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Constrained orthogonal polynomials

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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. We give explicit properties of such polynomials, generalizing Laguerre ones. The nature of the dimension 1 subspace completing such sets is described. A numerical example illustrates the use of such polynomials.

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1. 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, $\forall\, m$, $\int \mathrm{d}r\; w_m(r) = 0$. 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, $\int \mathrm{d}r\; w_n(r) = 0$, 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, $\mathrm{e}^{-\frac{1}{2}r^2}$.

The same functional approaches [2–4] are also of 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 this paper, we want to include two- and three-dimensional situations. We shall thus use weights of the form $e^{-\frac{1}{2}r}$, with $0 \leqslant r < \infty$, but integrals will carry a factor r^ν, with ν being a positive exponent, suitable for dimension d. This will lead to generalizations of Laguerre polynomials.

For any positive weight $\mu(r)$, and any dimension d, a constraint of vanishing average, $\int \mathrm{d}r\, r^\nu \mu(r)\Gamma_n(r) = 0$, 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 2. Section 3 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 4. A discussion and conclusion make section 5.

2. 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, $\int_0^\infty \mathrm{d}r\, r^{d-1}\, e^{-\frac{1}{2}r} G_0^d(r) = 0$, must be implemented. Hence, set integer labels $m \geqslant 1$ and $n \geqslant 1$ and define polynomials G_n^d by the conditions,

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

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 fulfils the constraint, then (ii) orthogonalize such seeds by a Gram–Schmidt algorithm. The first polynomials read

$$\begin{aligned} &G_1^1 = r - 2, \qquad G_2^1 = r^2 - 5r + 2, \qquad G_3^1 = r^3 - 10r^2 + 20r - 8, \\ &G_4^1 = r^4 - 17r^3 + 78r^2 - 108r + 24, \end{aligned} \tag{2a}$$

$$\begin{aligned} &G_1^2 = r - 4, \qquad G_2^2 = r^2 - 8r + 8, \qquad G_3^2 = r^3 - 14r^2 + 44r - 32, \\ &G_4^2 = r^4 - 22r^3 + 138r^2 - 288r + 144, \end{aligned} \tag{2b}$$

$$\begin{aligned} &G_1^3 = r - 6, \qquad G_2^3 = r^2 - 11r + 18, \qquad G_3^3 = r^3 - 18r^2 + 78r - 84, \\ &G_4^3 = r^4 - 27r^3 + 216r^2 - 606r + 468. \end{aligned} \tag{2c}$$

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 figure 1 also shows G_2^1, G_2^2 and L_2.

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, equations (2a)–(2c), by means of the following recursion formula

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

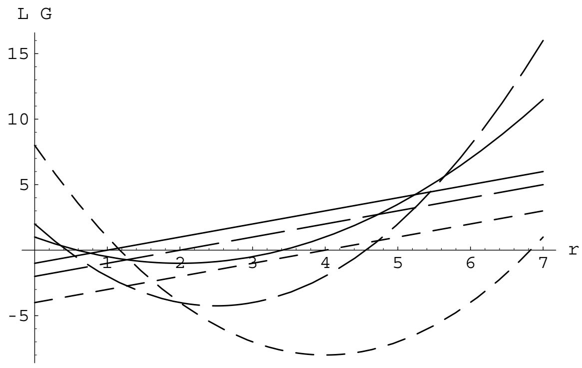

Figure 1. Comparison of Laguerre polynomials L_1, L_2 (full lines) with new polynomials G_1^1, G_2^1 (long dashes), G_1^2, G_2^2 (dashes).

