The unexplained accuracy of the Lagrange-mesh method

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The Lagrange-mesh method is an approximate variational calculation which resembles a mesh calculation because of the use of a Gauss quadrature. In order to analyze its accuracy, four different Lagrange-mesh calculations based on the zeros of Laguerre polynomials are compared with exact variational calculations based on the corresponding Laguerre basis. The comparison is performed for three solvable radial potentials: the Morse, harmonic-oscillator, and Coulomb potentials. The results show that the accuracies of the energies obtained for different partial waves with the different mesh approximations are very close to the variational accuracy, even in the presence of the centrifugal singularity. The same property holds for the approximate wave functions. This striking accuracy remains unexplained.

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I. INTRODUCTION

The Lagrange-mesh method is an approximate variational calculation which resembles a mesh calculation. This property is obtained by using a basis of Lagrange functions, i.e., orthonormal functions which vanish at all points but one in an associated mesh, and the Gauss quadrature corresponding to this mesh. The number of mesh points is equal to the basis size. The name Lagrange functions was introduced in Ref. [1] because of the resemblence to a basic property of the Lagrange interpolation polynomials. However, contrary to those polynomials, Lagrange functions are indefinitely differentiable.

Before describing the Lagrange-mesh method in more detail, let us first clarify one point. This method is sometimes considered [2] to be identical to the discrete-variable-representation (DVR) method [3]. In fact, in some cases, both approaches lead to the same mesh equations. However, we think that they follow different philosophies. The DVR method is designed to provide mesh equations and the selected mesh points can, in principle, be arbitrary [4]. The Lagrange-mesh method is valid only for meshes for which a Lagrange basis exists, i.e., for which the Lagrange conditions are satisfied [see Eq. (7) below]. These conditions usually ensure high accuracy. Therefore, the Lagrange-mesh method is a subset of the DVR method for which the Lagrange conditions provide an unusually high, and yet unexplained, accuracy. The Lagrange mesh equations have often been reobtained in different contexts. A recent example is given in Ref. [5].

Lagrange functions can be associated with every family of classical orthogonal polynomials [1]. In this case the associated Gauss quadrature is well known [6]. Recently, it has been shown that nonclassical orthogonal polynomials can also lead to useful Lagrange meshes [7]. The corresponding bases offer much more vast possibilities. They can, for example, provide an orthogonal basis equivalent to a set of shifted Gaussians [7,8]. In this case, nonstandard Gauss quadratures appear. An even more surprising property of the Lagrange bases is that they can be regularized, i.e., multiplied by some convenient factor, without losing their high accuracy, in spite of the fact that they become only approximately orthogonal [9–11]. This property is particularly important in treating the singularity of the centrifugal term when the orbital momentum is not zero.

The aim of the present paper is to describe the present status of our knowledge of the Lagrange-mesh method. To this end we shall concentrate on the example of the Laguerre meshes. We shall show that different meshes based on Laguerre polynomials can all give very accurate results with rather small numbers of mesh points. To evaluate the efficiency of the method, we shall compare the results of the Lagrange-mesh calculations with those of the exact variational calculations performed with the same Lagrange basis [11,7]. We shall emphasize the striking property that the Gauss approximation, which is the main difference beween both types of calculations, does lead to a very weak loss of accuracy in spite of the fact that the accuracy of the Gauss quadrature on individual matrix elements is rather poor. We shall also exemplify the qualitative differences of utility between meshes with tiny technical differences. Our hope is that the present analysis will stimulate mathematical results in the Lagrange-mesh approach.

The Lagrange-mesh method is summarized in Sec. II. Different Laguerre meshes, i.e., different meshes based on zeros of Laguerre polynomials, are presented in Sec. III. The accuracies with energies of solvable or approximately solvable potentials are presented and discussed in Sec. IV. Accuracies with wave functions are considered in Sec. V. Concluding remarks are presented in Sec. VI.

II. LAGRANGE-MESH METHOD

Let us consider a one-dimensional Schrödinger equation with kinetic energy $T=-d^2/dx^2$ over some interval (a,b),

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

To approximately solve this equation, we consider a variational approximation with N basis functions $f_i(x)$,

$$\psi(x)=\sum_{i=1}^{N} c_i f_i(x). \tag{2}$$

The corresponding variational equations read

$$\sum_{j=1}^{N} [T_{ij}+V_{ij}-EN_{ij}]c_j=0, \tag{3}$$

where

$$N_{ij}=\langle f_i|f_j\rangle, \tag{4}$$

$$T_{ij}=\langle f_i|T|f_j\rangle, \tag{5}$$

$$V_{ij}=\langle f_i|V|f_j\rangle. \tag{6}$$

The calculation of the V_{ij} may be tedious or time consuming. The resolution of Eq. (3) is more delicate when the basis is not orthogonal.

