, for calculations in subspaces, see [7] and [8]. For cases where the mapping between potential and density shows singularities, see [9]. For reviews of the rich multiplicity of derivations of DFs and KS solutions and their properties, we refer to [10] and [11], and, for nuclear physics, to [12].

Local or quasi local approximations use the continuous infinity of values $\rho(\mathbf{r}), \forall \mathbf{r}$, as the parameters of the problem. However, whether for atoms, molecules or nuclei, a finite number of parameters is enough to describe physical situations. For instance, Woods-Saxon nuclear profiles notoriously make good approximations, depending only on a handful of parameters, and it is easy to add a few parameters describing, for example, long tails and/or moderate oscillations of the density. (High frequency oscillations are unlikely, for they might cost large excitation energies.) We can stress here, in particular, the one-dimensional nature of the radial density functional (RDF) theory [13], valid for nuclei and/or atoms, isolated, described by rotationally-invariant Hamiltonians; the constrained density minimization of energy [14] returns isotropic densities, with radial profiles, $\rho(r), 0 \leqslant r < \infty$. The number of parameters to describe a nuclear density, therefore, can be restricted to maybe ~ 10 at most; situations with ~ 20 parameters are a luxury. For molecules, shapes are much more numerous, but a finite, while large number of parameters, truncating a list of multipoles for instance, still makes a reasonable frame. Practical DFs, therefore, can boil down to *functions* of a finite number of parameters. Functional variations can then be replaced by simple derivatives.

Herein, we show how information about both the density and the energy can be recast into polynomials. This allows eliminations of part of the parameters. Further polynomial manipulations locate energy extrema. Only density parameters are left. The same method gives KSPs. Finally we offer a discussion and conclusion.

Consider a basis of n orthonormalized, single-particle states, $\varphi_\alpha(\mathbf{r}\sigma\tau)$, where spin and isospin labels $\sigma\tau$ will be understood. The orthonormalized Slater determinants ϕ_i made out of the φ_α's for N fermions make a finite subspace, of some dimension $\mathcal{N}$, in which eigenstates of the physical Hamiltonian H can be approximated by configuration mixings, $\Psi = \sum_{i=1}^{\mathcal{N}}(C_i + iC'_i)\phi_i$. Here C_i and C'_i are the real and imaginary parts, respectively, of the mixing coefficients, but, in practice, with real matrix elements, $H_{ij} = \langle \phi_i | H | \phi_j \rangle$, of the Hamiltonian H, the imaginary parts C'_i vanish. Both the energy η and the normalization are *quadratic* functions of such coefficients,

$$\eta = \sum_{i,j=1}^{\mathcal{N}} C_i H_{ij} C_j, \ \ \sum_{i=1}^{\mathcal{N}} C_i^2 = 1. \tag{1}$$

Let $a_{\mathbf{r}}^\dagger$ and $a_{\mathbf{r}}$ be the usual creation and annihilation operators at position $\mathbf{r}$. Tabulate the matrix elements $\left\langle \phi_j \left| a_{\mathbf{r}}^\dagger a_{\mathbf{r}} \right| \phi_j \right\rangle$. The density corresponding to Ψ is, again, *quadratic* with respect to the C_i's,

$$\rho(\mathbf{r}) = \sum_{ij} C_i \left\langle \phi_j \left| a_{\mathbf{r}}^\dagger a_{\mathbf{r}} \right| \phi_j \right\rangle C_j, \tag{2}$$

and any parameter that is linear with respect to moments of the density is also a quadratic function of the C_i's.