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 rG_{n-1}^d. By partial integration, we see that

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

where again a prime means derivation with respect to r. Thus $\sigma_n^d \equiv \left(rG_{n-1}^d - 2rG_{n-1}^{d\prime} - 2dG_{n-1}^d\right)$ makes indeed a less trivial seed, compatible with the constraint. Note that the order n of this seed polynomial σ_n^d comes from the term rG_{n-1}^d only, the other two terms having order $n-1$. Note again that, in the table, equations (2), all polynomials G_n^d are monic. We can define G_n^d as monic, systematically. Since the product rG_{n-1}^d respects this 'monicity' and σ_n^d fulfils 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 $1 \leqslant m < n$, 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 $r^{d-1}\,\mathrm{e}^{-r}$, gives, by partial integration of the $G_{n-1}^{d\prime}$ term,

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

In the bracket [ ] in the last right-hand side of equation (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, equation (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 equation (3). Elementary manipulations also give

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

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

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

3. Projectors on the constrained subspace and on the codimensional subspace

The lack of a constant polynomial in our new set is not a sufficient description of the codimension imposed by the constraint. What is the projector on the 'cosubspace'? For the sake of the discussion and short notations, set first $d = 1$, $\mu(r) = \mathrm{e}^{-\frac{1}{2}r}$, and temporarily include factors of normalization to 1 into both Laguerre L_n and constrained G_n^1,

$$\begin{aligned} &\int_0^\infty \mathrm{d}r[\mu(r)]^2 L_m(r) L_n(r) = \delta_{mn}, \\ &\int_0^\infty \mathrm{d}r[\mu(r)]^2 G_m^1(r) G_n^1(r) = \delta_{mn}, \\ &\int_0^\infty \mathrm{d}r\, \mu(r) G_n^1(r) = 0. \end{aligned} \qquad (8)$$

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 $\mathcal{Q}_N - \mathcal{P}_N$ 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,

$$|\sigma_N\rangle = \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-\frac{1}{2}} \sum_{n=0}^N \langle z_n\rangle |z_n\rangle, \qquad \langle z_n\rangle = \int_0^\infty \mathrm{d}r \langle r|z_n\rangle, \qquad (9)$$

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

$$(\mathcal{Q}_N - |\sigma_N\rangle\langle\sigma_N|)\,|\tau\rangle = \sum_{n=0}^N \tau_n |z_n\rangle - \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-1} \left(\sum_{n=0}^N \langle z_n\rangle |z_n\rangle\right) \left(\sum_{p=0}^N \langle z_p\rangle \tau_p\right), \qquad (10)$$

one obtains

$$\begin{aligned} &\int_0^\infty \mathrm{d}r \langle r|\,(\mathcal{Q}_N - |\sigma_N\rangle\langle\sigma_N|)\,|\tau\rangle \\ &\quad = \sum_{n=0}^N \tau_n \langle z_n\rangle - \left(\sum_{m=0}^N \langle z_m\rangle^2\right)^{-1} \left(\sum_{n=0}^N \langle z_n\rangle\langle z_n\rangle\right) \left(\sum_{p=0}^N \langle z_p\rangle \tau_p\right) = 0. \end{aligned} \qquad (11)$$

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, equation (9), 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 $\langle z_{2p}\rangle^2 = \pi^{\frac{1}{2}} 2^{1-p}(2p-1)!!/p!$.

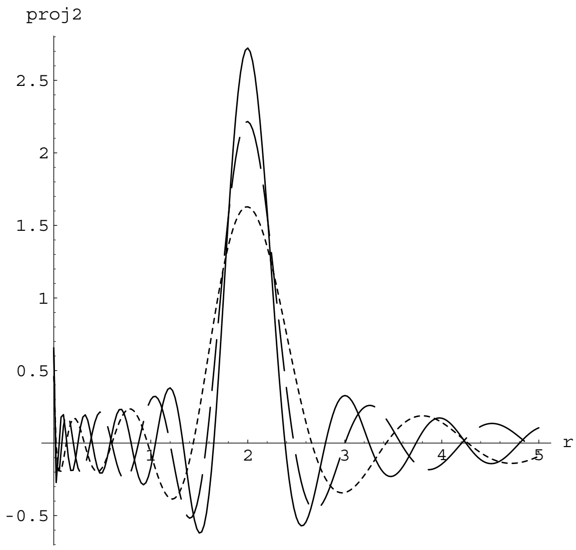

Figure 2. Shapes of projectors made of polynomials G_n^1. Full line, $\langle 2|\mathcal{P}_{150}|r\rangle$, long dashes, $\langle 2|\mathcal{P}_{100}|r\rangle$, short dashes $\langle 2|\mathcal{P}_{50}|r\rangle$.