Let us now define a Lagrange basis [1]. Such a basis is defined in relation with a set of N mesh points $x_i \in (a,b)$, called a Lagrange mesh. The Lagrange functions are N orthonormal functions $f_i(x)$ verifying at the N mesh points x_i the Lagrange conditions

$$f_i(x_j)=\lambda_i^{-1/2}\delta_{ij}, \tag{7}$$

i.e., each function $f_i(x)$ vanishes at all mesh points except at x_i. These conditions restrict the possible sets of mesh points. The constants λ_i appearing in Eq. (7) are the weights of the Gauss quadrature approximation associated with the mesh,

$$\int_a^b g(x)dx \approx \sum_{k=1}^{N} \lambda_k g(x_k). \tag{8}$$

As a result of the Lagrange conditions (7), the basis functions $f_i(x)$ are orthogonal at the Gauss approximation. They are even exactly orthonormal when the Gauss quadrature is exact for products of Lagrange functions,

$$\int_a^b f_i(x)f_j(x)dx=\sum_{k=1}^{N} \lambda_k f_i(x_k)f_j(x_k)=\delta_{ij}. \tag{9}$$

This is, for example, the case when Lagrange functions are constructed from orthogonal polynomials [1]. The first equality in Eq. (9) is then exact, because an N-point Gauss quadrature is exact for the product of the weight function with a polynomial of degree up to $2N-1$.

The philosophy of the Lagrange-mesh method is to apply the Gauss approximation to the potential matrix elements. The approximate potential matrix is then diagonal,

$$\int_a^b f_i(x)V(x)f_j(x)dx \approx \sum_{k=1}^{N} \lambda_k f_i(x_k)V(x_k)f_j(x_k)=V(x_i)\delta_{ij}. \tag{10}$$

With Eqs. (9) and (10), the approximate variational calculation (3) resembles a mesh calculation

$$\sum_{j=1}^{N} [T_{ij}+V(x_i)\delta_{ij}-E\delta_{ij}]c_j=0. \tag{11}$$

The kinetic energy matrix elements can also be calculated at the Gauss approximation as $T_{ij} \approx -\lambda_i^{1/2} f_j''(x_i)$. The resulting expressions only depend on the x_i and x_j. As discussed below, the Gauss approximation is often exact for the kinetic energy with Lagrange functions based on classical orthogonal polynomials.

Now we turn to a radial Schrödinger equation of the form (1) with a variable r defined over the interval $[0,\infty[$. Over such an interval, it is possible to scale a given mesh in order to adjust it to the physical problem. The N basis functions then read

$$F_i(r)=h^{-1/2}f_i(r/h). \tag{12}$$

The scale factor h can be treated as an approximate nonlinear variational parameter. The wave function is then expanded as

$$\psi(r)=\sum_{i=1}^{N} C_i F_i(r). \tag{13}$$

As before, this approximation and a Gauss quadrature over $[0,\infty[$ lead to the mesh equations

$$\sum_{j=1}^{N} [h^{-2}T_{ij}+V(hx_i)\delta_{ij}-E\delta_{ij}]C_j=0. \tag{14}$$

Notice that a radial wave function $\psi(r)$ is subject to the boundary condition

$$\psi(0)=0. \tag{15}$$

III. LAGUERRE MESHES

The radial equation can be solved variationally with the simple (but nonorthogonal) basis,

$$\chi_n(x)=x^n \exp(-x/2), \quad n=1,\ldots,N-1 \tag{16}$$

$(x \in [0,\infty[)$. The simplicity of this basis has recently been emphasized in Ref. [12]. However, because of the redundancy between the basis states, the size of this basis cannot much exceed $N=20$. The basis (16) is equivalent to a subset of the orthogonal basis

$$\varphi_k(x)=L_k(x)\exp(-x/2), \quad k=0,\ldots,N-1. \tag{17}$$

In fact, the basis functions (17) do not vanish at the origin and a constraint must be added to verify condition (15). Another basis, exactly equivalent to basis (17), and with basis (16) as a subset, is the orthonormal Lagrange-Laguerre basis

$$f_i(x)=(-1)^i x_i^{1/2}\frac{L_N(x)}{x-x_i}e^{-x/2}, \quad i=1,\ldots,N \tag{18}$$

