Constrained orthogonal polynomials

B.G. Giraud

Constrained orthogonal polynomials

B.G. Giraud,
giraud@spht.saclay.cea.fr, Service de Physique Théorique, DSM, CE Saclay, F-91191 Gif/Yvette, France
(November 8, 2018)

Abstract: We define sets of orthogonal polynomials satisfying the additional constraint of a vanishing average. These are of interest, for example, for the study of the Hohenberg-Kohn functional for electronic or nucleonic densities and for the study of density fluctuations in centrifuges. We give explicit properties of such polynomial sets, generalizing Laguerre and Legendre polynomials. The nature of the dimension 1 subspace completing such sets is described. A numerical example illustrates the use of such polynomials.

I. INTRODUCTION

Generalizations Γ_n of Hermite polynomials H_n were recently [1] proposed to describe, for instance, density perturbations constrained by a condition of matter conservation. Because of the constraint, such polynomials cannot form a complete set, but span a subspace well suited to specific applications. In particular, the polynomials Γ_n used in [1] were motivated by the consideration in nuclear physics of the Hohenberg-Kohn functional [2] and similar functionals along the Thomas-Fermi method [3,4]. Indeed, in such approaches, the ground state of a quantum system is shown to be a functional of its density $\rho(r)$, and there is a special connection between $\rho(r)$ and the mean field $u(r)$ driving the system. It was thus convenient to expand variations of ρ in a basis $\{w_m(r)\}$ of particle number conserving components, $\delta\rho(r) = \sum_m \delta\rho_m\, w_m(r)$, with the term-by-term constraint, $\forall m,\ \int dr\, w_m(r) = 0$. This spares, in the formalism, the often cumbersome use of a Lagrange multiplier. Simultaneously, it was convenient to expand variations of u in a basis orthogonal to the flat potential, because, trivially, a flat δu, as just a change in energy reference, cannot influence the density. The same basis can thus be used for $\delta u(r) = \sum_n \delta u_n\, w_n(r)$, since the very same condition, $\int dr\, w_n(r) = 0$, induces orthogonality to a constant δu. Because of the nuclear physics context of [1], harmonic oscillators shell models were considered and the basis contained a Gaussian factor, $e^{-\frac{1}{2}r^2}$.

The same functional approaches [2–4] are also of a general use in atomic and molecular physics, where Gaussian weights would be clumsy and radial properties are best fitted with simple exponential weights [5]. Furthermore, in [1], the discussion was restricted to one dimensional problems. In the present note, we want to include two and three dimensional situations. We shall thus use weights of the form $e^{-\frac{1}{2}r}$, with $0 \le r < \infty$, but integrals will carry a factor r^ν, with ν a positive exponent, suitable for dimension d. This will lead to generalizations of Laguerre polynomials.

This note is also concerned with compact domains, of the form $0 \le r \le 1$ for instance. This might correspond for instance to expansions of density fluctuations in cylindrical vessels used for chemical processes, where mass conservation is also in order, or maybe in centrifuges. Radial integrals with factors r and r^2 in both the constraint and orthogonalization conditions will lead to generalizations of Legendre polynomials.

For any positive weight $\mu(r)$, and any dimension d, a constraint of vanishing average, $\int dr\, r^\nu\, \mu(r)\, \Gamma_n(r) = 0$, is incompatible with a polynomial Γ of order $n = 0$. Therefore, in the following, the order hierarchy for the constrained polynomials runs from $n = 1$ to ∞, while that for the traditional polynomials runs from 0 to ∞. We study in some generality the "Laguerre" case in Section II. In turn, the "Legendre" case is the subject of Section III. A brief Section IV discusses possible applications to the study of density fluctuations in centrifuges. Section V answers a question which was omitted in [1], that of the nature of the projector onto the subspace spanned by the constrained states and the nature of the codimension of this subspace. A numerical application is provided in Section VI. A discussion and conclusion make Section VII.

II. MODIFICATION OF LAGUERRE POLYNOMIALS BY A CONSTRAINT OF ZERO AVERAGE

In this Section we consider basis states carrying a weight $e^{-\frac{1}{2}r}$, in the form $w_n(r) = e^{-\frac{1}{2}r}\, G_n^d(r)$, where G_n^d is a polynomial. It is clear that G_0^d cannot be a finite, non vanishing constant if the constraint, $\int_0^\infty dr\, r^{d-1}\, e^{-\frac{1}{2}r}\, G_0^d(r) = 0$, must be implemented. Hence set integer labels $m \ge 1$ and $n \ge 1$ and define polynomials G_n^d by the conditions,

$$\int_0^\infty dr\ r^{d-1}\, e^{-r}\, G_m^d(r)\, G_n^d(r) = g_n^d\, \delta_{mn}\,, \qquad \int_0^\infty dr\ r^{d-1}\, e^{-\frac{1}{2}r}\, G_n^d(r) = 0\,, \tag{1}$$

where δ_{mn} is the usual Kronecker symbol and the positive numbers g_n^d are normalizations, to be defined later.

It is elementary to generate such polynomials numerically, in two steps by brute force, namely i) first create "trivial seeds" of the form, $s_n^d(r) = r^n - \langle r^n \rangle_d$, where the subtraction of the average, $\langle r^n \rangle_d = 2^n\,(d-1+n)!/(d-1)!$, ensures that each trivial seed fulfills the constraint, then ii) orthogonalize such seeds by a Gram-Schmidt algorithm. The first polynomials read,

$$G_1^1 = r-2, \quad G_2^1 = r^2-5r+2, \quad G_3^1 = r^3-10r^2+20r-8, \quad G_4^1 = r^4-17r^3+78r^2-108r+24, \tag{2a}$$
$$G_1^2 = r-4, \quad G_2^2 = r^2-8r+8, \quad G_3^2 = r^3-14r^2+44r-32, \quad G_4^2 = r^4-22r^3+138r^2-288r+144, \tag{2b}$$
$$G_1^3 = r-6, \quad G_2^3 = r^2-11r+18, \quad G_3^3 = r^3-18r^2+78r-84, \quad G_4^3 = r^4-27r^3+216r^2-606r+468. \tag{2c}$$

All these are defined to be "monic", namely the coefficient of r^n is always 1. For an illustration we show in Figure 1 the new polynomials G_1^1 and G_1^2, together with Laguerre polynomial L_1. The same Fig. 1 also shows G_2^1, G_2^2 and L_2.