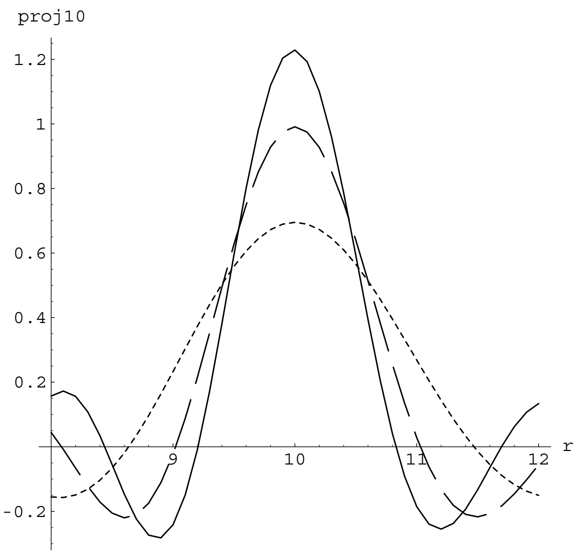

Figure 3. Shapes of projectors made of polynomials G_n^1. Full line, $\langle 10|\mathcal{P}_{150}|r\rangle$, long dashes, $\langle 10|\mathcal{P}_{100}|r\rangle$, short dashes $\langle 10|\mathcal{P}_{50}|r\rangle$.

It may be pointed out that the condition, $\int \mathrm{d}r\,\mu(r)f(r) = 0$, for functions f orthogonalized, like our polynomials, by a metric $[\mu(r)]^2$, might be interpreted as an orthogonality condition, $\int \mathrm{d}r\, f(r)[\mu(r)]^2 g(r) = 0$, with $g(r) = [\mu(r)]^{-1}$. This makes g a candidate for the subtractor form factor σ. 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. Figures 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,

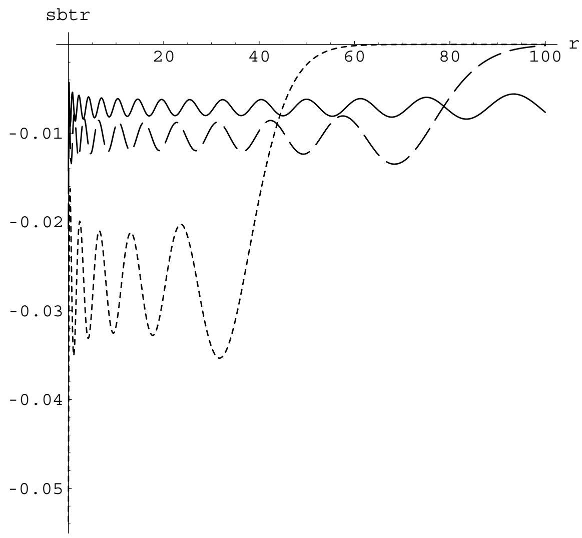

Figure 4. Subtractors made of G_n^1. Shapes centred at $r = 10$. Short dashes, $N = 10$, long dashes, $N = 20$, full line, $N = 30$.

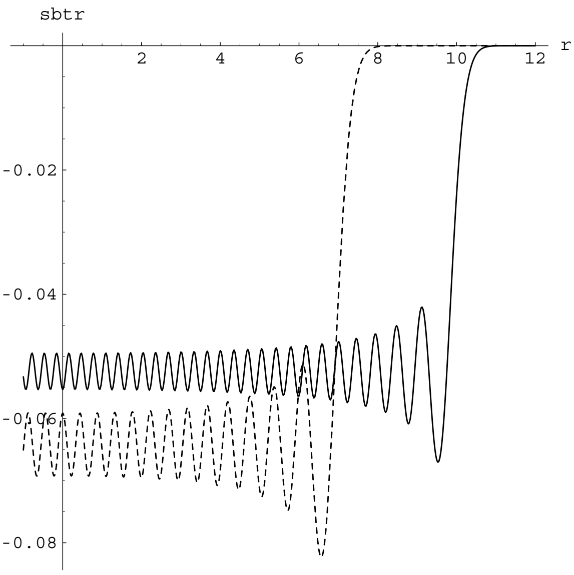

Figure 5. Subtractors made of Γ_n. Shapes centred at $r = 0$. Stronger wiggles, shorter cut-off, dashed line, $N = 50$. Weaker wiggles, larger cut-off, full line, $N = 100$.

