Semirelativistic Lagrange mesh calculations

C. Semay
Université de Mons-Hainaut, Place du Parc, 20, B-7000 Mons, Belgium

D. Baye and M. Hesse
Physique Nucléaire Théorique et Physique Mathématique, Case Postale 229, Université Libre de Bruxelles, B-1050 Brussels, Belgium

B. Silvestre-Brac
Institut des Sciences Nucléaires, IN2P3, CNRS, Université Joseph Fourier, Avenue des Martyrs 53, F-38026 Grenoble-Cedex, France
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The Lagrange mesh method is a very powerful procedure to compute eigenvalues and eigenfunctions of nonrelativistic Hamiltonians. The trial eigenstates are developed in a basis of well-chosen functions and the computation of Hamiltonian matrix elements requires only the evaluation of the potential at grid points. It is shown that this method can be used to solve semirelativistic two-body eigenvalue equations. As in the nonrelativistic case, it is very accurate, fast, and very simple to implement.

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I. INTRODUCTION

The Lagrange mesh method is a very accurate and simple procedure to compute eigenvalues and eigenfunctions of a two-body Schrödinger equation [1–3]. The trial eigenstates are developed in a basis of well-chosen functions and Hamiltonian matrix elements are obtained with a Gauss approximate quadrature. No numerical evaluation of matrix elements is required, only the computation of the potential at grid points. The spacings between grid points depend on the basis chosen and are not necessarily equal. This method can be extended to treat, very accurately, three-body systems as well in nuclear physics as in atomic physics (see, for instance, Ref. [4]). Recently, a general procedure for deriving new Lagrange meshes related to orthogonal or nonorthogonal bases has been developed [5].

The Fourier grid Hamiltonian method is another simple procedure to solve a two-body Schrödinger equation on a mesh [6,7]. It relies on the fact that the kinetic-energy operator is best represented in momentum space, while the potential energy is generally given in coordinate space. This method has been generalized to treat a semirelativistic operator in the three-dimensional space for bound states [8]. It has also been applied to the study of scattering equations [9]. This method requires a mesh of equally spaced grid points. As a consequence, a large number of points can sometimes be necessary to reach convergence.

It has recently been shown that the Fourier grid Hamiltonian method is equivalent to a Lagrange mesh calculation in which the matrix elements of the kinetic-energy operator are computed by a discrete Fourier transformation [10] (this makes possible the computation of bound states for semirelativistic kinematics). In order to escape from the constraint of equally spaced grid points, a new method is developed here to compute the kinetic matrix elements in the Lagrange mesh method. The idea, already used in Ref. [11] but in another context, is to compute the square root of an approximation to the square of the semirelativistic kinetic-energy operator. It is shown in this paper that very accurate eigenvalues and eigenfunctions of a semirelativistic Hamiltonian can be computed very fast and very easily with this modified Lagrange mesh method. It is worth noting that the Lagrange mesh technique can be applied if the potential is nonlocal, or if couplings exist between different channels.

The nonrelativistic and semirelativistic Lagrange mesh methods are described in Sec. II, while Sec. III presents an ansatz to easily compute the only nonlinear parameter of the method. Test calculations are presented in Sec. IV, and some concluding remarks are given in Sec. V.

II. METHOD

A Lagrange mesh is formed of N mesh points x_i associated with an orthonormal set of N indefinitely derivable functions $f_j(x)$ [1–3]. The Lagrange function f_j vanishes at all mesh points but one; it satisfies the Lagrange conditions

$$f_j(x_i)=\lambda_i^{-1/2}\delta_{ij}. \tag{1}$$

The x_i and λ_i are connected with a Gauss quadrature formula

$$\int_0^\infty g(x)dx \approx \sum_{k=1}^{N} \lambda_k g(x_k). \tag{2}$$

Here, the case of the Gauss-Laguerre quadrature is considered because the domain is $(0,\infty)$. The Gauss formula (2) is exact when $g(x)$ is a polynomial of degree $2N-1$ at most, multiplied by $\exp(-x)$. The Lagrange-Laguerre mesh is then based on zeros of a Laguerre polynomial of degree N [1],

$$L_N(x_i)=0. \tag{3}$$

The explicit form of the corresponding regularized Lagrange functions is given by

$$f_i(x)=(-1)^i x_i^{-1/2} x(x-x_i)^{-1} L_N(x)\exp(-x/2), \tag{4}$$

which is simply a polynomial of degree N, multiplied by an exponential function. They vanish at the origin and at x_j with

$j \neq i$. In fact, most calculations in the following can be performed without explicit expressions of the λ_i and $f_i(x)$; these quantities are only necessary to plot the wave functions. The factors λ_i must be computed in the case of a nonlocal interaction [10].

