Lagrange meshes from nonclassical orthogonal polynomials

D. Baye[1] and M. Vincke[2,1]
[1]*Physique Nucléaire Théorique et Physique Mathématique, Code Postal 229, Université Libre de Bruxelles, B 1050 Brussels, Belgium*
[2]*AIB-Vinçotte Nuclear, Avenue du Roi 157, B 1190 Brussels, Belgium*
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The Lagrange-mesh numerical method has the simplicity of a mesh calculation and the accuracy of a variational calculation. A flexible general procedure for deriving an infinity of new Lagrange meshes related to orthogonal or nonorthogonal bases is introduced by using nonclassical orthogonal polynomials. As an application, different Lagrange meshes based on shifted Gaussian functions are constructed. A simple quantum-mechanical example shows that the Lagrange-mesh method may become more accurate than the original variational calculation with a nonorthogonal basis. [S1063-651X(99)02706-3]

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The continuous expansion of computing power leads to attempts for solving with numerical techniques increasingly complicated problems. Consequently, efficient numerical approximations are needed more than ever. Ideally they should provide the highest accuracy with minimal computing efforts and maximal flexibility.

For well conditioned problems, i.e., when indefinitely differentiable solutions exist almost everywhere, global methods involving information from the whole domain of definition of the studied problem provide better accuracy than local methods. Among global approaches, two important and efficient approximations are the collocation and variational (or Galerkin) methods [1,2]. Nearly optimal techniques can be looked for by keeping the advantages of both approaches such as in the Lagrange-mesh method.

The Lagrange-mesh method is an approximate variational calculation, which resembles a mesh calculation in the spirit of collocation [3–6]. In the context of quantum mechanics, it is strikingly simple because the potential matrix is diagonal and only involves values of the potential at the different mesh points. These properties proceed from the existence of a Lagrange basis, i.e., an orthonormal family of infinitely differentiable functions, which vanish at all mesh points but one. When a variational calculation is performed with such a basis, the use of the associated Gauss quadrature leads to a diagonal potential matrix and to meshlike calculations. In spite of its extreme simplicity, this method is often very accurate with rather small numbers of mesh points. Its accuracy is comparable to the accuracy of the more complicated variational calculation performed with the associated Lagrange basis [5,6].

The Lagrange-mesh method provides accurate results for a number of bound-state and scattering calculations in atomic and nuclear physics [3–12]. It should also be useful in other areas of physics. However, until now, the development of the method was hindered by the fact that only a limited number of Lagrange meshes are available [13,14,3–6]. Most of them are based on zeros of classical orthogonal polynomials [3–6]. The condition of existence of a Lagrange mesh severely limited the number of possible underlying variational bases and offered poor flexibility. No alternative was available when the imposed repartition of mesh points did not match the physical properties of a problem.

The aim of the present paper is to overcome this limitation and to show that many more types of Lagrange meshes (infinitely many in principle) can be constructed with little computational effort. These meshes are still indirectly based on orthogonal polynomials, which belong to the broader nonclassical family, i.e., which do not satisfy a second-order differential equation. By selecting an appropriate weight function and by introducing a change of variable in the argument of the orthogonal polynomials, it becomes possible to reproduce wide classes of variational bases. As an example, we shall apply the general algorithm to deriving a mesh related to shifted Gaussian functions and illustrate it by an elementary application of quantum mechanics (see Ref. [6] for preliminary results). Equally spaced shifted Gaussian functions provide a flexible basis, which has proved useful in different areas of atomic and nuclear physics. During the completion of this paper, Karabulut and Sibert published a striking analytical study of a mesh based on shifted Gaussians [15]. Their mesh is different from the one we derive (see below) but the present algorithm also allows constructing the mesh of Ref. [15].