Let $\{S_\nu(\mathbf{r})\}, \ \nu = 1, \ldots, \infty$, be a complete orthonormal set of "vanishing average" functions. Namely, the two sets of conditions, $\int d\mathbf{r}\, S_\nu(\mathbf{r}) = 0, \forall \nu$, and, $\int d\mathbf{r} S_\mu(\mathbf{r}) S_\nu(\mathbf{r}) = \delta_{\mu\nu}, \forall \mu\nu$, are satisfied. Such sets are easy to find; in the case of one-dimensional problems, including radial ones, they can be implemented by means of orthogonal polynomials [15, 16] and a generalization to more dimensions is easy. Then subtract from ρ some reference density, ρ_0, obtained by some approximation relevant for the N fermions. The difference, $\Delta\rho = \rho - \rho_0$, is of a vanishing average, since, by definition, both ρ and ρ_0 integrate out to N. Then the Fourier coefficients,

$$\Delta_\nu = \int d\mathbf{r}\ S_\nu(\mathbf{r}) \Delta\rho(\mathbf{r}), \tag{3}$$

define ρ, as $\rho = \rho_0 + \sum_{n=1}^{\infty} \Delta_\nu S_\nu$. As already stated, this expansion of ρ can be truncated. at some realistic order $\mathcal{N}'$, lower than the number of independent parameters C_i. The Δ_ν's are *quadratic* in the C_i's,

$$\Delta_\nu = \sum_{ij} C_i \left[\int d\mathbf{r}\ S_\nu(\mathbf{r}) \left\langle \phi_j \left| a_{\mathbf{r}}^\dagger a_{\mathbf{r}} \right| \phi_j \right\rangle \right] C_j - \rho_{0\nu}. \tag{4}$$

Note the auxiliary numbers, $\rho_{0\nu} = \int d\mathbf{r}\, S_\nu(\mathbf{r})\, \rho_0(\mathbf{r})$.

It is then trivial to use the $\mathcal{N}'$ density constraints, Eqs. (4), and the normalization in Eqs. (1), to eliminate, for instance, the last $(\mathcal{N}' + 1)$ coefficients C_i. This leaves a polynomial relation, $\mathcal{R}(\eta, \Delta_1, \ldots, \Delta_{\mathcal{N}'}, C_1, \ldots, C_{\mathcal{N}-\mathcal{N}'-1}) = 0$, between the energy, the density parameters, and the remaining coefficients C_i. Finally, the energy must be minimized with respect to such remaining coefficients, via still polynomial conditions, $\partial\mathcal{R}/\partial C_i = 0, \ i = 1, \ldots, \mathcal{N} - \mathcal{N}' - 1$. This gives a polynomial relation, $\mathcal{E}(\eta, \Delta_1, \ldots, \Delta_{\mathcal{N}'}) = 0$, between the energy and the density parameters. This polynomial $\mathcal{E}$ is our "algebraic" DF. It accounts for all contributions to the energy, both without and with correlations, for only matrix elements of the full H are used.

The procedure can be further simplified in the following way. 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, two among the parameters $(\Delta_\nu + \rho_{0\nu})$. Set the equation, polynomial in all three variables $\varepsilon, \lambda_1, \lambda_2$,

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

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,

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

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.

For an illustrative toy model, we consider two fermions only and set the one-body part of H as, $K = -d^2/(2dr_1^2) - d^2/(2dr_2^2) + (r_1^2 + r_2^2)/2$, the sum of two harmonic oscillators, and its two-body part as a translation invariant, separable potential, defined in coordinate representation by,

$$\left\langle r_1 r_2 \left| V \right| r_1' r_2' \right\rangle = -V_0 \delta\left[(r_1 + r_2 - r_1' - r_2')/2\right] e^{-[(r_2 - r_1)^2 + (r_2' - r_1')^2]/4} (r_2 - r_1)(r_2' - r_1')/\sqrt{2\pi}. \tag{7}$$

Then, given the first 4 wave functions, $\varphi_0, \ldots, \varphi_3$, of the one-dimensional harmonic oscillator, we create, to prepare a configuration mixing, a basis of 4 negative parity Slater determinants. These read, in a transparent notation, $\{\varphi_0, \varphi_1\}, \{\varphi_0, \varphi_3\}, \{\varphi_2, \varphi_1\}, \{\varphi_2, \varphi_3\}$. We set $V_0 = 3$ for a numerical test. To constrain H, we choose the second moment operator, $r_1^2 + r_2^2$. The matrices representing H and the constraint in the toy subspace read,