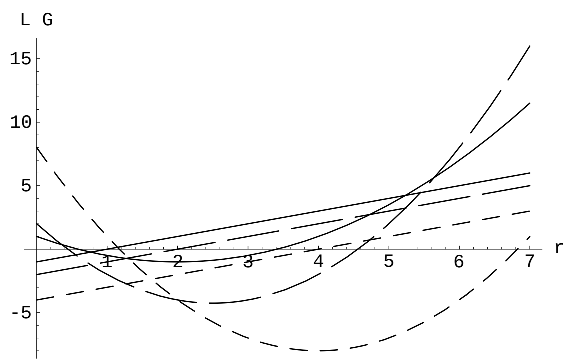

FIG. 1. Comparison of Laguerre polynomials L_1, L_2 (full lines) with new polynomials G_1^1, G_2^1 (long dashes), G_1^2, G_2^2 (dashes).

Rather using the Gram-Schmidt method, we find it easier, and more elegant, to generate the polynomials G_n^d, starting from the initial table, Eqs. (2a,2b,2c), by means of the following recursion formula,

$$G_n^d(r) = (r-d)\,G_{n-1}^d(r) - 2\,r\,G_{n-1}^{d\,\prime}(r) + (n+d-1)\,(n-2)\,G_{n-2}^d(r), \tag{3}$$

where the prime denotes the derivative with respect to r. Its simple structure can be proven analytically as follows:

i) Let us first create some kind of a "less trivial seed" at order n, assuming the polynomial G_{n-1}^d is known. For this, try $r\,G_{n-1}^d$. By partial integration, we see that,

$$\int_0^\infty dr\ r^{d-1}\,e^{-\frac{1}{2}r}\left[r\,G_{n-1}^d(r)\right] = 2\int_0^\infty dr\ e^{-\frac{1}{2}r}\left[r^d\,G_{n-1}^d(r)\right]', \tag{4}$$

where again a prime means derivation with respect to r. Thus $\sigma_n^d \equiv \left(r\,G_{n-1}^d - 2\,r\,G_{n-1}^{d\,\prime} - 2\,d\,G_{n-1}^d\right)$ makes indeed a less trivial seed, compatible with the constraint. Notice that the order n of this seed polynomial σ_n^d comes from the term $r\,G_{n-1}^d$ only, the other two terms having order $n-1$. Notice again that, in the table, Eqs. (2), all polynomials G_n^d are monic. We can define G_n^d as monic, systematically. Since the product $r\,G_{n-1}^d$ respect this "monicity", and since σ_n^d fulfills the constraint, we conclude that σ_n^d is a linear combination of G_n^d, with coefficient 1, and of all the lower order polynomials G_m^d, with $1 \le m < n$, but with yet unknown coefficients.

ii) It turns out that such coefficients vanish if $m < n-2$. Indeed, an integration of σ_n^d against G_m^d, weighted by $r^{d-1}e^{-r}$, gives, by partial integration of the $G_{n-1}^{d\,\prime}$ term,

$$\int_0^\infty dr\ e^{-r}\, r^{d-1}\, \sigma_n^d(r)\, G_m^d(r) \equiv \int_0^\infty dr\ r^{d-1} e^{-r} \left[(r-2d)\, G_{n-1}^d(r) - 2r\, G_{n-1}^{d\,\prime}(r)\right]\ G_m^d(r) =$$
$$\int_0^\infty dr\ e^{-r}\, r^{d-1}\, G_{n-1}^d(r)\, (r-2d)\, G_m^d(r) + 2\int_0^\infty dr\ G_{n-1}^d(r)\ \left[e^{-r}\, r^d\, G_m^d(r)\right]' =$$
$$\int_0^\infty dr\ e^{-r}\, r^{d-1}\, G_{n-1}^d(r) \left[-\sigma_{m+1}^d(r) - 2d\, G_m^d(r)\right]. \tag{5}$$

In the bracket [ ] in the last right-hand side of Eq. (5) the seed σ_{m+1}^d has order $m+1$ and, by definition, G_m^d is of order m. By definition also, G_{n-1}^d, of order $n-1$, is orthogonal to all those polynomials of lower order, that are compatible with the constraint. This integral, Eq. (5), thus vanishes as long as $m+1 < n-1$. It can be concluded that the difference, $\sigma_n^d - G_n^d$, contains only two contributions, namely those from G_{n-2}^d and G_{n-1}^d. Explicit forms for their coefficients are obtained by elementary manipulations, leading to Eq. (3). Elementary manipulations also give,

$$2\, r\, G_n^{d\,\prime\prime} - (r-2d)\, G_n^{d\,\prime} + n\, G_n^d = (n-1)\,(n+d)\, G_{n-1}^d\,. \tag{6}$$

Here, in the same way as a prime means first derivative with respect to r, we used double primes for second derivatives. Finally the normalization of the polynomials is obtained easily as,

$$g_n^d \equiv \int_0^\infty dr\ e^{-r}\, r^{d-1}\, [G_n^d(r)]^2 = (n-1)!\,(n+d)!\,. \tag{7}$$