The Lagrange-mesh approach offers a close similarity (and sometimes provides identical results) with the discrete-variable representation (DVR) method [16,17]. The main difference lies in the philosophy of the methods. The Lagrange-mesh method is basically variational. Fulfilling the condition of existence of a Lagrange basis entails a high accuracy of the results (at the cost of an imposed mesh). In the DVR, the freedom of choice of the mesh is the most important aspect but a good accuracy is obtained when an implicit Lagrange basis exists. The direct use of this basis significantly simplifies the DVR. The Lagrange-mesh method may be considered as some accurate subset of the DVR. Let us also briefly mention two other approaches related to some extent with—but different from—the present paper. Schneider [18] uses a generalization of nonclassical orthogonal polynomials. Wei *et al.* [19] employ a basis inspired from Lagrange polynomials. Both methods fall out of the Lagrange-mesh technique either because the Lagrange conditions are not always satisfied in Ref. [18] or because the basis is not orthogonal in Ref. [19].

Consider the one-dimensional Schrödinger equation,

$$[T+V(x)]\psi(x)=E\psi(x), \tag{1}$$

where $T=-d^2/dx^2$ is the kinetic-energy operator, $V(x)$ is a local potential, and $\psi(x)$ is a bound-state wave function at energy E.

In a variational calculation, the wave function is approximated by a linear combination $\Sigma_i C_i f_i(x)$ with variational coefficients C_i of N orthonormal basis functions $f_i(x)$. The system of variational equations reads

$$\sum_{j=1}^{N}(T_{ij}+V_{ij})C_j=EC_i, \tag{2}$$

where $T_{ij}=\langle f_i|T|f_j\rangle$ and $V_{ij}=\langle f_i|V|f_j\rangle$. With a good basis choice, this method can give accurate results but the calculation of the potential matrix may be difficult and time consuming.

A Lagrange basis is defined as the association of N mesh points x_i and of N Lagrange functions $f_i(x)$, orthonormal on some interval (a,b). The infinitely differentiable functions $f_i(x)$ satisfy the Lagrange conditions,

$$f_i(x_j)=\lambda_i^{-1/2}\delta_{ij}, \tag{3}$$

i.e., $f_i(x)$ vanishes at all mesh points x_j except x_i. The mesh points x_i and constants λ_i provide a Gauss quadrature approximation associated with the mesh [3],

$$\int_a^b g(x)dx\approx\sum_{k=1}^{N}\lambda_k g(x_k). \tag{4}$$

Because of conditions (3), the potential matrix is diagonal at the Gauss approximation (4),

$$V_{ij}=\int_a^b f_i(x)V(x)f_j(x)dx\approx V(x_i)\delta_{ij}, \tag{5}$$

and the variational equations (2) take a form similar to mesh equations as in finite-difference methods. With scaled basis functions $h^{-1/2}f_i(x/h)$ defined over the interval (ah,bh), the Lagrange-mesh equations read

$$\sum_{j=1}^{N}[h^{-2}T_{ij}+V(hx_i)\delta_{ij}]C_j=EC_i. \tag{6}$$

The scale factor h can often be treated as an approximate variational parameter but the results are not very sensitive to its precise value when N is large enough.

The number of conditions (3) is much larger than the number of mesh points. Nevertheless, they are met in a number of cases: a Lagrange mesh can be associated with each family of classical orthogonal polynomial [3,4] and with the Fourier [3,5,13] and sinc [14] functions. Here we address a general question: Can one associate a Lagrange mesh with other families of basis functions, such as, for example, shifted Gaussian functions? We show below that many new types of Lagrange meshes can be defined starting from nonclassical orthogonal polynomials.