For example, let us consider the eigenvalue equation

$$[T(\vec{p}^2)+V(r)]|\psi\rangle = E|\psi\rangle, \tag{5}$$

where $T(\vec{p}^2)$ is the kinetic-energy term of the Hamiltonian and $V(r)$ the potential that depends only on the radial coordinate r. A variational calculation is performed with the trial state

$$|\psi\rangle = \sum_{j=1}^{N} C_j |f_j\rangle, \tag{6}$$

where

$$\langle \vec{r}|f_j\rangle = \frac{f_j(r/h)}{\sqrt{h}r} Y_{\ell m}(\hat{r}), \tag{7}$$

and where ℓ is the orbital angular-momentum quantum number. The coefficients C_j are linear variational parameters and the scale factor h is a nonlinear parameter aimed at adjusting the mesh to the domain of physical interest. With Eqs. (2) and (1), the coefficients read

$$C_i = \sqrt{h\,\lambda_i}\,u(hx_i), \tag{8}$$

where $u(r)$ is the regularized radial part of the trial wave function. They provide a direct picture of the wave function at mesh points. However, contrary to some other mesh methods, the wave function is also defined between mesh points by Eqs. (4), (6), and (7).

At the Gauss approximation, $\langle f_i|f_j\rangle \approx \delta_{ij}$, and the potential matrix elements are given by

$$\langle f_i|V(r)|f_j\rangle \approx V(hx_i)\,\delta_{ij}. \tag{9}$$

The potential matrix is both simple to obtain and diagonal. Let us assume that the matrix elements $\langle f_i|T|f_j\rangle \approx T_{ij}$ are known. With Eqs. (6) and (9), the variational method applied to Eq. (5) provides a system of N mesh equations

$$\sum_{j=1}^{N} [T_{ij} + V(hx_i)\,\delta_{ij} - E\,\delta_{ij}] C_j = 0. \tag{10}$$

We shall see that, in this system, the first term is easy to compute. The second one is diagonal and only involves values of the potential at scaled mesh points.

A. Nonrelativistic Hamiltonian

For a nonrelativistic Hamiltonian, the operator $T(\vec{p}^2)$ is simply given by $\vec{p}^2/(2\mu)$, where μ is the reduced mass. With Eq. (2), radial kinetic matrix elements are given by

$$T_{ij} = \frac{1}{2\mu h^2}\left(t_{ij} + \frac{\ell(\ell+1)}{x_i^2}\,\delta_{ij}\right), \tag{11}$$

where ($\hbar = 1$)

$$t_{ij} = \int_0^\infty f_i(x)\left(-\frac{d^2}{dx^2}\right) f_j(x)\;\; dx \approx -\lambda_i^{1/2} f_j''(x_i). \tag{12}$$

This compact expression is exact for some Lagrange meshes. This is not the case for the regularized Laguerre mesh. An exact expression can easily be obtained (see appendix in Ref. [2]). However, as shown in Ref. [3], it is preferable to use the approximations (11) and (12). The kinetic matrix elements are then even easier to obtain and read [3]

$$t_{ij} = \begin{cases} (-)^{i-j}(x_i x_j)^{-1/2}(x_i + x_j)(x_i - x_j)^{-2} & (i \neq j), \\ (12x_i^2)^{-1}[4 + (4N+2)x_i - x_i^2] & (i = j). \end{cases} \tag{13}$$

The simplicity of this approach is obvious on Eq. (10). Another striking property, which is not obvious at all, has been observed on many examples [1–3]: the accuracy of the mesh approximation remains close to the accuracy of the original variational calculation without the Gauss approximation.