III. MODIFICATION OF LEGENDRE POLYNOMIALS BY A CONSTRAINT OF ZERO AVERAGE

Legendre polynomials, and their associates and generalizations (Gegenbauer, Chebyshev, Jacobi) are defined with respect to the $[-1,1]$ segment. Exceptionally in the literature, one finds shifted Legendre polynomials, adjusted to the $[0,1]$ segment. We are here interested in applications to radial densities in cylinders, or the small circles of toruses, or spheres. Hence we shall use $0 \le r \le 1$. It is clear that the case, $d=1$, does not make an original problem, since Legendre polynomials, whether translated and/or scaled or not, already average to 0 as soon as their order n is ≥ 1. We keep the case, $d=1$, for the sake only of completeness and in this Section we consider $d=1,2,3$, with a geometry factor r^{d-1}. The weight is $\mu(r)=1$, hence our states are described by just a polynomial $\mathcal{G}_n^d$ of order n. It is again obvious that $\mathcal{G}_0^d$ cannot be a non vanishing constant if the constraint, $\int_0^1 dr\, r^{d-1}\, \mathcal{G}_0^d(r)=0$, is implemented. Hence set $m \ge 1$, $n \ge 1$, and define polynomials $\mathcal{G}_n^d$ from conditions,

$$\int_0^1 dr\ r^{d-1}\, \mathcal{G}_m^d(r)\, \mathcal{G}_n^d(r) = \gamma_n^d\, \delta_{mn}\,, \qquad \int_0^1 dr\ r^{d-1}\, \mathcal{G}_n^d(r) = 0\,, \tag{8}$$

where the normalizations γ_n^d are again to be defined later. It is obvious that the shifted (and shrunk) Legendre polynomials $\mathcal{L}_n(2r-1)$, $n \ge 1$, satisfy both constraint and orthogonality relations for $d=1$, because they are orthogonal to any constant polynomial, of order 0. The polynomials $\mathcal{G}_n^1 = \mathcal{L}_n(2r-1)$ thus make nothing new. We turn therefore to $d=2$ and $d=3$, with a brute force construction as in the previous Section. But the defining conditions, Eqs. (8), show a difference with Eqs. (1): both orthogonality and constraint conditions now carry the same weight, namely $\mu^2=\mu$, while in the previous case, Eqs. (1), there were different weights, because of the exponentials e^{-r} and $e^{-\frac{1}{2}r}$. A similar difference between μ^2 and μ happened in the "Hermite" case, naturally.

Hence now, in this Legendre case, we can Gram-Schmidt orthogonalize even more trivial seeds r^n, without subtractions, and accept those orthogonal polynomials with order $m \ge 1$. The table of first results reads,

$$\mathcal{G}_1^1 = 2r-1, \quad \mathcal{G}_2^1 = 6r^2-6r+1, \quad \mathcal{G}_3^1 = (2r-1)(10r^2-10r+1), \quad \mathcal{G}_4^1 = 70r^4-140r^3+90r^2-20r+1, \tag{9a}$$
$$\mathcal{G}_1^2 = 3r-2, \ \mathcal{G}_2^2 = 10r^2-12r+3, \quad \mathcal{G}_3^2 = 35r^3-60r^2+30r-4, \quad \mathcal{G}_4^2 = 126r^4-280r^3+210r^2-60r+5, \tag{9b}$$
$$\mathcal{G}_1^3 = 4r-3, \ \mathcal{G}_2^3 = 15r^2-20r+6, \ \mathcal{G}_3^3 = 56r^3-105r^2+60r-10, \ \mathcal{G}_4^3 = 210r^4-504r^3+420r^2-140r+15. \tag{9c}$$

Easy, but slightly tedious manipulations validate the following recursion relations,

$$n\, \mathcal{G}_n^1 = (2n-1)\,(2r-1)\, \mathcal{G}_{n-1}^1 - (n-1)\, \mathcal{G}_{n-2}^1\,, \tag{10a}$$
$$(n+1)\,(2n-1)\, \mathcal{G}_n^2 = 2\,[\,(4n^2-1)r - 2n^2\,]\, \mathcal{G}_{n-1}^2 - (n-1)\,(2n+1)\, \mathcal{G}_{n-2}^2\,, \tag{10b}$$
$$n^2\,(n+2)\, \mathcal{G}_n^3 = (2n+1)\,[\,2n(n+1)r - (n^2+n+1)\,]\, \mathcal{G}_{n-1}^3 - (n-1)\,(n+1)^2\ \mathcal{G}_{n-2}^3\,. \tag{10c}$$

and the differential equation,

$$r\,(r-1)\,\mathcal{G}_n^{d\,\prime\prime}+[\,(d+1)\,r-d\,]\,\mathcal{G}_n^{d\,\prime}-n\,(n+d)\,\mathcal{G}_n^d=0. \tag{11}$$

Finally the normalization of the polynomials reads,

$$\gamma_n^d\equiv\int_0^\infty dr\;r^{d-1}\,[\mathcal{G}_n^d(r)]^2=1/(2n+d)\,. \tag{12}$$

We show in Figure 2 the plots of $\mathcal{G}_n^d$ for $n=1,2$ and $d=1,2,3$.

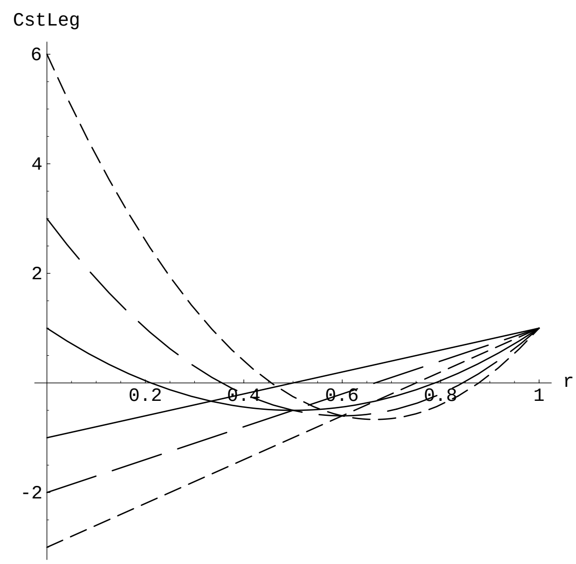

FIG. 2. Modified Legendre polynomials $\mathcal{G}_1^1$, $\mathcal{G}_2^1$ (full lines), $\mathcal{G}_1^2$, $\mathcal{G}_2^2$ (long dashes), $\mathcal{G}_1^3$, $\mathcal{G}_2^3$ (dashes).