Let us consider a weight function $\rho(u)$ and the corresponding normalized polynomials $p_k(u)$ orthogonal over some interval (c,d). Nonclassical orthogonal polynomials possess two important properties, i.e., a simple three-term recurrence relation [see Eq. (15) below] and the Christoffel-Darboux relation [20]. Let us denote as $u_i(i=1,N)$ the zeros of $p_N(u)$,

$$p_N(u_i)=0. \tag{7}$$

With the N first polynomials, the Christoffel-Darboux relation leads to the property [3],

$$\sum_{k=0}^{N-1}p_k(u_i)p_k(u_j)=[\lambda_i\rho(u_i)]^{-1}\delta_{ij}. \tag{8}$$

Equation (8) provides a way of calculating the Christoffel numbers λ_i entering the Gauss formula (4). Now we introduce an infinitely differentiable bijective mapping $u=t(x)$ of (a,b) on (c,d) and the orthonormal family

$$\varphi_k(x)=[w(x)]^{1/2}p_k(t(x)) \tag{9}$$

with the included weight

$$w(x)=\rho(t(x))t'(x), \tag{10}$$

where t' is the derivative of t. Because of the freedom we have in the choices of $\rho(u)$ and of $t(x)$, it is possible to design functions φ_k with some definite properties.

When the functions φ_k are selected, Lagrange functions are defined as

$$f_i(x)=\left[\frac{w(x)}{\lambda_i w(x_i)}\right]^{1/2}\frac{p_N(t(x))}{(t(x)-u_i)p_N'(u_i)}, \tag{11}$$

which correspond to linear combinations of the φ_k. The Lagrange mesh points are given by

$$x_i=t^{-1}(u_i). \tag{12}$$

One easily verifies with Eqs. (12) and (7) that condition (3) is satisfied. The orthonormality of the f_i follows from the fact that the Gauss approximation over (c,d) is exact for $\rho(u)$ multiplied by polynomials in u up to degree $2N-1$ [20],

$$\int_a^b f_i(x)f_j(x)dx=\sum_{k=1}^{N}\lambda_k f_i(x_k)f_j(x_k)=\delta_{ij}. \tag{13}$$

Contrary to the case of classical polynomials, the T_{ij} cannot easily be obtained in compact form. We shall thus compute them numerically from

$$T_{ij}=\int_a^b f_i'(x)f_j'(x)dx. \tag{14}$$

Also unlike the classical case [3], the Gauss approximation (4) is, in general, neither exact nor even very accurate in Eq. (14).

The calculation of the zeros of p_N follows a standard strategy [21]. The orthonormal polynomials are linked by the recurrence relations,

$$\beta_k p_k(u)=(u-\alpha_k)p_{k-1}(u)-\beta_{k-1}p_{k-2}(u), \tag{15}$$

TABLE I. Errors ϵ_ν on energies of the Morse potential (22) from variational calculations with basis (19) and from the corresponding mesh calculations. The powers of 10 are indicated in brackets.

	N	a	h	ϵ_0	ϵ_5	ϵ_{10}	ϵ_{15}
Var.	10	0.3	0.12	9[−13]	6[−6]		
Mesh		0.3	0.12	−1[−12]	−1[−5]		
Var.	20	0.4	0.11	−1[−18]	2[−11]	5[−6]	
Mesh		0.3	0.12	−2[−15]	−4[−12]	−4[−7]	
Var.	30	0.5	0.10	1[−19]	−1[−15]	1[−10]	1[−5]
Mesh		0.3	0.12	5[−16]	2[−15]	2[−11]	4[−6]
Var.	40	0.5	0.10	−5[−20]	−2[−15]	2[−12]	1[−9]
Mesh		0.3	0.13	−5[−14]	4[−13]	5[−13]	2[−10]
Ref. [19]	80			−1[−11]	−1[−10]	−2[−10]	−3[−10]

with $p_{-1}(u)=0$ and $p_0(u)=1/\beta_0$. The coefficients α_k and β_k are easily obtained with the Stieltjes procedure [22,18]. The normalization coefficient β_0 is given by

$$\beta_0^2=\int_c^d \rho(u)du=\int_a^b w(x)dx. \tag{16}$$

By expressing all integrals with the variable x, the other coefficients can be obtained by recurrence,

$$\alpha_k=\int_a^b w(x)t(x)\{p_{k-1}[t(x)]\}^2dx \tag{17}$$

and

$$\beta_k^2=\int_a^b w(x)\{[t(x)-\alpha_k]p_{k-1}[t(x)] - \beta_{k-1}p_{k-2}[t(x)]\}^2dx. \tag{18}$$

The zeros u_i are the eigenvalues of the symmetric tridiagonal matrix with α_1 to α_N on the diagonal and β_1 to β_{N-1} off diagonal.