B. Semirelativistic Hamiltonian

In natural units ($\hbar = c = 1$), a semirelativistic Hamiltonian is written

$$H = \sqrt{\vec{p}^2 + m_1^2} + \sqrt{\vec{p}^2 + m_2^2} + V(r). \tag{14}$$

The eigenvalue equation associated with this Hamiltonian is generally called the spinless Salpeter equation. To apply the method described above, it is necessary to compute the matrix elements $\langle f_i|\sqrt{\vec{p}^2 + m^2}|f_j\rangle$. This can be performed using a four-step method suggested in Ref. [11] (see also references therein):

(i) Computation of the matrix M^2 whose elements are

$$(M^2)_{ij} = \langle f_i|\vec{p}^2 + m^2|f_j\rangle. \tag{15}$$

They are calculated as in the nonrelativistic case with Eqs. (11) and (12).

(ii) Diagonalization of the matrix M^2. If D^2 is the diagonal matrix formed by the eigenvalues of M^2, we have

$$M^2 = SD^2S^{-1}, \tag{16}$$

where S is the transformation matrix composed of the normalized eigenvectors.

(iii) Computation of D, the diagonal square root matrix of D^2, by taking the positive square roots of all diagonal elements of D^2.

(iv) Determination of the square root matrix M in the original basis by using the transformation (16)

$$M = SDS^{-1}. \tag{17}$$

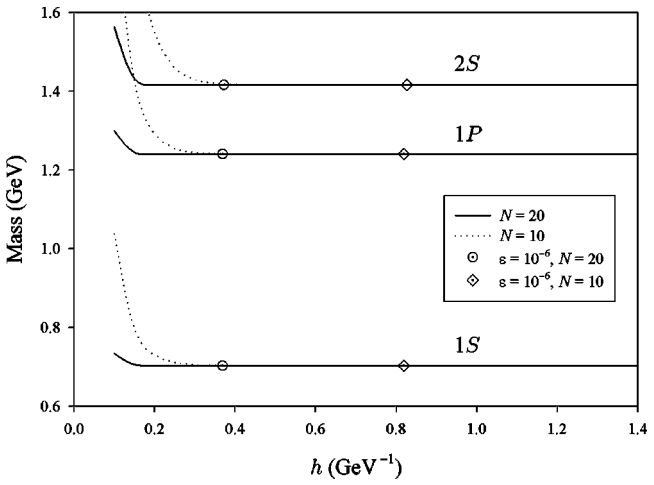

FIG. 1. Masses of the $1S$, $2S$, and $1P$ $u\bar{u}$ mesons, with the semirelativistic model of Ref. [11], as a function of the scale parameter h, for two numbers of mesh points $N=10$ and 20. The values of h predicted by the algorithm described in Sec. III are also indicated for a value of $\epsilon=10^{-6}$.

The elements M_{ij} of the matrix computed with Eq. (17) are approximations of the numbers $\langle f_i|\sqrt{\vec{p}^2+m^2}|f_j\rangle$. The calculation is not exact for two reasons. First, the elements $(M^2)_{ij}$ are computed with approximate formulas (11) and (12). Second, the diagonalization is performed in the limited definition space of the trial function (6). In order to compute exactly the matrix elements of the operator $\sqrt{\vec{p}^2+m^2}$, it is necessary to compute exactly all eigenvalues of the infinite matrix whose elements are $\langle\vec{p}^2+m^2\rangle$, again exactly computed. This is obviously not possible. We shall see in Sec. IV that the procedure proposed here can give very good results.

The kinetic matrix elements being calculated not exactly for the reasons given above, and the potential matrix elements being computed at the Gauss approximation (9), the variational character of the method cannot be guaranteed. This is only possible if an exact quadrature is performed. In practice for a sufficiently high number of basis states, the method is often variational (eigenvalues computed are all upper bounds) or antivariational (eigenvalues computed are all lower bounds). Examples will be given below.

III. SCALE PARAMETER

The accuracy of the eigenvalues and eigenfunctions depends on two parameters: The number of mesh points N and the value of the scale parameter h. The dependence of the eigenvalues on h is illustrated in Fig. 1 for the semirelativistic model of Ref. [11]. This behavior is typical; it is obtained for all states and for all potentials studied here, as well for nonrelativistic as semirelativistic kinematics. When h increases from zero, a rapid decrease of the eigenvalues is first obtained, followed by a long plateau. As the method is not variational, there is no obvious procedure to determine the best value of h. When h is too large, all points of the Lagrange mesh are located in the asymptotic tail of the wave functions and it is then impossible to obtain a good value of the eigenvalue. Fortunately, the plateau is very long and the value of h can be taken in a wide range.