IV. POLYNOMIALS FOR CENTRIFUGES

The case of centrifuges is worth a short comment. As soon as the matter under centrifugation is compressible, the density becomes much larger at the outer edge, $r=1$, than at the rotation axis, $r=0$. Let h be the height of the centrifuge. Assume, for the sake for the argument, that one studies fluctuations about a reference density of the form, $\rho(r)=\rho_c\,e^{Kr^2}$, where the parameter K contains all informations about the angular velocity, compressibility, etc. of the process. The factor, $\rho_c=M\,\left[h\int_0^1 dr\,r\,\rho(r)\right]^{-1}=M\,h^{-1}\,2\,K\,\left[e^K-1\right]^{-1}$, ensures the conservation of the mass M included in the vessel. If a cause for fluctuations of ρ is an instability of K, the first order for density change is,

$$\frac{\partial\rho}{\partial K}(r)=2\,\frac{K\,r^2\,\left[e^K-1\right]+e^K-Ke^K-1}{\left[e^K-1\right]^2}\,e^{Kr^2}\,,\qquad\int_0^1 dr\,r\,\frac{\partial\rho}{\partial K}(r)=0, \tag{13}$$

namely a polynomial of order 2 multiplied by e^{Kr^2}. Higher derivatives with respect to K will generate similar, even order polynomials, with the same property, $\int_0^1 dr\,r\,\partial^n\rho/\partial K^n(r)=0$. An orthogonalization, under a metric $\propto e^{2Kr^2}$, might be useful. This new set of polynomials will depend on K, however, since r is already scaled to a radius 1 for the cylinder and thus K cannot be scaled away. Because of this K dependence we do not elaborate further on this issue. For a large list of *ad hoc* polynomials and integration weights, see [6].

V. PROJECTOR ON THE CONSTRAINED SUBSPACE

For the sake of the discussion and short notations, set first $d = 1$, $\mu(r) = e^{-\frac{1}{2}r}$, and temporarily include normalization to unity factors into both the Laguerre polynomials L_n and the constrained G_n^1. This summarizes as,

$$\int_0^\infty dr\ [\mu(r)]^2\, L_m(r)\, L_n(r) = \delta_{mn}, \qquad \int_0^\infty dr\ [\mu(r)]^2\, G_m^1(r)\, G_n^1(r) = \delta_{mn}, \qquad \int_0^\infty dr\ \mu(r)\, G_n^1(r) = 0, \tag{14}$$

Then the kets and bras defined by $\langle r|w_n\rangle = \langle w_n|r\rangle = w_n(r) = \mu(r)\, G_n^1(r)$ and $\langle r|z_n\rangle = \langle z_n|r\rangle = z_n(r) = \mu(r)\, L_n(r)$ provide two "truncation" projectors, $\mathcal{P}_N = \sum_{n=1}^N |w_n\rangle\langle w_n|$ and $\mathcal{Q}_N = \sum_{n=0}^N |z_n\rangle\langle z_n|$, available for subspaces where polynomial orders do not exceed N. Their respective ranks N and $N+1$, and the embedding and commutation relation, $[\mathcal{P}_N, \mathcal{Q}_N] = \mathcal{P}_N$, are obvious. Obvious also is the limit, $\lim_{N\to\infty} \mathcal{Q}_N = 1$. The role of the rank one $|\sigma_N\rangle\langle\sigma_N|$ difference $\mathcal{P}_N - \mathcal{Q}_N$ is to subtract from any test state, $|\tau\rangle = \sum_{n=0}^N \tau_n |z_n\rangle$, that part which violates the condition of vanishing average. We shall show that the elementary ansatz,

$$|\sigma_N\rangle = \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-\frac{1}{2}} \sum_{n=0}^N \langle z_n\rangle\ |z_n\rangle, \qquad \langle z_n\rangle = \int_0^\infty dr\, \langle r|z_n\rangle, \tag{15}$$

defines the proper "subtractor" operator $|\sigma_N\rangle\langle\sigma_N|$. Indeed, from

$$(\,\mathcal{Q}_N - |\sigma_N\rangle\langle\sigma_N|\,)\ |\tau\rangle = \sum_{n=0}^N \tau_n\, |z_n\rangle - \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-1} \left(\sum_{n=0}^N \langle z_n\rangle\, |z_n\rangle\right) \left(\sum_{p=0}^N \langle z_p\rangle\, \tau_p\right), \tag{16}$$

one obtains

$$\int_0^\infty dr\, \langle r|\, (\mathcal{Q}_N - |\sigma_N\rangle\langle\sigma_N|)\ |\tau\rangle = \sum_{n=0}^N \tau_n\, \langle z_n\rangle - \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-1} \left(\sum_{n=0}^N \langle z_n\rangle\, \langle z_n\rangle\right) \left(\sum_{p=0}^N \langle z_p\rangle\, \tau_p\right) = 0. \tag{17}$$

Hence $\mathcal{Q}_N - |\sigma_N\rangle\langle\sigma_N|$ is the projector $\mathcal{P}_N$. Incidentally, the Laguerre result for σ_N is very simple, because $\langle z_m\rangle = 2,\ \forall m$. But the ansatz for σ_N, Eq.(15), generalizes to all cases. For instance, with Hermite polynomials, odd orders already satisfy the constraint when integrated from $-\infty$ to ∞, naturally, and thus do not contribute to σ_N. Even orders contribute, and it is easy to verify, upon integrating from $-\infty$ to ∞ again, that $\langle z_{2p}\rangle^2 = \pi^{\frac{1}{2}}\, 2^{1-p}\, (2p-1)!!/p!$.

It may be pointed out that the condition, $\int dr\, \mu(r)\, f(r) = 0$, for functions f orthogonalized, like our polynomials, by a metric $[\mu(r)]^2$, might be interpreted as an orthogonality condition, $\int dr\, f(r)\, [\mu(r)]^2\, g(r) = 0$, with $g(r) = [\mu(r)]^{-1}$. This makes g a candidate for the subtractor form factor σ. This is of some interest for the centrifuge case, where a state function such as, for instance, e^{-Kr^2}, remains finite when $0 \le r \le 1$. But there is little need to stress that, when the support of μ extends to ∞, then μ^{-1} does not belong to the Hilbert space and cannot be used for σ.