As an application, we consider the interval $(-\infty,\infty)$ and the N shifted Gaussian functions,

$$\chi_n(x)=\exp[-(x-an)^2/2]. \tag{19}$$

[$n=-(N-1)/2$ to $(N-1)/2$, N even]. The parameter a controls the spacing-to-width ratio. The basis consisting of the N functions χ_n is equivalent to the orthogonal basis,

$$\varphi_k(x)=\exp\left(-\frac{x^2}{2}\right)\left[\cosh\left(\frac{ax}{2}\right)\right]^{N-1}p_k\left[\tanh\left(\frac{ax}{2}\right)\right], \tag{20}$$

with $k=0,N-1$, i.e., both bases span the same subspace. The polynomials p_k are either even or odd and lead to symmetric meshes. From Eq. (20), we choose $t(x)=\tanh(ax/2)$, which maps $(-\infty,\infty)$ on $(-1,1)$. The weight function is defined as

$$w_N(x)=A_N\exp(-x^2)[\cosh(ax/2)]^{2N-2}, \tag{21}$$

where A_N is a coefficient that can be chosen for convenience. Notice that $w_N(x)$ depends on N. The choice $A_N=2^{2N-2}\exp[-(N-1)^2a^2/4]$ keeps constant the order of magnitude of $w(x)$. The numerical integrations in Eqs. (16) to (18) and in Eq. (14) are performed with a constant step Δx. This technique is very accurate with infinitely differentiable functions [23]. The Lagrange basis is then equivalent to the bases (19) and (20). The derivatives $f_i'(x)$ are calculated with Eqs. (11) and (21).

Karabulut and Sibert [15] construct a Lagrange basis from shifted Gaussians with simple analytical expressions of the α_k and β_k. Their weight function is independent of N. Their mesh is different from the mesh deduced from Eqs. (20) to (21). It can be shifted symmetrically with respect to the origin but the basis then has no symmetry. Alternatively, shifting their basis can make it equivalent to Eqs. (19) and (20) but the mesh is then asymmetric.

As an example, we consider a system of reduced mass μ in the Morse potential (Ref. [19]),

$$V(x)=D[\exp(-2\alpha x)-2\exp(-\alpha x)+1], \tag{22}$$

where $\alpha=0.9374$, $D=\omega\beta/4$, and $\mu=\alpha^2\beta/2\omega$ with $\beta=156.047\,612\,535$ and $\omega=0.000\,574\,183\,728\,6$. These values precisely correspond to Table I of Ref. [19]. Potential (22) allows simple variational calculations and an exact evaluation of the error.

Table I displays absolute errors ϵ_ν on the energies of the ground state and of the 5th, 10th, and 15th excited states for different calculations with optimized parameters a and h. For small N, the Lagrange mesh provides excellent results not far from those of the exact variational calculation, i.e., a variational calculation performed with the nonorthogonal set of N basis functions χ_n with exact expressions for all matrix elements. When N increases, the nonorthogonality of the basis prevents the use of the optimal value of $a(\approx 0.3)$ in calculations with 15 significant digits. No such problem exists in the mesh approach. The mesh results become better than the variational results, except for small quantum numbers where they are limited by the accuracy on the zeros (for $\Delta x=0.02$). A similar accuracy requires a larger number of mesh points in Ref. [19]. The Lagrange meshes inspired by Ref. [15] provide slightly less good results.