Nevertheless, it could be interesting to have a procedure to estimate directly a good value of h in order to avoid a search, which is always time consuming. We have remarked that the best results are obtained when the mesh covers the main part of the wave function and that the last mesh points are located in its asymptotic tail. So, if we choose a point r_a in the tail of the wave function, the value of h can be obtained by $h=r_a/x_N$, where x_N is the last zero considered.

A value of r_a can be computed using the technique developed in Ref. [8]. The first step is to find a potential $V_\infty(r)$ that matches, at best, the potential $V(r)$ for $r\to\infty$. The second step is to choose a trial state $|\lambda\rangle$ that depends on one parameter λ, taken for instance, as the inverse of a distance. The best matching between the state studied and the trial state is obtained by means of the variational principle. The value of λ is determined by the usual condition

$$\frac{\partial\langle\lambda|T+V_\infty(r)|\lambda\rangle}{\partial\lambda}=0, \tag{18}$$

where T is the kinetic part of the Hamiltonian considered. In the case of the spinless Salpeter equation, the variational solution is computed using the fundamental inequality

$$\langle\sqrt{\vec{p}^2+m^2}\rangle\leqslant\sqrt{\langle\vec{p}^2\rangle+m^2}. \tag{19}$$

The regularized radial part $u_\lambda(r)$ of the trial state $|\lambda\rangle$ is then analyzed to find the value of r_ϵ that satisfies the following condition

$$\frac{u_\lambda(r_\epsilon)}{\max[u_\lambda(r)]}\leqslant\epsilon, \tag{20}$$

where ϵ is a number small enough to neglect the contribution of $u_\lambda(r)$ for values of r greater than r_ϵ. This value of r_ϵ is then taken as the value r_a. Details on this procedure, which is very fast, are given in Ref. [8]. With this method, we have always obtained a value of h within the plateau (see Fig. 1), provided small enough values of ϵ are considered (typically in the range 10^{-4}–10^{-7}). If necessary, the value of h obtained can be a starting point for a new and better determination of the scale parameter.

For a given value of r_a, the accuracy increases with the number of mesh points N. But there is a limit on the values of N that can be used. The points of the mesh are the zeros of the Laguerre polynomial. So it is necessary to compute these zeros with enough precision not to spoil the accuracy of the method. With standard routines [12], up to the 80 first zeros can be calculated with high precision. With specific techniques, this number can reach 120.

It is worth noting that in an usual variational method, like in Ref. [11], the addition of new basis states does not modify the Hamiltonian matrix elements calculated with the smaller basis. The situation is different for the Lagrange mesh method. The N zeros of the polynomial L_N are located between the $N+1$ zeros of the polynomial L_{N+1}. As a consequence, all matrix elements are changed when the number N

TABLE I. Masses of $1S$, $2S$, and $1P$ states, in arbitrary units, for the Kratzer potential with nonrelativistic kinetic energy, and for parameter values: $m=1$, $D=0.5$, and $a=1.5$. The computation is performed with $i\times 10$ basis functions for the Lagrange mesh method and with i Gaussian wave functions. The value of r_a is the one predicted by the algorithm described in Sec. III ($\epsilon=10^{-5}$). The exact results are also given for $i=\infty$.