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 figures 2 and 3. The slower convergence in figure 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 figures 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 (figure 4) and Hermite (figure 5) type, respectively. (For graphical convenience, the polynomials Γ_n^1 and H_n used for the Hermite case, figure 5, are tuned to a weight e^{-r^2} rather than $\mathrm{e}^{-\frac{1}{2}r^2}$, 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. An intuitive image of this may help, like that of the Dirac δ as an infinitely narrow and high 'peak' with integral 1: the limit of the subtractor makes an infinitely broad and flat 'pancake' with integral -1.

4. Illustrative examples: trajectories in density space

Return temporarily 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 $H_0=\frac{1}{2}(-d^2/\mathrm{d}r^2+r^2)$. The ground-state density reads $\rho(r)=\sum_{i=1}^{Z}[\psi_i(r)]^2$. Let $i=1,\ldots,Z$ and $I=Z+1,\ldots,\infty$ label 'hole' and 'particle' orbitals, respectively. Add a perturbation $\delta u(r)$ to $r^2/2$. The variation of ρ is

$$\delta\rho(r)=2\sum_{iI}\psi_i(r)\psi_I(r)\frac{\langle I|\delta u|i\rangle}{i-I}. \tag{12}$$

If we expand δu and $\delta\rho$ in that basis $\{w_n\}$ provided by the new polynomials, the formula, equation (12), becomes

$$\delta\rho_m=2\sum_{iIn}\mathcal{D}_{miI}\frac{1}{i-I}\mathcal{D}_{niI}\delta u_n,\qquad \mathcal{D}_{niI}\equiv\int\mathrm{d}r\,w_n(r)\psi_i(r)\psi_I(r), \tag{13}$$

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 suitable 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.

In figures 6 and 7 we show, with $Z=4$, results from $\mathcal{H}_4=H_0+\lambda_4 2(2\pi)^{-\frac{1}{4}}15^{-\frac{1}{2}}(8r^4-14r^2+1)\,\mathrm{e}^{-r^2}$ and $\mathcal{H}_6=H_0+\lambda_6(2\pi)^{-\frac{1}{4}}105^{-\frac{1}{2}}(32r^6-128r^4+94r^2-11)\,\mathrm{e}^{-r^2}$, respectively. The case, $\mathcal{H}_2=H_0+\lambda_2 2(2/\pi)^{\frac{1}{4}}3^{-\frac{1}{2}}(2r^2-1)\,\mathrm{e}^{-r^2}$, almost makes a harmonic oscillator for small values of λ_2 and is probably of academic interest only; anyhow we verified that it 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 $\mathrm{e}^{-\frac{1}{2}r^2}$ 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.