More interesting is the limiting process, $N \to \infty$, as illustrated by Figures 2-5. Figs. 2 and 3 show the shapes, in terms of r, of $\langle 2|\mathcal{P}_N|r\rangle$ and $\langle 10|\mathcal{P}_N|r\rangle$, respectively, when the projectors are made of the modified Laguerre polynomials G_n^1. The build up of an approximate δ-function when N increases from $N = 50$ (short dashes) to $N = 100$ (long ones) and $N = 150$ (full lines) is transparent, although the convergence is faster when peaks are closer to the origin, compare Figs. 2 and 3. The slower convergence in Fig. 3 is due to the cut-off imposed by exponential weights as long as N is finite. Given N, there is a "box effect", the range of the box being of order $\sim N$. A similar build up is observed for our other families of constrained polynomials, with slightly different details of minor importance such as, for instance, a box range $\sim \sqrt{N}$ for the Hermite case.

The box effect is even more transparent in Figs. 4 and 5, which show the shapes of subtractors $\langle 10|\sigma_N\rangle\langle\sigma_N|r\rangle$ and $\langle 0|\sigma_N\rangle\langle\sigma_N|r\rangle$ deduced from constrained polynomials of the Laguerre (Fig. 4) and Hermite (Fig. 5) type, respectively. (For graphical convenience, the polynomials Γ_n^1 and H_n used for the Hermite case, Fig. 5, are tuned to a weight e^{-r^2} rather than $e^{-\frac{1}{2}r^2}$, but this detail is not critical.)

It seems safe to predict that, given an effective length $\Lambda(N)$ for the box, the wiggles of the subtractor will smooth out when $N \to \infty$ and that only a background $\sim -1/\Lambda(N)$ will then remain.

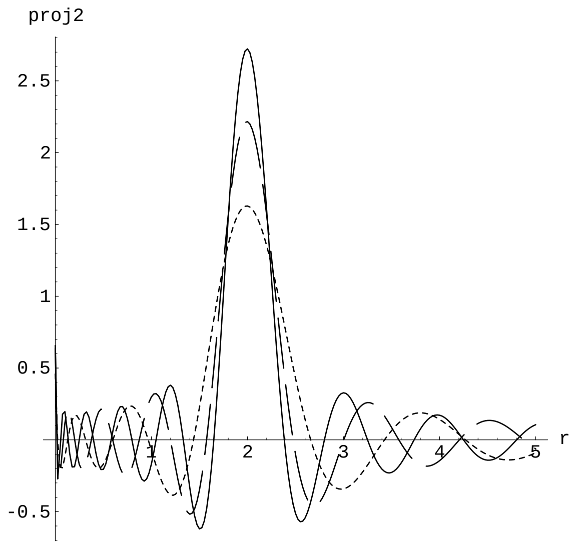

FIG. 3. Shapes of projectors made of polynomials G_n^1. Full line, $\langle 2|\mathcal{P}_{150}|r\rangle$, long dashes, $\langle 2|\mathcal{P}_{100}|r\rangle$, short dashes $\langle 2|\mathcal{P}_{50}|r\rangle$.

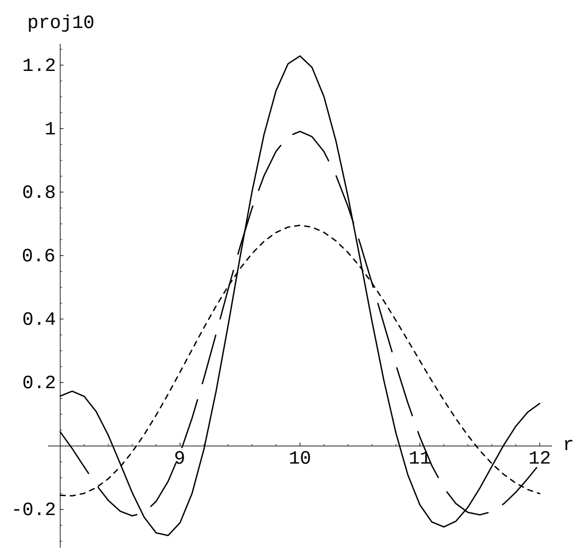

FIG. 4. Shapes of projectors made of polynomials G_n^1. Full line, $\langle 10|\mathcal{P}_{150}|r\rangle$, long dashes, $\langle 10|\mathcal{P}_{100}|r\rangle$, short dashes $\langle 10|\mathcal{P}_{50}|r\rangle$.

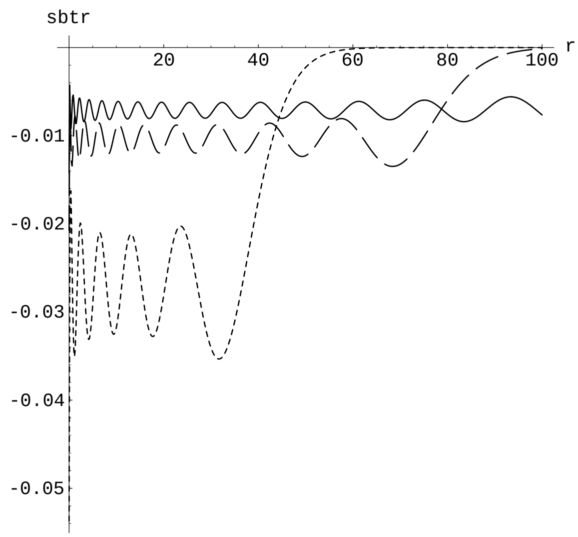

FIG. 5. Subtractors made of G^1_n. Shapes centered at $r = 10$. Short dashes, $N = 10$, long dashes, $N = 20$, full line, $N = 30$.