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

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

$$\begin{aligned} P_{\text{toy}}(\varepsilon, \lambda) = {}& -360 + 154\varepsilon + 344\varepsilon^2 - 154\varepsilon^3 + 16\varepsilon^4 + 1464\lambda \\ & + 1692\varepsilon\lambda - 1636\varepsilon^2\lambda + 256\varepsilon^3\lambda + 725\lambda^2 - 5140\varepsilon\lambda^2 + \\ & 1408\varepsilon^2\lambda^2 - 4192\lambda^3 + 3072\varepsilon\lambda^3 + 2064\lambda^4 = 0, \\ Q_{\text{toy}}(D, \varepsilon, \lambda) = {}& -1464 - 1692\varepsilon + 1636\varepsilon^2 - 256\varepsilon^3 - 1450\lambda + \\ & 10280\varepsilon\lambda - 2816\varepsilon^2\lambda + 12576\lambda^2 - 9216\varepsilon\lambda^2 - 8256\lambda^3 + \\ & (154 + 688\varepsilon - 462\varepsilon^2 + 64\varepsilon^3 + 1692\lambda - 3272\varepsilon\lambda + \\ & 768\varepsilon^2\lambda - 5140\lambda^2 + 2816\varepsilon\lambda^2 + 3072\lambda^3)D = 0. \end{aligned} \tag{9}$$

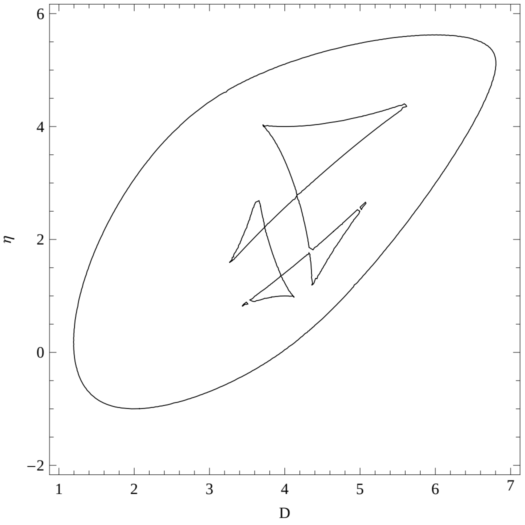

Figure 1. Contour $\mathcal{E}_{\rm toy}(\eta, D) = 0$ for the configuration mixing model with 4×4 matrices, as described in the text.

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

We show in Fig. 1 the contour line, $\mathcal{E}_{\rm toy}(\eta, D) = 0$. The ground state is found at the lowest point of the oval envelope, with coordinates, $D = 2, \eta = -1$. The highest and lowest eigenvalues of $\mathcal{H}$ are, 45/8 and -1, and those of $\mathcal{D}$ are, $4 \pm \sqrt{4 + \sqrt{15}}$, namely ~ 6.81 and ~ 1.19. This is confirmed by the extremal points, up, down, right and left, of the oval. The inside pattern refers to excited states. The concavity of the lowest part of the envelope and convexity of its highest part are transparent properties of the theory. They generalize for any dimension of the subspace and any number of constraints; we tested this generalization with further toy models. Moreover, when, via embedded subspaces, the dimension $\mathcal{N}$ of the matrices, $\mathcal{H}, \mathcal{D}_i$, grows while H and the constraints are kept the same, a growth of the envelope is found and the bottom of the envelope converges towards a limit, as expected. This gives numerical estimates for an extrapolation of this concave part towards its limit for $\mathcal{N} \to \infty$.

Such concavities should also occur in DF theories with a continuous infinity of constraints. But they are often difficult to verify, and are, therefore, overlooked, although they are an important test of soundness.

A byproduct of the procedure consists of a polynomial relating the potential energy to the constraints. Set the Hamiltonian as, $H = h + V$, with $V = -V_0 \mathcal{V}$, where V_0 is an interaction strength and $\mathcal{V}$ gives all details of interaction shapes. Nothing prevents one from considering V_0 as a Lagrange multiplier and obtain, via the polynomial method pushed one step further, a polynomial, $\mathcal{F}(\langle h \rangle, \langle \mathcal{V} \rangle, D_1, \dots, D_{\mathcal{N}'})$, linking $\langle h \rangle$ to the expectation values of $\mathcal{V}$ and the constraints. A standard result of this Legendre transform is, $\partial \langle h \rangle / \partial \langle \mathcal{V} \rangle = V_0$, *i.e.*,

$$\mathcal{G}(V_0, \langle h \rangle, \langle \mathcal{V} \rangle, D_1, \dots, D_{\mathcal{N}'}) \equiv (\partial \mathcal{F} / \partial \langle h \rangle)\, V_0 - \partial \mathcal{F} / \partial \langle \mathcal{V} \rangle = 0. \tag{10}$$