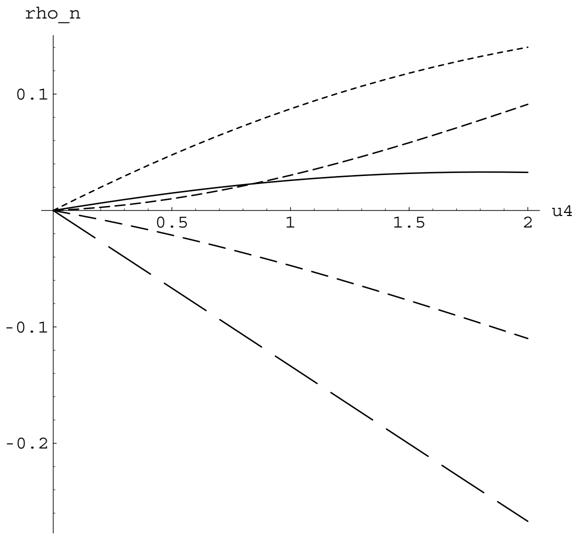

Figure 6. Harmonic oscillator toy model. Coordinates of the perturbation density $\Delta\rho$ created by a perturbing potential $\Delta u = \lambda_4 w_4$. Full line: $2\Delta\rho_2$. Long dashes: $\Delta\rho_4$. Medium dashes: $2\Delta\rho_6$. Short dashes: $4\Delta\rho_8$. Very short dashes: $8\Delta\rho_{10}$.

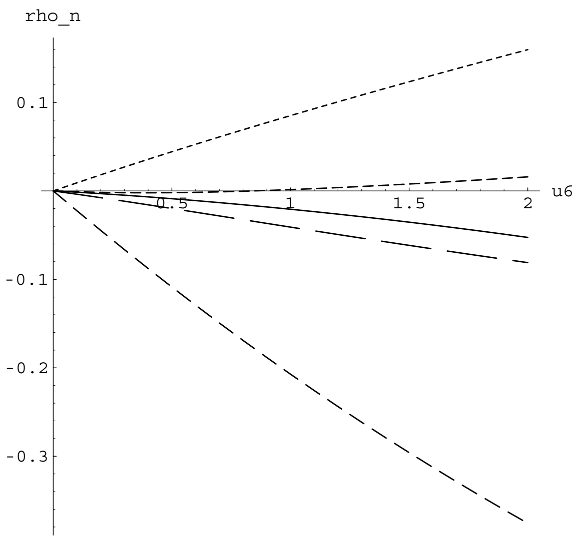

Figure 7. Same as figure 6, but now $\Delta u = \lambda_6 w_6$. Full line: $4\Delta\rho_2$. Long dashes: $2\Delta\rho_4$. Medium dashes: $\Delta\rho_6$. Short dashes: $2\Delta\rho_8$. Very short dashes: $4\Delta\rho_{10}$.

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 figures 6 and 7, we had indeed to magnify 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

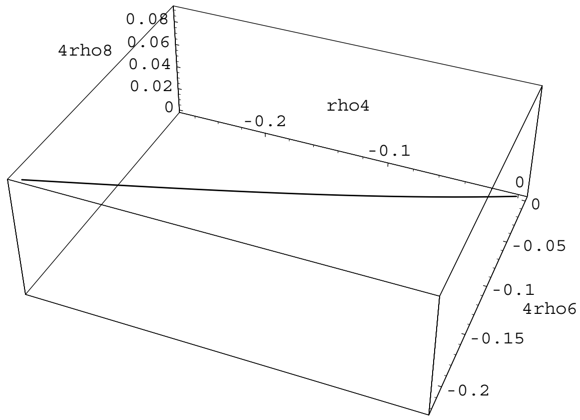

Figure 8. 3D trajectory in density space. $\Delta\rho_4$, $\Delta\rho_6$ and $\Delta\rho_8$ taken from figure 6; the latter two coordinates magnified four times.

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 figures 6 and 7, and also in figure 8, where the three $\Delta\rho_4$, $\Delta\rho_6$, $\Delta\rho_8$ sets of data shown by figure 6 are converted into a parametric plot for a trajectory. For graphical purposes again, $\Delta\rho_6$ and $\Delta\rho_8$ are magnified four times to create figure 8. 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 arises: 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 $\rho(r,0) = \pi^{-\frac{1}{2}}(8r^6 - 12r^4 + 18r + 9)\,\mathrm{e}^{-r^2}/6$. 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 $\mathcal{P}(r)$:

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

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 $\mathrm{d}\bar{\mathcal{P}}/\mathrm{d}r$. 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 9. Generalizations to more $\Delta\rho$ parameters are obvious, with more cumbersome resultants $\mathcal{R}$.