	$1S$		$2S$		$1P$	
i	Lagrange	Gauss	Lagrange	Gauss	Lagrange	Gauss
r_a	20.32		47.72		47.72	
1	1.7 989 491 271	1.8 090 140 683	1.9 212 831 800		1.8 970 189 881 308	1.9 020 584 965 588
2	1.7 989 357 935	1.8 026 218 788	1.9 212 503 621	1.9 236 462 941	1.8 970 179 601 704	1.8 973 990 442 706
3	1.7 989 353 246	1.7 999 271 967	1.9 212 496 211	1.9 217 084 733	1.8 970 179 570 392	1.8 970 487 465 924
4	1.7 989 351 384	1.7 991 388 244	1.9 212 495 444	1.9 215 316 924	1.8 970 179 569 203	1.8 970 267 073 117
5	1.7 989 351 013	1.7 990 179 046	1.9 212 495 247	1.9 213 213 780	1.8 970 179 568 941	1.8 970 199 788 150
6	1.7 989 350 909	1.7 989 714 114	1.9 212 495 100	1.9 212 845 605	1.8 970 179 568 899	1.8 970 187 892 477
7	1.7 989 350 873	1.7 989 445 797	1.9 212 495 048	1.9 212 595 866	1.8 970 179 568 893	1.8 970 181 291 186
8	1.7 989 350 860	1.7 989 382 512	1.9 212 495 026	1.9 212 525 000	1.8 970 179 568 892	1.8 970 181 007 165
∞	1.7 989 350 844		1.9 212 495 003		1.8 970 179 568 882	

is modified. Moreover, if the value of h is not changed, the value of r_a is modified, and vice versa. Let us recall that $r_a=hx_N$.

IV. NUMERICAL TESTS

We have tested the accuracy of our method with a large number of different potentials (Coulomb-type, finite range, confining, coupled channels, nonlocal interaction, etc.) and with a wide range of particle masses. We shall present here our results for three potentials in the case of two identical particles $m=m_1=m_2$. Only masses of the $1S$, $2S$, and $1P$ states are given. The number of points of the mesh, that is to say, the number of basis states, is limited to 80.

To check our method, we have also compared our results with those obtained with a variational method: The development of the trial state with Gaussian functions [13]. This last method is known to yield very precise results in the two-body and many-body quantum problems. In this paper, each Gaussian function depends on two parameters: its amplitude, which is a linear variational parameter, and its size, which is a nonlinear parameter. The sizes of the various Gaussian functions can be determined stochastically or with an effective formula (arithmetic progression for instance). In this paper, we chose to compute these parameters with a full minimization procedure, in order to obtain the best possible lower bound. But it is very difficult to obtain results with more than eight functions because these functions are not orthogonal and redundancies appear in the size parameters. Let us note that the first radial excitation must be computed with at least two Gaussian functions.

The precision of the Lagrange mesh method is known to be very good for nonrelativistic models [1–3]. Nevertheless, we present here the results obtained for the Kratzer potential ([14] p. 178)

$$V=-2D\left(\frac{a}{r}-\frac{a^2}{2r^2}\right). \tag{21}$$

Supplemented by a nonrelativistic kinetic energy, the binding energies are given by the following analytical formula as a function of the radial quantum number n (0,1, . . .) and the orbital angular momentum ℓ

$$E=-\frac{2\mu a^2D^2}{(n+1/2+\sqrt{2\mu a^2D+(\ell+1/2)^2})^2}. \tag{22}$$

Results for the Kratzer potential with nonrelativistic kinematics are gathered in Table I. For a fixed number of ''basis'' states, the Gaussian method gives better results than the Lagrange mesh method. Nevertheless, the number of Lagrange functions can be easily increased and a very high precision can be reached. In this case, the Lagrange mesh method is variational, but counterexamples exist [10].

We have also tested our method with a semirelativistic model used to describe mesons as quark-antiquark states [11]. The short-range part of the interaction is of Coulomb-type, while the long-range is a confining potential

$$V=-\frac{\kappa}{r}+ar+C, \tag{23}$$

with $\kappa=0.437$, $a=0.203$ GeV^2, and $C=-0.599$ GeV. For the quark u, we have $m=0.150$ GeV. Masses of some $u\bar{u}$ mesons for this model are presented in Table II. No exact result is known, but the masses obtained with the two methods are in good agreement. Because of the redundancy problem with the Gaussian functions, a better convergence can be obtained for the Lagrange mesh method, which is antivariational in this case.

The eigenvalue equation with a semirelativistic Hamiltonian supplemented by a Coulomb-type potential

$$V=-\frac{\kappa}{r} \tag{24}$$

is often called the Herbst's equation (κ is a positive number without dimension). It has been intensively studied, but the

TABLE II. Masses in GeV of $1S$, $2S$, and $1P$ $u\bar{u}$ mesons, with the semirelativistic model of Ref. [11]. The computation is performed with $i\times 10$ basis functions for the Lagrange mesh method and with i Gaussian wave functions. The value of r_a is the one predicted by the algorithm described in Sec. III ($\epsilon=10^{-7}$). The results obtained in Ref. [11] are also given.