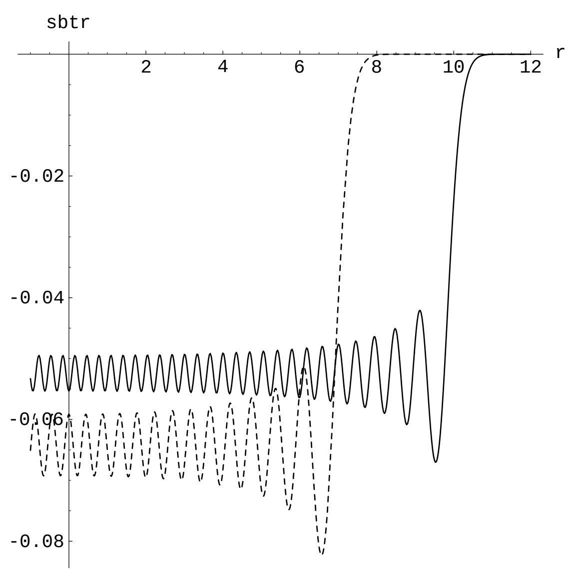

FIG. 6. Subtractors made of Γ_n. Shapes centered at $r = 0$. Stronger wiggles, shorter cut-off, dashed line, $N = 50$. Weaker wiggles, larger cut-off, full line, $N = 100$.

VI. ILLUSTRATIVE EXAMPLE: TRAJECTORIES IN DENSITY SPACE

We return here to the toy model discussed in [1] and the corresponding, modified Hermite polynomials. The model consists of Z non interacting, spinless fermions, driven by a one dimensional harmonic oscillator $H_0 = \frac{1}{2}(-d^2/dr^2 + r^2)$. The ground state density from the Z lowest orbitals reads, $\rho(r) = \sum_{i=1}^{Z} [\psi_i(r)]^2$. Let $i = 1, .., Z$ and $I = Z + 1, ... \infty$ label "hole" and "particle" orbitals, respectively. Add a perturbation $\delta u(r)$ to the initial potential $r^2/2$. The first order variation of the density is,

$$\delta\rho(r) = 2 \sum_{iI} \psi_i(r)\psi_I(r) \frac{\langle I|\delta u|i\rangle}{i - I} . \tag{18}$$

If we expand δu and $\delta\rho$ in that basis $\{w_n\}$ provided by the new polynomials, the formula, Eq. (18), becomes,

$$\delta\rho_m = 2 \sum_{iI\,n} \mathcal{D}_{m\,iI} \frac{1}{i - I} \mathcal{D}_{n\,iI}\, \delta u_n, \qquad \mathcal{D}_{n\,iI} \equiv \int dr\, w_n(r)\, \psi_i(r)\psi_I(r), \tag{19}$$

where $\mathcal{D}$ denotes both a particle-hole matrix element of a potential perturbation and the projection of a particle-hole product of orbitals upon the basis $\{w_n\}$. In [1] we briefly studied the eigenvalues and eigenvectors of this symmetric matrix, $\mathcal{F} = \mathcal{D}\,(E_0 - H_0)^{-1}\,\tilde{\mathcal{D}}$, where $(E_0 - H_0)^{-1}$ is a short notation to account for the denominators and the particle-hole summation, and the tilde indicates transposition. It is clear that the invertible $\mathcal{F}$ represents the functional derivative $\delta\rho_m/\delta u_n$ and is suited for *infinitesimal* perturbations. We shall now take advantage of the representation provided by $\{w_n\}$ to study *finite* trajectories $\rho(u)$.

For this, we consider a variable Hamiltonian, $\mathcal{H}_m(\lambda) = H_0 + \lambda\, w_m(r)$, made of the initial harmonic oscillator, but with a finite perturbation Δu along one "mode" w_m. It is trivial to diagonalize $\mathcal{H}_m(\lambda)$ with an excellent numerical accuracy and thus obtain, given Z, the ground state density $\rho(r, \lambda)$. Then it is trivial to expand the finite variation, $\Delta\rho = \rho(r, \lambda) - \rho(r, 0)$, in the basis $\{w_n\}$. This defines coordinates $\Delta\rho_n(\lambda; m)$ for trajectories, parametrized by the intensity of the chosen mode m for Δu.

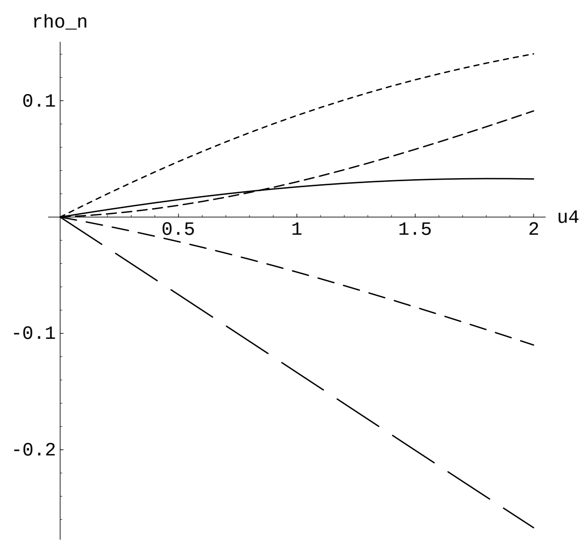

FIG. 7. Coordinates of the perturbation density $\Delta\rho$ created by a perturbing potential $\Delta u = \lambda_4\, w_4$. Full line: $2\,\Delta\rho_2$. Long dashes: $\Delta\rho_4$. Moderate dashes: $2\,\Delta\rho_6$. Short dashes: $4\,\Delta\rho_8$. Very short dashes: $8\,\Delta\rho_{10}$.

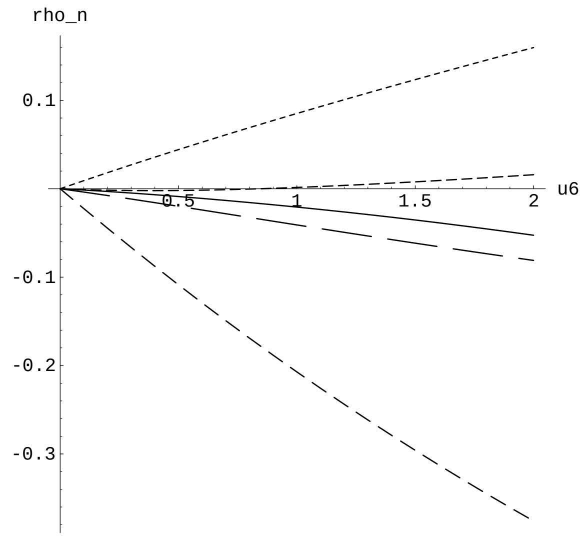

FIG. 8. Same as Fig. 7, but now $\Delta u = \lambda_6\, w_6$. Full line: $4\,\Delta\rho_2$. Long dashes: $2\,\Delta\rho_4$. Moderate ones: $\Delta\rho_6$. Short ones: $2\,\Delta\rho_8$. Very short dashes: $4\,\Delta\rho_{10}$.