with the mesh points x_1 to x_N given by

$$L_N(x_i)=0. \tag{19}$$

The Gauss-Laguerre quadrature is then obtained with the weights

$$\lambda_i = \frac{e^{x_i}}{x_i [L'_N(x_i)]^2}. \tag{20}$$

Notice that the λ_i are not needed in the mesh equations but only in the expression of the wave function. Since the basis functions (18) do not satisfy condition (15), the kinetic energy matrix elements must be written as $T_{ij} = \langle f'_i | f'_j \rangle$ in order to keep Hermiticity. These expressions can be evaluated exactly at the Gauss approximation using $T_{ij} = f_i(0) f'_j(0) - \langle f_i | f''_j \rangle$ as

$$T_{ii} = (12x_i^2)^{-1}[4(4N+2)x_i - x_i^2 - 20] \tag{21}$$

and, for $i \neq j$,

$$T_{ij} = (-1)^{i-j}(x_i x_j)^{-1/2}\left[N + \frac{1}{2} - \frac{1}{x_i} - \frac{1}{x_j} + \frac{x_i + x_j}{(x_i - x_j)^2}\right]. \tag{22}$$

Although it may accidentally give good results (see the next section), this mesh approximation is not fully satisfactory since the basis does not satisfy condition (15). It is not valid for $l > 0$ since the integrals do not converge. Another basis must be used for $l > 0$. We shall compare three different ways of solving these problems. In each case we shall compare the mesh approximation with exact variational calculations performed with the same basis.

First we can define the basis

$$\overline{f}_i(x) = f_i(x) - (-1)^{N-i}(x_N/x_i)^{1/2} f_N(x), \quad i = 1, \ldots, N-1. \tag{23}$$

With Eq. (18), one easily verifies that condition (15) is satisfied by each basis function. The price to pay is that the basis is not orthogonal. However, a generalized eigenvalue problem involving $N-1$ mesh equations can easily be derived from the mesh equations (14) of the previous case.

A second orthonormal basis strictly equivalent to basis (16) reads

$$\tilde{\varphi}_k(x) = h_k^{-1/2} x L_k^{(2)}(x) \exp(-x/2), \quad k = 0, \ldots, N-1, \tag{24}$$

where $L_k^{(2)}$ is an associate Laguerre polynomial and $h_k = (k+1)(k+2)$ [13]. Each basis function satisfies condition (15). As proposed in Ref. [1], an equivalent orthonormal Lagrange-Laguerre basis is given by

$$\tilde{f}_i(x) = (-1)^i (\tilde{x}_i/h_N)^{1/2} \frac{x L_N^{(2)}(x)}{x - \tilde{x}_i} e^{-x/2}, \quad i = 1, \ldots, N. \tag{25}$$

Here the mesh points are given by

$$L_N^{(2)}(\tilde{x}_i) = 0 \tag{26}$$

and the Gauss weights by [13]

$$\tilde{\lambda}_i = h_N \frac{e^{\tilde{x}_i}}{\tilde{x}_i^3 [L_N^{(2)\prime}(\tilde{x}_i)]^2}. \tag{27}$$

The exact kinetic-energy matrix elements read [1]

$$\tilde{T}_{ii} = (9/4)\tilde{x}_i^{-2} + S_{ii} \tag{28}$$

and, for $i \neq j$,

$$\tilde{T}_{ij} = (-1)^{i-j}\left[\frac{3}{2}(\tilde{x}_i \tilde{x}_j)^{-1/2}(\tilde{x}_i^{-1} + \tilde{x}_j^{-1}) - S_{ij}\right] \tag{29}$$

with

$$S_{ij} = (\tilde{x}_i \tilde{x}_j)^{1/2} \sum_{k \neq i,j} \frac{1}{\tilde{x}_k (\tilde{x}_k - \tilde{x}_i)(\tilde{x}_k - \tilde{x}_j)}. \tag{30}$$

The corresponding mesh equations take the form (14). As shown below, this mesh is excellent for the *s* wave. However, the Gauss quadrature is *a priori* very bad for $1/r^2$ so that higher partial waves are not expected to be accurately treated on this mesh. In Ref. [1], other meshes are proposed for $l > 0$ which provide accurate results for nonsingular potentials. This solution has the drawback that different partial waves correspond to different meshes and that coupled-channel or three-body problems cannot be considered.

A third approach starts from the nonorthogonal basis,

$$\hat{\varphi}_k(x) = x L_k(x) \exp(-x/2), \quad k = 0, \ldots, N-1 \tag{31}$$

which is equivalent to Eqs. (16), (23), (24), and (25). As established implicitly in Ref. [9] and explicitly in Ref. [14], an equivalent Lagrange-Laguerre basis can also be defined as

$$\hat{f}_i(x) = \frac{x}{x_i} f_i(x) = (-1)^i x_i^{-1/2} \frac{x L_N(x)}{x - x_i} e^{-x/2}, \quad i = 1, \ldots, N \tag{32}$$

with x_i given by Eq. (19). An important difference with basis (25) is that the Gauss quadrature with the same λ_i as in Eq. (20) is here exact for the centrifugal form factor $1/r^2$. Another difference is that basis (32) is nonorthogonal. Its exact overlap matrix elements are easily obtained as explained in the appendix of Ref. [9],

$$N_{ij} = \int_0^\infty \hat{f}_i(x) \hat{f}_j(x) dx = \delta_{ij} + (-1)^{i-j}(x_i x_j)^{-1/2}. \tag{33}$$