Replace, in $\mathcal{F}$ and $\mathcal{G}$, the quantity $\langle h \rangle$ by $\eta + \langle \mathcal{V} \rangle V_0$. Then eliminate η and V_0 between $\mathcal{E}$ and such modified $\mathcal{F}$ and $\mathcal{G}$. This links $\langle \mathcal{V} \rangle$, hence $\langle V \rangle$, to the D_i. It must be stressed here that now $\langle \mathcal{V} \rangle$ should *not* be minimized with respect to the D_i; rather, those D_i values to be used are those that minimize the total energy η.

A similar argument provides the kinetic energy, or any other part of η, in the same context of total energy constrained minimization. Such results are of interest for a detailed analysis of corrections induced by correlations.

An issue which will arise in all future models using this polynomial method is that the final minimization of η must be performed within a convex domain of densities: what conditions selected parameters (moments, local values, etc), satisfy to maintain ρ positive? This question was recently [18] solved by means of the Sturm criterion, for a general class of positive functions having positive Fourier transforms. The criterion gives the number of real roots of a polynomial, and can be used to ensure that a polynomial has no real roots. As seen in the toy model, the detailed structure of the calculation can be a guide to define the physically acceptable domain of parameters. For more subtle questions about the topology of acceptable functional spaces of densities and trial functions, we refer to [19], but will state, without proof, that here with traditional functions (harmonic, Coulomb) and their configuration mixing, the positivity of ρ should be sufficient.

There is also the question of spurious solutions. For more complicated systems, spurious solutions [7, 8] might certainly pop up, but an analysis for their detection remains easy. In particular, for other toy models that we tested, spurious solutions were found to induce values of physical parameters out of their allowed range, and/or even complex values while only real ones are acceptable. We can insist that the final, polynomial equation for the energy, $\mathcal{S}(\eta)=0$, can only create a finite number of candidate solution branches to be investigated.

A constructive derivation of KSPs is available. For instance, truncate some single particle basis and let $\mathcal{P}$ be the projector upon the resulting, finite dimensional subspace for a system of N fermions, with their Hamiltonian H, or rather now, $\mathcal{P}H\mathcal{P}$. Given the kinetic energy operator T, choose a local potential $w_0(r)$, hence a one-body operator $W_0=\sum_{i=1}^{N} w_0(r_i)$, hence a one-body Hamiltonian $H_0=T+W_0$, so that the ground state of $\mathcal{P}H_0\mathcal{P}$, a Slater determinant Φ_0, be non degenerate and providing an approximate density ρ_0 for the system. For any density ρ in the subspace, the integral, $\int \Delta\rho$, of the difference, $\Delta\rho=\rho-\rho_0$, vanishes as already stated. (Here and in the following, the integral sign, $\int$, means $\int r^{d-2}\,dr$ depending on the d-dimensional problem under consideration.) Expand, as already discussed, $\Delta\rho$ in a basis of orthonormal functions $S_\beta(r)$, "constrained by vanishing averages" [15, 16], $\Delta\rho(r)=\sum_{\beta=1}^{\infty} b_\beta\, S_\beta(r)$. Truncate the expansion at some suitable order $\mathcal{N}'$. Again, given a determinant Φ with the parameters $c_{n\ell m}^{\alpha}$ of its orbitals, or given a correlated state, $\Psi=\sum_q C_q\,\Phi_q$, the constraints, $\Phi\Rightarrow b_\beta$ or $\Psi\Rightarrow b_\beta$, are polynomials of the parameters. Given H_0, the polynomial method returns a polynomial $\mathcal{K}(\kappa, b_1,\dots,b_{\mathcal{N}'})$ for a reference functional, such that the lowest root of the equation, $\mathcal{K}=0$, represents the constrained minimum, $\kappa'=\mathrm{Min}_{\Phi\Rightarrow b_1,\dots,b_{\mathcal{N}'}}\langle\Phi|H_0|\Phi\rangle$, for the determinants in the subspace. In the same way, given the full H, the method gives a polynomial $\mathcal{E}(\eta, b_1,\dots,b_{\mathcal{N}'})$, the lowest η root of which is the constrained minimum, $\eta'=\mathrm{Min}_{\Psi\Rightarrow b_1,\dots,b_{\mathcal{N}'}}\langle\Psi|H|\Psi\rangle$, for correlated states in the subspace. Then it is trivial to derive from $\mathcal{K}$ and $\mathcal{E}$ a polynomial, $\Omega(\omega; b_1,\dots,b_{\mathcal{N}'})$, for the difference, $\omega=\eta-\kappa$. The diagonalization of $\mathcal{P}H\mathcal{P}$ then reads,