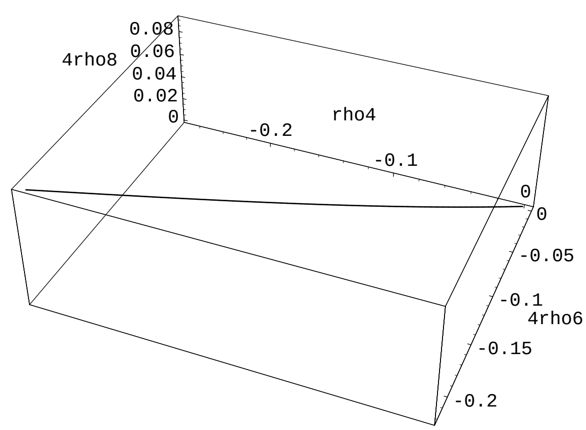

FIG. 9. 3D trajectory in density space. $\Delta\rho_4$, $\Delta\rho_6$ and $\Delta\rho_8$ taken from Fig. 7, the latter two coordinates blown 4 times.

In Figures 7 and 8 we show, with $Z = 4$, results from $\mathcal{H}_4 = H_0 + \lambda_4\, 2\,(2\pi)^{-\frac{1}{4}}\, 15^{-\frac{1}{2}}\,(8r^4 - 14r^2 + 1)\, e^{-r^2}$ and $\mathcal{H}_6 = H_0 + \lambda_6\,(2\pi)^{-\frac{1}{4}}\, 105^{-\frac{1}{2}}\,(32r^6 - 128r^4 + 94r^2 - 11)\, e^{-r^2}$, respectively. The case, $\mathcal{H}_2 = H_0 + \lambda_2\, 2\,(2/\pi)^{\frac{1}{4}}\, 3^{-\frac{1}{2}}\,(2r^2 - 1)\, e^{-r^2}$, makes almost a harmonic oscillator and is probably of academic interest only; anyhow we verified that its confirms the results with $\mathcal{H}_4$ and $\mathcal{H}_6$. We use a basis $\{w_n\}$ containing a factor e^{-r^2} rather than $e^{-\frac{1}{2}r^2}$ to better match the same factor e^{-r^2} created by products of harmonic oscillator orbitals in the calculation of matrix elements $\langle z_p|\Delta u|z_q\rangle$, but this technicality is not important for the physics.

The main result to be observed seems to be the lack of "collectivity" for such modes and for such elementary Hamiltonians. Indeed, for $\lambda_4 = 2$, the first five coordinates of $\Delta\rho$ read $\{0.016, -0.267, -0.055, 0.023, 0.018\}$, with a strong dominance of $\Delta\rho_4$, while for $\lambda_6 = 2$, these read $\{-0.013, -0.041, -0.376, 0.008, 0.040\}$, with a strong dominance of $\Delta\rho_6$. To clarify Figs. 7 and 8, we had indeed to blow up each $\Delta\rho_n$ by a factor $2^{|n-m|}$, where m is the index of the driver mode in potential space. Other modes than $m = 4$ and $m = 6$ show the same property: in the density space, a trajectory driven by $\Delta u = \lambda w_m$ stays close to the same w_m axis in that density space, although curvatures effects, while somewhat modest, are not absent. Such non linearity, slight curvatures are seen in Figs. 7-8, and also in Figure 9, where the three $\Delta\rho_4, \Delta\rho_6, \Delta\rho_8$ sets of data shown by Fig. 7 are converted into a parametric plot for a trajectory. For graphical purposes again, $\Delta\rho_6$ and $\Delta\rho_8$ are blown up 4 times to create Fig. 9. It can be concluded, temporarily, that the "flexibility" matrix $\mathcal{F}$ is not too far from being diagonal in the $\{w_n\}$ basis, or in other words, that the w_n modes indicate an approximately natural hierarchy in both the potential and the density spaces.

A subsidiary question pops up: that of the positivity of ρ. Indeed, while the space of potentials is basically a linear space, with arbitrary signs for $u(r)$ when the position r changes, densities $\rho(r)$ must remain positive for every r. This creates severe constraints for any linear parametrization of $\Delta\rho$ in terms of the basis $\{w_n\}$. In our toy model, it turns out that $\rho(r, 0) = \pi^{-\frac{1}{2}}(8r^6 - 12r^4 + 18r + 9)\, e^{-r^2}/6$. Hence, if we truncate $\Delta\rho$ to have two components only, w_2 and w_4 for instance, then ρ is the product of e^{-r^2} and a polynomial $\mathcal{P}(r)$,

$$6\,\pi^{\frac{1}{2}}\,\mathcal{P}(r) = 8r^6 - 12r^4 + 18r^2 + 9 + \Delta\rho_2\, 12\,(2\pi)^{\frac{1}{4}}\, 3^{-\frac{1}{2}}\,(2r^2 - 1) + \Delta\rho_4\, 12\,(\pi/2)^{\frac{1}{4}}\, 15^{-\frac{1}{2}}\,(8r^4 - 14r^2 + 1). \tag{20}$$

Rescale out inessential factors, for a simpler polynomial, $\bar{\mathcal{P}} = 8r^6 - 12r^4 + 18r^2 + 9 + \Delta R_2(2r^2 - 1) + \Delta R_4(8r^4 - 14r^2 + 1)$. Eliminate r between $\bar{\mathcal{P}}$ and $d\bar{\mathcal{P}}/dr$. The resultant $\mathcal{R}(\Delta R_2, \Delta R_4)$, when it vanishes, gives the border of the convex domain of parameters $\Delta R_2, \Delta R_4$ where $\bar{\mathcal{P}}$ remains positive definite. This domain contains the origin, because of $\rho(r, 0)$. The precise form of $\mathcal{R}$ is a little cumbersome and does not need to be published here. But the resulting border is shown in Figure 10. Generalizations to more $\Delta\rho$ parameters are obvious, with more cumbersome resultants $\mathcal{R}$.