The Gauss approximation $\hat{T}_{ij}^G = -\lambda_i^{1/2} \hat{f}''_j(x_i)$ for the kinetic energy matrix elements reads [10]

$$\hat{T}_{ii}^G = (12x_i^2)^{-1}[4 + (4N+2)x_i - x_i^2] \tag{34}$$

and, for $i \neq j$,

$$\hat{T}^G_{ij}=(-1)^{i-j}(x_ix_j)^{-1/2}(x_i+x_j)(x_i-x_j)^{-2}. \tag{35}$$

The exact kinetic energy matrix elements can be calculated starting from the Gauss approximation as explained in the appendix of Ref. [9]. They read

$$\hat{T}_{ij}=\hat{T}^G_{ij}-\frac{1}{4}(-1)^{i-j}(x_ix_j)^{-1/2}. \tag{36}$$

With the exact expressions (33) and (36), the mesh equations take the form

$$\sum_{j=1}^{N}[h^{-2}\hat{T}_{ij}+V(hx_i)\delta_{ij}-EN_{ij}]C_j=0, \tag{37}$$

i.e., lead to a generalized eigenvalue problem. However, according to Eq. (9), the basis (32) is orthonormal at the Gauss approximation. When this approximation is used for the overlap and for the kinetic energy [Eqs. (34) and (35)], one recovers the nongeneralized eigenvalue problem (14). As observed in Ref. [10], this additional approximation does not cause any real loss of accuracy. However, the main advantage of the so-called regularized mesh, under the form (37) or under the simpler Gauss form (14), is that it now allows us to accurately treat singular terms behaving as r^{-1} and r^{-2} at the Gauss approximation. Therefore the regularized mesh is also valid for $l>0$. In fact, looking at the expression (32) of the basis functions $\hat{f}_i(x)$, one observes that the matrix elements $\langle\hat{f}_i|r^{-1}|\hat{f}_j\rangle$ and $\langle\hat{f}_i|r^{-2}|\hat{f}_j\rangle$ are exact at the Gauss approximation.

IV. ACCURACY OF ENERGIES IN SOLVABLE EXAMPLES

In this section, we illustrate the properties discussed in the previous section with different solvable potentials: the Morse, three-dimensional harmonic oscillator, and Coulomb potentials. The selected Morse potential [10] is regular everywhere and displays a strong repulsive barrier at the origin. The oscillator potential is also regular but vanishes at the origin. The Coulomb potential provides an example of singularity. We can thus compare the mesh methods under progressively more difficult conditions.

As in Refs. [10,11,7], the Morse potential is defined as

$$V(r)=D\{\exp[-2a(r-r_e)]-2\exp[-a(r-r_e)]\}, \tag{38}$$

where $D=0.102\,62$, $r_e=2$, $a=0.72$, and $2m=1836$. For the s wave, this potential is very close to solvable. It is exactly solvable over $]-\infty,+\infty[$ [15]. Over $[0,+\infty[$, the strong exponential barrier forces the wave function to be exponentially small at the origin. The eigenvalues are given extremely accurately (i.e., with an accuracy much better than 10^{-15}) by

$$E_{n_r}=-D+\left(n_r+\frac{1}{2}\right)a(2D/m)^{1/2}-\left(n_r+\frac{1}{2}\right)^2a^2/2m \tag{39}$$

TABLE I. Energies of the $n_r=0$ and $n_r=5$ states of the Morse potential. In the $l=0$ case, the values are deduced from the analytical expression (39). The $l=1$ and $l=2$ energies are obtained by a Lagrange mesh calculation (14) with $N=60$ mesh points (19), kinetic energy (34) and (35), and the scale factor $h=0.05$.

l	$n_r=0$	$n_r=5$
0	−0.097 307 739 656 379	−0.051 949 842 102 521
1	−0.097 040 301 141 149	−0.051 735 382 273 815
2	−0.096 507 541 478 194	−0.051 308 827 503 494

for $n_r=0$ to 15. For $l>0$, the eigenvalues are calculated numerically. Typical energies are gathered in Table I. The Morse potential has also the advantage that its matrix elements can be calculated exactly for the different bases discussed above. For the oscillator and Coulomb potentials, we compare the results with the standard expressions in natural units, i.e., $E_{n_r}=2n_r+l+\frac{3}{2}$ and $E_{n_r}=\frac{1}{2}(n_r+l+1)^{-2}$, respectively.