Another model, that uses Laguerre and our modified Laguerre polynomials, is in order. Consider a hydrogenoid, suitably scaled Hamiltonian, $H_0 = -\mathrm{d}^2/\mathrm{d}r^2 - 2/r$. We use here s-wave, radial forms only. All subsequent integrations will mean $\int_0^\infty r^2\,\mathrm{d}r$, naturally. With the usual spectrum $-1, -1/4, -1/9$, etc the lowest three orbitals of H_0 then read, $\psi_1 = 2\,\mathrm{e}^{-r}$, $\psi_2 = (1 - r/2)\,\mathrm{e}^{-r/2}/\sqrt{2}$, $\psi_3 = 2\sqrt{3}(1 - 2r/3 + 2r^2/27)\,\mathrm{e}^{-r/3}/9$. These will make a reference density ρ_0 in a $Z = 3$ hydrogenoid toy model with just s-waves. Then we perturb the Hamiltonian by means of a potential proportional to mode G_1^3. More precisely,

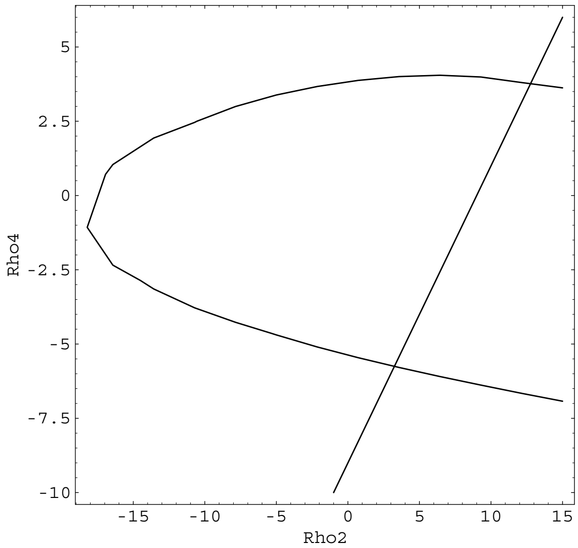

Figure 9. Domain of values of ΔR_2 and ΔR_4 acceptable for the positivity of the density of the harmonic oscillator toy model. The domain sits inside the full line curve and left of the straight line. It contains the origin.

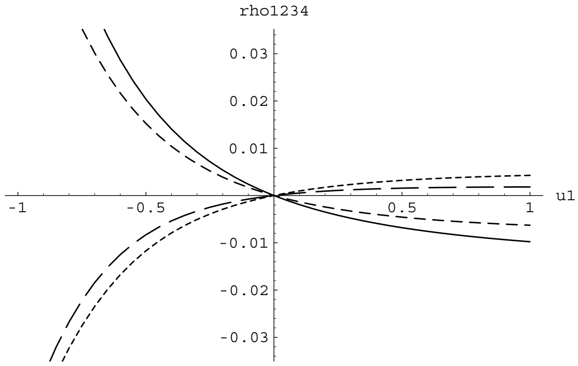

Figure 10. Second toy model, $Z = 3$ hydrogenoid s-density perturbed by mode G_1^3. Components of the density perturbation: $\Delta\rho_1$, full line; $\Delta\rho_2$, long dashes; $\Delta\rho_3$, medium dashes; $\Delta\rho_4$, small dashes.

set $H = H_0 + u_1(r-6)\,\mathrm{e}^{-r/2}/(2\sqrt{6})$. Obtain the density $\rho(r, u_1)$ from the lowest three s-wave eigenstates of H. 'Coordinates' in density space result from projecting the difference $\Delta\rho = \rho(r, u_1) - \rho_0$ upon the basis spanned by the G_n^3 polynomials, suitably weighted and normalized, namely $\Delta\rho_n(u_1) = \int_0^\infty r^2\,\mathrm{d}r\,\Delta\rho(r, u_1)\,\mathrm{e}^{-r/2} G_n^3(r)/\sqrt{(n-1)!(n+3)!}$. Results for the first four components, $\Delta\rho_1, \ldots, \Delta\rho_4$, are shown in figure 10. One sees that, in contrast to the previous toy model, that with Hermite-like polynomials, the component with the same order as the perturbing potential does not seem to dominate the response $\Delta\rho$. A few components, however, seem to suffice for the reconstruction of $\Delta\rho$. For instance, for that value $u_1 = -1$ which corresponds to the strongest response we calculated, the squares of eight components $\{\Delta\rho_1, \ldots, \Delta\rho_8\} = \{0.0945, -0.0534, 0.0736, -0.0576, 0.0576, -0.0336, 0.0176, -0.0107\}$, add up to 0.025 39, to be compared with