Now we turn to a radial problem on the interval $(0,\infty)$ with the basis,

$$\chi_n(r)=\exp[-(r-an)^2/2]-\exp[-(r+an)^2/2], \tag{23}$$

TABLE II. Errors ϵ_ν on energies of a radial Morse potential from variational calculations with basis (23) and from two mesh calculations (see text). Laguerre-mesh results from Refs. [5,6] are also displayed. Powers of 10 are indicated in brackets.

	N	a	h	ϵ_0	ϵ_1	ϵ_5	ϵ_{10}
Var.	10	0.5	0.42	3[−8]	5[−6]		
Mesh 1		0.5	0.42	3[−7]	1[−6]		
Mesh 2		0.5	0.42	2[−7]	−6[−6]		
Var.	20	0.5	0.42	−1[−10]	1[−8]	6[−6]	
Mesh 1		0.3	0.44	−4[−13]	−1[−11]	4[−8]	
Mesh 2		0.3	0.44	−9[−13]	−3[−12]	2[−10]	
Var.	30	0.5	0.42	−5[−10]	7[−9]	3[−7]	
Mesh 1		0.3	0.49	8[−14]	−3[−12]	−3[−9]	6[−7]
Mesh 2		0.3	0.46	6[−15]	9[−14]	5[−10]	3[−8]
[5,6]	40		0.04	1[−15]	−1[−14]	−2[−10]	−3[−7]

$[n=1/2$ to $(N-1)/2,\quad N$ even$]$. Lagrange meshes corresponding to this basis can be obtained in several ways. First, one can simply keep the positive sector of the previous mesh and project the Lagrange functions (11) on negative parity [4] (Mesh 1). Second, one can apply the algorithm directly. The basis (23) is, for example, equivalent to the orthogonal basis,

$$\varphi_k(r)=\exp(-r^2/2)\sinh(ar/2)p_k[\sinh^2(ar/2)], \quad (24)$$

with $k=0, N-1$. This provides the weight

$$w(r)=\exp(-r^2)\sinh^2(ar/2) \quad (25)$$

and $t(r)=\sinh^2(ar/2)$ (Mesh 2).

As an example, we consider a radial Morse potential with equilibrium distance r_e as in Ref. [5]. It corresponds to the H_2^+ molecular ion with $\alpha=0.72$, $r_e=2$, $D=0.102\,62$, and $2\mu=1836$, precisely. Here, the analytical expressions of the eigenvalues are not exact but they are accurate to better than 10^{-15}. Both mesh calculations are compared in Table II with an exact variational calculation performed with basis (23). The errors ϵ_ν with respect to the analytical expressions are displayed in Table II. The striking result is again that the accuracy of the different Lagrange-mesh calculations is close to the accuracy of the variational calculation when the same a value is used. A similar effect has already been observed with the constant-step mesh [5] and with the Laguerre mesh [6]. Here, however, in the variational calculation, the nonorthogonality of the basis restricts the choice of a to values larger than the optimal one. The mesh calculation can be performed for the optimal a and provides better results.

In summary, a general procedure for deriving an infinity of new Lagrange variational bases and the associated Lagrange meshes has been introduced. For large classes of orthogonal or nonorthogonal bases, an equivalent orthogonal Lagrange basis can be constructed, which yields a very simple mesh approximation. Because of its orthogonality, the Lagrange basis does not suffer from the redundancy problem of a nonorthogonal basis. Therefore, a Lagrange-mesh approximation may provide more accurate results than the variational calculation with the original nonorthogonal basis, which is restricted by the finite accuracy of computers. We have applied the general technique to shifted Gaussians and obtained several meshes, one of which has been obtained analytically by other authors [15]. A comparison with variational calculations on simple examples shows that the loss of accuracy due to the mesh approximation is surprisingly weak and is sometimes compensated by a broader choice of values for the variational parameters. The existence of a large number of meshes with additional flexibility that provide a high accuracy for well-conditioned problems and the fact that the Lagrange mesh method leads to sparse matrices in multidimensional problems should be useful in various areas of numerical physics.

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