For the three Lagrange meshes discussed above, we compare exact variational calculations with the Lagrange mesh results for the same number of points and values of the scale parameter h. In fact, the variational bases (16), (23), (24), (25), (31), and (32) being equivalent, they should provide the same variational results. The equivalent bases (17) and (18) are different since the spanned vector space contains an additional component proportional to $\varphi_0(x)$ and should not be relevant here. On the contrary, the three mesh calculations based on Eqs. (23), (25), and (32) are expected to provide different results.

All the results from exact variational calculations obtained with *orthogonal* bases are identical and are displayed as "var." in Tables II–VII. The results obtained with the weakly nonorthogonal bases (23), (31), and (32) are essentially identical. Those obtained with the strongly nonorthogonal basis (16) are also identical for $N\leqslant 10$ but their accuracy becomes less good beyond that value. For $N=20$, the accuracy on the ground state is only 3×10^{-6}. Between $N=10$ and 20, the accuracy is progressively degraded because the overlap reduction algorithm behaves worse and worse. Beyond $N=20$, numerical problems appear with the positive character of the overlap matrix.

Four different mesh calculations are compared in Table II with the variational results for the s, p, and d waves of the Morse potential. The scale factor is fixed at $h=0.05$. This value corresponds to a rough optimization of the meshes. Finely tuned optimizations depending on the state and partial wave might improve the results but the improvement is usually not important. The errors on the energies are defined as

$$\epsilon_{n_r}=E^{\text{approx}}_{n_r}-E_{n_r} \tag{40}$$

for the different approximations. The different columns successively correspond to the variational calculation (3) with one of the equivalent orthogonal Laguerre bases, the mesh calculation (14) modified according to Eq. (23) with mesh x_i and T_{ij} given by Eqs. (21) and (22), the mesh calculation

TABLE II. Errors ϵ_{n_r} [Eq. (40)] in the energies of the $n_r=0$ and $n_r=5$ states of the Morse potential in the *s*, *p*, and *d* waves obtained for $h=0.05$ with the variational equations (3), with x_i and T_{ij} in the mesh equations (14) modified according to Eq. (23), with $\tilde{x}_i$ and $\tilde{T}_{ij}$ in the mesh equations (14), with x_i and $\hat{T}_{ij}$ in the mesh equations (37), and with x_i and $\hat{T}^G_{ij}$ in the mesh equations (14). The powers of ten are indicated in square brackets.

l	n_r	N	Var.	(x_i, T_{ij})	$(\tilde{x}_i, \tilde{T}_{ij})$	$(x_i, \hat{T}_{ij})$	$(x_i, \hat{T}^G_{ij})$
0	0	20	3.8[−7]	1.6[−6]	4.6[−7]	6.3[−7]	4.2[−7]
		40	<1[−14]	1.4[−14]	<1[−14]	1.4[−14]	1.4[−14]
	5	20	4.0[−3]	1.5[−2]	5.5[−3]	8.0[−4]	9.6[−4]
		40	1.1[−9]	4.0[−9]	3.0[−9]	−4.8[−9]	−4.6[−9]
1	0	20	4.1[−7]	1.6[−6]	4.8[−7]	7.0[−7]	5.0[−7]
		40	<1[−14]	1.4[−14]	<1[−14]	1.4[−14]	1.4[−14]
	5	20	4.4[−3]	1.6[−2]	5.7[−3]	1.0[−3]	1.2[−3]
		40	1.1[−9]	4.2[−9]	3.1[−9]	−4.3[−9]	−4.2[−9]
2	0	20	4.5[−7]	1.7[−6]	5.0[−7]	8.2[−7]	6.5[−7]
		40	<1[−14]	1.5[−14]	<1[−14]	1.5[−14]	1.6[−14]
	5	20	4.7[−3]	1.7[−2]	6.0[−3]	1.5[−3]	1.7[−3]
		40	1.1[−9]	4.4[−9]	3.1[−9]	−3.4[−9]	−3.2[−9]

TABLE III. Errors ϵ_{n_r} [Eq. (40)] in the energies of the $n_r=0$ and $n_r=5$ states of the harmonic oscillator potential obtained in different cases (see Table II) for $h=0.1$.