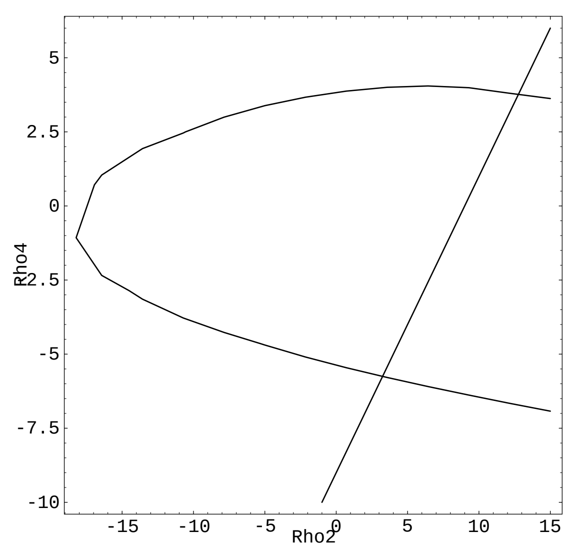

FIG. 10. Domain of values of ΔR_2 and ΔR_4 acceptable for the positivity of the density of the toy model. The domain sits inside the full line curve and left of the straight line. It contains the origin.

VII. DISCUSSION AND CONCLUSION

The subject of orthogonal polynomials has been so treated and overtreated that any claim to novelty must contain much more than a change of the integration measure. We took therefore a different approach, motivated by a law of physics and/or chemistry, matter conservation. This means a constraint of a vanishing average for the states described by weighted polynomials.

For a support $[0,\infty[$ and a simple exponential weight such as $e^{-\frac{1}{2}r}$, a non trivial generalization of Laguerre polynomials occurs. This extends the generalization of Hermite polynomials described in [1] with the support $]-\infty,\infty[$ and Gaussian weights such as $e^{-\frac{1}{2}r^2}$.

We also took care of cylindrical and spherical geometries, by replacing $\int dr$ with $\int dr\, r$ and $\int dr\, r^2$, respectively. The new sets of constrained polynomials are clearly sensitive to the geometry.

For finite supports such as $[0,1]$ and constant weights, the constraint is already satisfied by the usual brand of orthogonal polynomials as soon as their order is ≥ 1. In that sense, we did not find significantly original generalizations of Legendre polynomials, although we generated polynomials fitted to the cylindrical and spherical geometries. The cause of the failure is transparent: when the weight $\mu(r)$ is a constant, there is no difference between the orthogonality metric μ^2 and the constraint weight μ.

For each set of new polynomials we found a recursion relation and a differential equation. There seems to be a systematic property for those cases where the constraint generates truly original polynomials, namely when $\mu^2 \neq \mu$. In such cases, recursion and differentiation seem to be necessarily entangled. This does not happen for traditional orthogonal polynomials, indeed, and this "entanglement" may deserve some future attention.

Constrained polynomials expressing matter conservation in centrifuges do make an original set if the fluid under centrifugation is compressible; a non constant reference weight μ is indeed in order there. But the set depends on the precise form of μ via potentially many physical parameters. We found it difficult to design, through scaling, a sufficiently "universal" set. "Centrifuge polynomials" will have to be calculated specifically for each practical situation.

For those new polynomials generalizing the Hermite and Laguerre ones, we found a description of the subspace accounting for their defect of completeness. A codimension 1 is the consequence of the constraint, expressed at first by the obvious lack of a polynomial of order $n = 0$.

Finally the use of such polynomials was illustrated by a toy model for the Hohenberg-Kohn functional. A slightly surprising result was found: our polynomials, those of low order at least, define potential perturbations which are reflected by density perturbations having almost the same shapes. This occurs despite the delocalization created by the kinetic energy operator, hints at short ranges in effective interactions and validates the localization spirit of the Thomas-Fermi method. Whether such hints are good when the full zoology of the density functional is investigated is, obviously, an open question; for a review of the richness of the functional, we refer to [7]. If long range forces are active, a significant amount of delocalization between the "potential cause" and the "density effect" is not excluded. It would be interesting indeed to discover collective degrees of freedom in this connection between potential and density. In any case, our main conclusion may be that the new polynomials provide, for the context of matter conservation, a discrete and full set of modes and coordinates, hence a systematic and constructive representation of phenomena.

It is a pleasure to thank Y. Abe, J.-P. Boujot, B. Eynard, C. Normand, R. Peschanski and A. Weiguny for stimulating discussions.

---

[1] B.G. Giraud, M.L. Mehta and A. Weiguny, *C. R. Physique* **5** (2004) 781
[2] P. Hohenberg and W. Kohn, Phys. Rev. **136** 3B (1964) B864
[3] N. D. Mermin, Phys. Rev. **137** 5A (1965) A1441
[4] R. Berg and L. Wilets, Proc. Phys. Soc. A, LXVIII, (1955) 229; W. Kohn and L. J. Sham, Phys. Rev. **140** 4A (1965) A1133
[5] A. Messiah, Mécanique Quantique, Dunod ed. Paris (1962) p. 362
[6] J.-P. Boujot, Thèse de 3e cycle, Calcul de moments appliqués à l'évaluation numérique d'intégrales, Faculté des sciences de l'universié de Paris (1964)
[7] J.P. Perdew and S. Kurth, in *A Primer in Density Functional Theory*, C. Fiolhais, F. Nogueira and M. Marques, eds., Lecture Notes in Physics, **620**, Springer, Berlin (2003)