	$1S$		$2S$		$1P$	
i	Lagrange	Gauss	Lagrange	Gauss	Lagrange	Gauss
r_a	26.81 $(\mathrm{GeV})^{-1}$		26.74 $(\mathrm{GeV})^{-1}$		26.64 $(\mathrm{GeV})^{-1}$	
1	0.70 237 255	0.73 445 725	1.4 154 184		1.2 402 390 936	1.2 581 207 451
2	0.70 257 022	0.70 812 172	1.4 158 542	1.4 263 285	1.2 402 381 667	1.2 416 398 117
3	0.70 258 437	0.70 403 501	1.4 158 778	1.4 179 611	1.2 402 381 681	1.2 404 159 078
4	0.70 258 719	0.70 304 037	1.4 158 826	1.4 167 156	1.2 402 381 688	1.2 402 686 201
5	0.70 258 805	0.70 274 634	1.4 158 840	1.4 163 172	1.2 402 381 697	1.2 402 444 923
6	0.70 258 839	0.70 264 838	1.4 158 846	1.4 160 095	1.2 402 381 710	1.2 402 396 711
7	0.70 258 854	0.70 261 279	1.4 158 849	1.4 159 263	1.2 402 381 729	1.2 402 386 124
8	0.70 258 863	0.70 259 896	1.4 158 850	1.4 159 018	1.2 402 381 754	1.2 402 383 528
Ref.	0.703		1.416		1.240	

spectra is not known analytically. Nevertheless, approximations are available for some eigenvalues. For the ground state, we have compared our results with a lower bound due to Martin and Roy [15]

$$E_0 \geqslant 2m\sqrt{\frac{1+\sqrt{1-\kappa^2}}{2}} \quad \text{for} \quad \kappa<1, \tag{25}$$

and with an upper bound due to Lucha and Schöberl [16]

$$E_0 \leqslant \min_{\chi}\left\{\left[\frac{128}{15\pi}F\left(-\frac{1}{2},2;\frac{7}{2};1-\frac{m^2}{\chi^2}\right)-\kappa\right]\chi\right\}$$
$$\text{for} \quad \kappa \leqslant \frac{16}{3\pi}, \tag{26}$$

where F is an hypergeometric function [17], and where χ is a minimization parameter. For a vanishing angular momentum, an approximation for all radial quantum numbers is known up to order κ^7 [18]. The precision of all these approximate formulas increases when κ decreases. Results for the Herbst's equation are shown in Tables III and IV for two values of κ. The two methods give similar results and are in agreement with the bounds and approximation available. Again, the Lagrange mesh method is antivariational and allows a better convergence than the Gaussian method.

It is worth noting that with 80 basis states the method proposed here can be several times faster than the Gaussian method with eight functions (by a factor that can reach 100 in some cases). The diagonalization is more time consuming for the Lagrange mesh method, but there is no lengthy determination of nonlinear parameters to perform.

TABLE III. Masses in GeV of $1S$, $2S$, and $1P$ states for Herbst's equation with $m=0.5$ GeV and $\kappa=0.05$. The computation is performed with $i\times 10$ basis functions for the Lagrange mesh method and with i Gaussian wave functions. The value of r_a is the one predicted by the algorithm described in Sec. III ($\epsilon=10^{-6}$). A lower bound (L), an approximation up to order κ^7 (A), and an upper bound (U) are given when they are available (see Sec. IV).