$0.025\,43 = \int_0^\infty r^2\,\mathrm{d}r[\Delta\rho(r,-1)]^2$. This seems to mean a satisfactory reconstruction with few degrees of freedom. For the sake of rigour, however, the conclusion must be suspended, pending an estimate of continuum components in the eigenorbitals, for the present results are based on expansions in discrete hydrogenoid orbitals only.

In any case, it can be stressed that the density, while being a highly non-linear physical 'effect' with respect to potential 'causes' and resulting orbitals and correlations, can conveniently be considered as a vector to be expanded in the bases spanned by our weighted, constrained polynomials.

5. 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 $\mathrm{e}^{-\frac{1}{2}r}$, 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 $\mathrm{e}^{-\frac{1}{2}r^2}$.

We also took care of cylindrical and spherical geometries, by replacing $\int \mathrm{d}r$ with $\int \mathrm{d}r\, r$ and $\int \mathrm{d}r\, r^2$, respectively. The new set of constrained polynomials is 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 $\geqslant 1$. The reason for such a trivial result 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 the new polynomials generalizing Laguerre ones, we found a recursion relation and a differential equation. Recursion and differentiation are entangled. The same oddity occurs in the 'constrained Hermite' [1] case. This does not happen for traditional orthogonal polynomials, and this 'entanglement' may deserve some future attention.

For both new polynomials generalizing the Hermite and Laguerre ones, we found a precise 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 toy models for the Hohenberg–Kohn connection between density and potential. A slightly surprising result was found: our polynomials, those of low order at least, sometimes may define potential perturbations reflected by density perturbations having almost the same shapes. This occurs despite the delocalization due to 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 [6]. 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.

Acknowledgments

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Appendix

The formula given by an anonymous referee to relate the polynomials G_n^d to usual Laguerre polynomials reads

$$G_n^d(r) = -\sum_{j=1}^{n} j2^j (d+1+j)_{n-j}(1-n)_{j-1} L_j^{d-1}\left(\frac{r}{2}\right), \tag{A.1}$$

where $(m)_i$ is the 'Pochhammer rising factorial', $(m)_i = m(m+1)\cdots(m+i-1)$. We copy here his derivation.

Since the usual Laguerre polynomials,

$$L_n^\alpha(r) = (\alpha+1)_n/n! \sum_{j=0}^{n} (-n)_j/(\alpha+1)_j r^j/j!, \tag{A.2}$$

are orthogonal when integrated with metric measure $\mathrm{d}r r^\alpha\,\mathrm{e}^{-r}$, it is trivial that the polynomials $L_n^\alpha\left(\frac{1}{2}r\right)$ are orthogonal when integrated with metric measure $\mathrm{d}r r^\alpha\,\mathrm{e}^{-\frac{1}{2}r}$. In particular, since $L_0^\alpha = 1, \forall\,\alpha$, then $\int_0^\infty \mathrm{d}r\, r^\alpha\,\mathrm{e}^{-\frac{1}{2}r} 1 \times L_n^\alpha\left(\frac{1}{2}r\right) = 0$, provided $n \geqslant 1$. Set therefore $\alpha = d-1$. The constraint of a vanishing average in dimension d is thus satisfied by an expansion of the polynomials $G_m^d(r)$ in the polynomials $L_n^{d-1}\left(\frac{1}{2}r\right), n \geqslant 1$.