l	n_r	N	Var.	(x_i, T_{ij})	$(\tilde{x}_i, \tilde{T}_{ij})$	$(x_i, \hat{T}_{ij})$	$(x_i, \hat{T}^G_{ij})$
0	0	20	3.1[−14]	8.9[−14]	3.7[−14]	1.3[−13]	1.1[−13]
		40	2.8[−14]	−3.0[−13]	<1[−14]	1.4[−14]	−4.9[−14]
	5	20	1.2[−4]	4.4[−4]	9.4[−5]	−3.2[−3]	−3.5[−4]
		40	<1[−14]	−4.1[−14]	6.6[−14]	−1.8[−14]	−5.7[−14]
1	0	20	1.2[−12]	1.1[−13]	−9.6[−7]	−2.2[−12]	−1.4[−12]
		40	3.3[−14]	−3.4[−14]	−1.4[−7]	−4.7[−14]	−3.8[−14]
	5	20	2.6[−4]	2.2[−3]	1.5[−4]	−7.5[−3]	6.6[−4]
		40	3.3[−13]	2.7[−13]	−1.6[−6]	−8.1[−13]	−3.0[−13]
2	0	20	8.8[−12]	3.6[−11]	7.3[−12]	−6.2[−11]	−2.7[−11]
		40	<1[−14]	6.3[−14]	<1[−14]	1.1[−13]	−1.4[−14]
	5	20	1.7[−3]	3.4[−3]	1.5[−3]	2.9[−3]	3.4[−3]
		40	3.4[−13]	2.8[−12]	1.4[−13]	−1.5[−12]	8.5[−13]

TABLE IV. Errors ϵ_{n_r} [Eq. (40)] in the energies of the $n_r=0$ and $n_r=5$ states of the Coulomb potential obtained in different cases (see Table II) for $h=1.5$.

l	n_r	N	Var.	(x_i, T_{ij})	$(\tilde{x}_i, \tilde{T}_{ij})$	$(x_i, \hat{T}_{ij})$	$(x_i, \hat{T}^G_{ij})$
0	0	20	2.1[−10]	7.5[−10]	2.8[−2]	2.1[−10]	−4.0[−10]
		40	<1[−14]	<1[−14]	8.9[−3]	<1[−14]	3.1[−14]
	5	20	3.6[−8]	1.5[−7]	1.3[−4]	3.6[−8]	7.4[−8]
		40	<1[−14]	<1[−14]	4.1[−5]	<1[−14]	<1[−14]
1	0	20	<1[−14]	<1[−14]	−9.2[−5]	<1[−14]	<1[−14]
		40	<1[−14]	<1[−14]	−1.3[−5]	<1[−14]	<1[−14]
	5	20	2.0[−5]	4.9[−5]	1.6[−5]	2.0[−5]	3.1[−5]
		40	<1[−14]	<1[−14]	−4.0[−7]	<1[−14]	<1[−14]
2	0	20	<1[−14]	<1[−14]	<1[−14]	<1[−14]	<1[−14]
		40	<1[−14]	<1[−14]	<1[−14]	<1[−14]	<1[−14]
	5	20	4.6[−4]	7.5[−4]	4.6[−4]	4.6[−4]	5.8[−4]
		40	1.4[−11]	4.2[−11]	1.4[−11]	1.4[−11]	2.4[−11]

TABLE V. Comparison of errors η [Eq. (41)] in the wave functions of the $n_r=0$ and $n_r=5$ states for the Morse potential: exact, variational, and $(x_i,\hat{T}^G_{ij})$ Lagrange-mesh calculations (32) with $h=0.05$.

		$n_r=0$			$n_r=5$		
l	N	Mesh/ex.	Var./ex.	Mesh/var.	Mesh/ex.	Var./ex.	Mesh/var.
0	20	1.9[−4]	4.2[−4]	5.6[−4]	0.15	0.10	0.09
	40	3.3[−9]	2.4[−8]	2.7[−8]	4.4[−6]	2.8[−5]	3.2[−5]
1	20			5.5[−4]			8.6[−2]
	40			2.7[−8]			3.1[−5]
2	20			5.4[−4]			8.3[−2]
	40			2.7[−8]			3.0[−5]

(14) with mesh $\tilde{x}_i$ and $\tilde{T}_{ij}$ given by Eqs. (28) and (29), the mesh calculation (37) with mesh x_i and $\hat{T}_{ij}$ given by Eq. (36), and the mesh calculation (14) with mesh x_i and $\hat{T}^G_{ij}$ given by Eqs. (34) and (35). The first mesh calculation is related to basis (23) and requires solving a generalized eigenvalue problem of dimension $N-1$. The other ones correspond to dimension N. The accuracy of the mesh calculations is limited by the accuracy on the zeros of the Laguerre polynomials which is itself restricted by the computer accuracy. For this reason, we do not explicitly show the errors that we have obtained when they are smaller than 10^{-14}. The errors on the variational calculation are always positive as expected when the computer accuracy is not reached, but the errors on the mesh calculations may be negative. Let us start the discussion with the *s* wave.