$$\frac{\partial\kappa}{\partial b_\beta}+\frac{\partial\omega}{\partial b_\beta}=0,\quad \beta=1,\dots,\mathcal{N}'. \tag{11}$$

With the ratio, $v_\beta=-(\partial\Omega/\partial b_\beta)/(\partial\Omega/\partial\omega)$, representing $\partial\omega/\partial b_\beta$, define the one-body, local potential, $v_\Delta(r)=\sum_{\beta=1}^{\mathcal{N}'} v_\beta\, S_\beta(r)$. Let Φ be the ground state of $\mathcal{P}\left[H_0+\sum_{i=1}^{N} v_\Delta(r_i)\right]\mathcal{P}$. Notice that $\langle\Phi|\mathcal{P}S_\beta\mathcal{P}|\Phi\rangle=\langle\Phi|S_\beta|\Phi\rangle$. Then the energy E of Φ has derivatives,

$$\partial E/\partial v_\beta=\int(\Delta\rho+\rho_0)\,S_\beta=b_\beta+b_{\beta 0}, \tag{12}$$

because of the orthonormality of the S_β's. The numbers, $b_{\beta 0}=\int\rho_0\,S_\beta$, are easily pretabulated. The quantities, v_β and $(b_\beta+b_{\beta 0})$, are Legendre conjugates, and, moreover, $\partial/\partial(b_\beta+b_{\beta 0})=\partial/\partial b_\beta$. The conditions, Eqs. (11), read as the diagonalization for a determinant Φ with the same density

ρ as that of the eigenstate Ψ of $\mathcal{PHP}$. The potential, $\mathcal{P}(w_0 + v_\Delta)\mathcal{P}$, is a KSP valid for the subspace, up to the convergence of the truncation with $\mathcal{N}'$ terms.

This polynomial method most often uses a very non local parametrization of ρ, that deviates from the quasi-local tradition of the field. In every case, our unconventional parametrization of ρ creates a new zoology of DFs. Nothing of this zoology is known to us, but its interest is obvious, since manipulations of polynomials and properties of their roots, including bounds, are basic subjects. Moreover, extrapolations of polynomials, and criticism of such extrapolations, are easy. The number of *available, exactly solvable* models is *huge*. It is limited only by computational power. For nuclei or atoms, the models will be "radial" [13], somewhat simple. For nuclear physics, our ultimate goal will be to see whether particle number can be used as a constraint, to generate a mass formula. For electrons in molecules or extended systems (metals, thin layers, etc.), however, a necessary algebra of functions of 2 or 3 variables will burden the models. Anyhow, one can always test whether our polynomials from "smaller" models may remain good approximations for "larger" ones, if, for instance, scaling properties can be established. Asymptotic properties of a sequence of "DF polynomials" might guide towards derivations of more traditional DFs. In particular, the polynomial models allow comparisons between the KS and the true kinetic energies of correlated systems. They also provide explicit terms for those correlation energies due to interactions.

In conclusion, this algebraic method simplifies density functional theory into energy minimization under finite numbers of constraints, under very elementary manipulations of polynomials. It retains all essential informations about the density and all components of the energy.

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