	$1S$		$2S$		$1P$	
i	Lagrange	Gauss	Lagrange	Gauss	Lagrange	Gauss
r_a	1414.63 $(\mathrm{GeV})^{-1}$		3274.43 $(\mathrm{GeV})^{-1}$		3274.43 $(\mathrm{GeV})^{-1}$	
1	0.999 687 256 848	0.999 734 683 111	0.999 921 835 334		0.9 999 218 678 794	0.9 999 292 609 670
2	0.999 687 260 874	0.999 696 226 562	0.999 921 835 623	0.999 926 963 018	0.9 999 218 678 794	0.9 999 229 386 266
3	0.999 687 262 433	0.999 689 200 665	0.999 921 835 944	0.999 922 679 874	0.9 999 218 678 794	0.9 999 220 389 573
4	0.999 687 262 779	0.999 687 740 479	0.999 921 836 103	0.999 922 071 982	0.9 999 218 678 794	0.9 999 219 965 679
5	0.999 687 262 876	0.999 687 397 211	0.999 921 836 163	0.999 922 010 639	0.9 999 218 678 794	0.9 999 218 831 427
6	0.999 687 262 910	0.999 687 365 466	0.999 921 836 186	0.999 921 996 493	0.9 999 218 678 794	0.9 999 218 744 770
7	0.999 687 262 925	0.999 687 320 679	0.999 921 836 196	0.999 921 990 438	0.9 999 218 678 794	0.9 999 218 719 455
8	0.999 687 262 932	0.999 687 286 164	0.999 921 836 200	0.999 921 846 628	0.9 999 218 678 794	0.9 999 218 712 517
L	0.999 687 255 538					
A	0.999 687 262 947		0.999 921 836 208			
U	0.999 687 267 936					

TABLE IV. Same as Table III but with $m=0.5$ GeV and $\kappa=0.5$.

	$1S$		$2S$		$1P$	
i	Lagrange	Gauss	Lagrange	Gauss	Lagrange	Gauss
r_a	137.01 $(\mathrm{GeV})^{-1}$		324.90 $(\mathrm{GeV})^{-1}$		324.90 $(\mathrm{GeV})^{-1}$	
1	0.96 645 459	0.97 287 140	0.99 178 095		0.9 921 160 226 777	0.9 928 911 718 096
2	0.96 653 341	0.96 818 509	0.99 180 940	0.99 252 953	0.9 921 160 108 390	0.9 922 346 609 017
3	0.96 654 234	0.96 703 865	0.99 181 276	0.99 198 052	0.9 921 160 110 896	0.9 921 363 722 236
4	0.96 654 384	0.96 670 985	0.99 181 348	0.99 186 778	0.9 921 160 111 002	0.9 921 199 615 358
5	0.96 654 431	0.96 660 465	0.99 181 372	0.99 183 946	0.9 921 160 111 013	0.9 921 168 705 023
6	0.96 654 450	0.96 656 792	0.99 181 382	0.99 182 810	0.9 921 160 111 014	0.9 921 162 242 900
7	0.96 654 459	0.96 655 426	0.99 181 386	0.99 181 883	0.9 921 160 111 015	0.9 921 161 028 139
8	0.96 654 463	0.96 654 883	0.99 181 389	0.99 181 581	0.9 921 160 111 015	0.9 921 160 815 791
L	0.96 592 583					
A	0.96 664 937		0.99 182 664			
U	0.96 694 460					

V. CONCLUDING REMARKS

In this paper, we have shown that the Lagrange mesh method can be used to solve nonrelativistic and semirelativistic two-body eigenvalue equations. This method is very convenient:

The technique is very easy to implement: It requires only the evaluation of the potential at some grid points and not the calculation of matrix elements in a given basis. The kinetic matrix elements are computed with a standard procedure. The method generates directly the values of the radial part of the wave function at grid points. However, contrary to some other mesh methods, the wave function is also defined between mesh points. Moreover, the extension of the method to the cases of nonlocal interactions or coupled channel equations is trivial.

It is very precise: The accuracy of the solutions depends only on two parameters: The number of grid points and the scale parameter. The eigenvalues are not sensitive to this last factor. Moreover, a very good estimation of this parameter can be easily obtained by using the procedure described above. The number of grid points can be automatically increased until a convergence is reached for the eigenvalues. This number can be as small as 20.

It is very fast: The method involves the use of symmetric real matrices of order N, the number of grid points, which does not exceed 100. The most time-consuming part of the method is the diagonalization of the Hamiltonian matrices. This is not a problem for modern computers. Moreover, several powerful techniques for finding eigenvalues and/or eigenvectors exist and can be used at the best convenience.

This method is very competitive with all other techniques to solve two-body eigenvalue equations.

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