The accuracy of the (x_i,T_{ij}) calculation is only slightly poorer than the accuracy of the variational calculation. Surprisingly, identical results are obtained with the mesh corresponding to basis (18) which does not satisfy condition (15). However, this property is not true for the other potentials. This can be understood as follows. The results obtained with the mesh equations derived from bases (18) and (23), respectively, correspond to even and odd solutions of the Morse potential symmetrized over $]-\infty,+\infty[$. Since this potential has a strong repulsive barrier at the origin, even and odd solutions are degenerate to a high accuracy. The same reason explains why Eq. (39) provides essentially exact values for the present radial Morse potential.

The results obtained with the mesh $(\tilde{x}_i,\tilde{T}_{ij})$ are even slightly better. For the regularized mesh (19) derived from basis (32), two different calculations with the mesh x_i are presented without and with Gauss approximation for the overlap and kinetic-energy matrices. The first calculation is a generalized eigenvalue problem [Eq. (37)] with the exact kinetic energy (36). The second one is the eigenvalue problem (14) with the approximate kinetic energy (34) and (35). The accuracy is excellent in both cases and the simpler approximate approach is surely not less good than the other one.

Let us now emphasize that all these very accurate results of the mesh calculations are obtained in spite of the fact that *the Gauss approximation is not very good for individual matrix elements of the potential*. Indeed, when comparing the exact potential matrix elements calculated for the variational calculation with those of the regularized-mesh basis (32), for example, one finds that the relative accuracy on diagonal matrix elements is never better than 2% for $N=20$ and 0.05% for $N=40$, and is often far worse. Nondiagonal matrix elements which are approximated by zero at the Gauss approximation cannot be given a relative accuracy but their absolute accuracy is not better than for diagonal elements. Hence the excellent accuracy obtained with $N=40$ (absolute error of about 10^{-14} for the ground state) is obtained with potential matrix elements with absolute errors not better than 2×10^{-6}. This property must be taken into account when interpreting the Lagrange-mesh method. The accuracy of that method is *not* due to a high accuracy of the Gauss approximation on individual matrix elements.

All the different Laguerre meshes might not withstand the introduction of a singularity at the origin under the form of a centrifugal barrier. The results for the *p* and *d* waves are also compared with the exact variational results in Table II. One hardly sees a difference of accuracy with the *s* wave case. As

TABLE VI. Comparison of errors η [Eq. (41)] in the wave functions of the $n_r=0$ and $n_r=5$ states for the harmonic oscillator potential: exact, variational, and $(x_i,\hat{T}^G_{ij})$ Lagrange-mesh calculations (32) with $h=0.1$.

		$n_r=0$			$n_r=5$		
l	N	Mesh/ex.	Var./ex.	Mesh/var.	Mesh/ex.	Var./ex.	Mesh/var.
0	20	8.3[−10]	8.3[−9]	8.8[−9]	1.5[−4]	6.5[−4]	7.5[−4]
	40	<1[−14]	<1[−14]	<1[−14]	2.2[−10]	5.4[−9]	5.6[−9]
1	20	3.9[−9]	5.7[−8]	6.1[−8]	5.1[−4]	5.6[−4]	8.8[−4]
	40	1.3[−14]	1.8[−13]	1.9[−13]	5.5[−10]	1.5[−8]	1.6[−8]
2	20	1.3[−8]	1.5[−7]	1.6[−7]	7.0[−4]	1.9[−3]	2.3[−3]
	40	<1[−14]	4.3[−13]	4.3[−13]	1.4[−9]	1.4[−8]	1.5[−8]

TABLE VII. Comparison of errors η [Eq. (41)] in the wave functions of the $n_r=0$ and $n_r=5$ states for the Coulomb potential: exact, variational, and $(x_i,\hat{T}^G_{ij})$ Lagrange-mesh calculations (32) with $h=1.5$.

		$n_r=0$			$n_r=5$		
l	N	Mesh/ex.	Var./ex.	Mesh/var.	Mesh/ex.	Var./ex.	Mesh/var.
0	20	6.4[−8]	1.8[−6]	1.9[−6]	1.1[−5]	2.5[−5]	3.4[−5]
	40	3.8[−14]	2.4[−12]	2.4[−12]	6.7[−14]	6.6[−13]	7.2[−13]
1	20	1.5[−14]	4.4[−13]	4.6[−13]	1.5[−3]	9.4[−4]	7.0[−4]
	40	<1[−14]	<1[−14]	<1[−14]	2.6[−10]	1.7[−9]	1.9[−9]
2	20	<1[−14]	<1[−14]	<1[−14]	1.3[−2]	1.2[−2]	2.9[−3]
	40	<1[−14]	<1[−14]	<1[−14]	7.8[−8]	3.1[−7]	3.9[−7]

we shall learn from the other examples, this is due to the strong repulsive barrier of the Morse potential.