There remains the need of a reorthogonalization of such polynomials $L_n^{d-1}\left(\frac{1}{2}r\right)$ with respect to $\mathrm{d}r r^{d-1}\,\mathrm{e}^{-r}$. Obtain first the scalar product of $L_m^\alpha\left(\frac{1}{2}r\right)$ and $L_n^\alpha\left(\frac{1}{2}r\right)$. It derives from the coefficient of $s^m t^n$ in the expansion of the following scalar product of generating functions

$$\begin{aligned}
&\int_0^\infty \mathrm{d}r\, r^\alpha\,\mathrm{e}^{-r}(1-s)^{-\alpha-1}\exp\left(-\frac{sr/2}{1-s}\right)(1-t)^{-\alpha-1}\exp\left(-\frac{tr/2}{1-t}\right)\\
&\qquad = (1-s)^{-\alpha-1}(1-t)^{-\alpha-1}\int_0^\infty \mathrm{d}r\, r^\alpha \exp\left[-r\frac{1-(s+t)/2}{(1-s)(1-t)}\right]\\
&\qquad = \Gamma(\alpha+1)\left(1-\frac{s+t}{2}\right)^{-\alpha-1} = \Gamma(\alpha+1)\sum_{j=0}^{\infty}\frac{(\alpha+1)_j(s+t)^j}{j!2^j},
\end{aligned} \tag{A.3}$$

and hence

$$\int_0^\infty \mathrm{d}r\, r^\alpha\,\mathrm{e}^{-r} L_m^\alpha\left(\frac{r}{2}\right) L_n^\alpha\left(\frac{r}{2}\right) = \Gamma(\alpha+1)\frac{(\alpha+1)_{m+n}}{2^{m+n}m!n!}. \tag{A.4}$$

Now consider that map which, $\forall\,n \geqslant 0$, replaces r^n by $[(\alpha+1)(\alpha+2)]^{-\frac{1}{2}}2^{n+1}(n+1)!L_{n+1}^\alpha\left(\frac{1}{2}r\right)$. The map will induce an *isometry*, by linear extension, from $L^2[(0,\infty); \Gamma(\alpha+3)^{-1}r^{\alpha+2}\,\mathrm{e}^{-r}]$ into $L^2[(0,\infty); \Gamma(\alpha+1)^{-1}r^\alpha\,\mathrm{e}^{-r}]$. Indeed, recall the scalar product, $\int_0^\infty \mathrm{d}r\, r^{\alpha+2}\,\mathrm{e}^{-r}r^m r^n = \Gamma(\alpha+3)(\alpha+3)_{m+n}$, and compare it with the right-hand side of equation (A.4). One can now use, to orthogonalize the set, $\left\{L_1^\alpha\left(\frac{1}{2}r\right), L_2^\alpha\left(\frac{1}{2}r\right), L_3^\alpha\left(\frac{1}{2}r\right), \ldots\right\}$, that same construction of an orthogonal basis in space $L^2\left[(0,\infty); \Gamma(\alpha+3)^{-1}r^{\alpha+2}\,\mathrm{e}^{-r}\right]$, which consisted in making the polynomials $L_n^{\alpha+2}(r), n = 0,1,2,\ldots,$ etc from the monomials $r^n, n = 0,1,2,\ldots,$ etc.

Thus, inside $(n-1)!L_{n-1}^{\alpha+2}(r)$, see equation (A.2) with $\alpha+2$ instead of α and $(n-1)$ instead of n, replace each monomial r^j, $j = 0, 1, \ldots, n-1$, by $2^{j+1}(j+1)!L_{j+1}^{\alpha}\left(\frac{1}{2}r\right)$. This produces a polynomial proportional to $G_n^d(r)$, with $n \geqslant 1$. A calculation with leading coefficients finishes the derivation. Since $\int_0^\infty \mathrm{d}r\, r^{\alpha+2}\,\mathrm{e}^{-r} L_m^{\alpha+2}(r)L_n^{\alpha+2}(r) = \delta_{mn}\Gamma(\alpha+3)(\alpha+3)_n/n!$, then $\int_0^\infty \mathrm{d}r\, r^{d-1}\,\mathrm{e}^{-r} G_m^d G_n^d(r) = \delta_{mn}\Gamma(d)(d)_{n+1}(n-1)!$.

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