The results for the harmonic oscillator are displayed in Table III for the same conditions. The scale factor is fixed at $h=0.1$. For the s wave, the accuracies behave similarly to those of the Morse potential except that the convergence is faster. For the ground state, the accuracy is already close to the computer accuracy for $N=20$. A difference, however, appears for the p wave. The mesh $(\tilde{x}_i,\tilde{T}_{ij})$ is far less accurate than the other ones. This difference can be attributed to the centrifugal term whose value is not given exactly by the Gauss quadrature in that case. Surprisingly, this problem disappears for higher partial waves: the d wave results are again very similar for all meshes and very close to the variational accuracy.

The results for the Coulomb potential are presented in Table IV. The scale factor is fixed at $h=1.5$. For the s wave, the accuracies behave similarly as those of the other potentials except for the mesh $(\tilde{x}_i,\tilde{T}_{ij})$ whose accuracy is very poor. Again this problem is related to the singularity of the Coulomb potential. As before, it becomes less serious with increasing l.

We conclude this section by noting that several Lagrange-mesh calculations are able to provide the same accuracy as the corresponding variational calculation. One of the meshes, $(\tilde{x}_i,\tilde{T}_{ij})$, may be less accurate in the presence of a singularity. Among the other ones, the simplest one is the regularized mesh with full Gauss approximation $(x_i,\hat{T}^G_{ij})$ because it leads to a nongeneralized eigenvalue problem. We consider only this mesh in the next section.

V. ACCURACY OF WAVE FUNCTIONS

In previous works, we only considered the accuracy in energies. Now we extend the analysis by considering the accuracy of the Lagrange-mesh wave functions. We compare the results of mesh $(x_i,\hat{T}^G_{ij})$ to the exact wave functions as well as to the corresponding variational approximation. We define the distance between two (exact or approximate) wave functions ψ_1 and ψ_2 as

$$\eta=N^{-1}\sum_{i=1}^{N}|\psi_1(hx_i)-\psi_2(hx_i)|. \tag{41}$$

This definition is based on the values at mesh points only. We have also considered distances based on equally spaced points but the results are qualitatively similar, so that we do not show them in detail.

The distances η for the Morse potential are given in Table V. A comparison with the ''exact'' analytical wave function is only possible for the s wave. For a variational calculation, the accuracy on the wave function is less good than the accuracy on the energy, i.e., the error on the wave function is expected to be of the order of the square root of the error on the energy. This rule seems to be followed qualitatively. One observes that the mesh wave function seems to be slighly more accurate than the variational one.

More information can be obtained with the harmonic-oscillator (Table VI) and Coulomb (Table VII) potentials because the exact wave functions are available for all partial waves. Here the errors on the mesh and variational calculations are sometimes restricted by the computer accuracy. For both states of both potentials, one observes that the mesh wave function is systematically slightly better than the variational one. However, this property is only valid for a distance calculated from values at mesh points. With a distance calculated with 200 equally spaced mesh points located between 0 and hx_N, the accuracies on the variational wave functions do not change much from those shown in Tables VI and VII but the variational approximations are now often slightly better than the mesh approximations.

VI. CONCLUSIONS

In order to analyze the accuracy of the Lagrange-mesh method, different variants based on the zeros of Laguerre polynomials are compared with exact variational calculations based on the corresponding Laguerre basis. Tests are performed on radial equations, where the wave function has to vanish at the origin, for three solvable potentials: the Morse, harmonic-oscillator, and Coulomb potentials.

The results show that the accuracies of the energies obtained for different partial waves with the different mesh approximations are very close to the variational accuracy, even in the presence of the centrifugal singularity. We observe that the same property holds for the approximate wave functions. It must be stressed that the Gauss approximation is far less accurate on individual matrix elements than on energies and wave functions. We think that DVR-like calcula-

tions require that the Lagrange conditions be satisfied, exactly or almost exactly, in order to be highly accurate.

The different mesh equations usually provide similar accuracies. However, when the Gauss approximation does not exactly treat r^{-1} and r^{-2} singularities, the accuracy may drop. Strangely, in the examples considered, the lost accuracy is recovered when l increases.

The simplest mesh is the regularized Laguerre mesh with full use of the Gauss approximation. The eigenvalue problem is not generalized and the accuracy is excellent. This might arise from the consistent use of the Gauss approximation in all terms. This striking accuracy remains unexplained. Nevertheless, the Lagrange-Laguerre mesh makes it possible to accurately treat various physical problems such as semirelativistic two-body systems [16] or atomic and molecular three-body systems [17].

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