Lagrange-mesh calculations and Fourier transform

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The Lagrange-mesh method is a very accurate procedure for computing eigenvalues and eigenfunctions of a two-body quantum equation written in the configuration space. Using a Gauss quadrature rule, the method only requires the evaluation of the potential at some mesh points. The eigenfunctions are expanded in terms of regularized Lagrange functions, which vanish at all mesh points except one. Using the peculiarities of the method, it is shown that the Fourier transform of the eigenfunctions, computed in the configuration space, can easily be obtained with good accuracy in the physical domain of the momentum space. Also, observables in this space can easily be computed with good accuracy only using matrix elements and eigenfunctions computed in the configuration space.

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I. INTRODUCTION

The Lagrange-mesh method is a very accurate procedure for computing eigenvalues and eigenfunctions of a two-body Schrödinger equation [1–5] as well as a semirelativistic Hamiltonian [6–9]. The trial eigenstates are developed in a basis of well chosen functions, the Lagrange functions. Using their special properties, the potential matrix elements are simply the values of the potential at mesh points if they are computed with a Gauss quadrature. At first sight, this method could look like a discrete variational method, but this is absolutely not the case since the eigenfunctions can be computed at any position. Because of the use of the Gauss quadrature scheme, the method is not variational, but nevertheless, great accuracy can be reached [10]. The method presented here relies on a mesh of points built with the zeros of a Laguerre polynomial, but a general procedure for deriving other Lagrange meshes related to orthogonal or nonorthogonal bases has also been developed [11]. It is worth mentioning that this method can be extended to treat three-body systems very accurately in nuclear physics as well as in atomic physics (see, for instance, Ref. [12]).

At the beginning, this method was developed in the position space. As we see below, the potential matrix elements are very easy to compute if the interaction is known in terms of the distance r between the interacting particles. This is also true for mean values of observables depending on r. For some problems, it can also be useful to compute the eigenfunctions in the momentum space by the Fourier transform as well as observables depending on the relative momentum between the particles. We will show that the Lagrange-mesh method can provide these types of data very efficiently and very easily using the fundamental properties of the Lagrange functions.

The Lagrange-mesh method in configuration space is described in Sec. II, while Sec. III presents some results in momentum space. An ansatz to easily compute the only nonlinear parameter of the method is described in Sec. IV. Test calculations are presented in Sec. V, and some concluding remarks are given in Sec. VI.

II. METHOD IN POSITION SPACE

A. Lagrange functions

The basic ingredients for the Lagrange-mesh method are a mesh of N points x_i associated with an orthonormal set of N indefinitely derivable functions $f_j(x)$ [1–3]. The Lagrange function $f_j(x)$ satisfies the Lagrange conditions,

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

that is to say, it vanishes at all mesh points except one. The x_i and λ_i, respectively, are the abscissas and the weights of a Gauss quadrature formula,

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

As we work with the radial part of the wave functions, we consider the case of the Gauss-Laguerre quadrature because the domain of interest 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 the zeros of a Laguerre polynomial of degree N [1], and the mesh points are given by $L_N(x_i) = 0$. These zeros can be determined with high precision using the usual methods to find the roots of a polynomial [13] (the MATHEMATICA expression Root does the job efficiently) or as the eigenvalues of a particular tridiagonal matrix [14]. The weights can be computed by the following formula [10]:

$$\ln \lambda_i = x_i - \ln x_i + 2 \ln \Gamma(N+1) - \sum_{j\neq i=1}^{N} \ln(x_i - x_j)^2. \tag{3}$$

It is worth noting that, for most calculations, it is not necessary to compute the weights λ_i. The original Lagrange functions do not vanish at the origin, so it is preferable to use the regularized Lagrange functions whose explicit form is given by

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

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which is a polynomial of degree N, multiplied by an exponential function. Such a function $f_i(x)$ vanishes at the origin and at x_j with $j \neq i$.

With the Lagrange-mesh method, the solution of a quantum equation reduces (as is often the case) to the determination of eigensolutions of a given matrix. 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 $V(r)$ is the potential that only depends on the radial coordinate $r = |\vec{r}|$. In the following, we will always work in natural units: $\hbar = c = 1$. A trial state $|\psi\rangle$, an approximation of the genuine eigenstate, is expanded on a basis built with these regularized Lagrange functions,

$$|\psi\rangle = \sum_{j=1}^{N} C_j |f_j\rangle, \quad \text{with} \quad \langle \vec{r}|f_j\rangle = \frac{f_j(r/h)}{\sqrt{h}r} Y_{lm}(\hat{r}), \tag{6}$$

with $\hat{r} = \vec{r}/r$. 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. Contrary to some other mesh methods, the wave function is defined between mesh points by Eqs. (4) and (6).

Basis states $|f_i\rangle$, built with the regularized Lagrange functions, are not exactly orthogonal. But, at the Gauss approximation, we have $\langle f_j|f_i\rangle = \delta_{ji}$. So, in the following, all mean values will be performed using the Gauss quadrature formula (2). In this case, the potential matrix elements are given by

$$\langle f_i|V(r)|f_j\rangle = V(hx_i)\delta_{ij}. \tag{7}$$

The potential matrix is simple to obtain and is diagonal. Let us assume that the matrix elements $\langle f_i|T|f_j\rangle \approx T_{ij}$ are known. Their computation will be explained in the next section. With Eqs. (6) and (7), the variational method applied to Eq. (5) provides a system of N mesh equations,

$$\sum_{j=1}^{N} [T_{ij} + V(hx_i)\delta_{ij} - E\delta_{ij}]C_j = 0. \tag{8}$$

In the Lagrange-mesh method, the Hamiltonian matrix elements are not exactly calculated but are computed at the Gauss approximation. So, the variational character of the method cannot be guaranteed, except 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). It has been observed [1–3] that the accuracy of the mesh approximation remains close to the accuracy of the original variational calculation without the Gauss approximation. So, in most cases, very high accuracy can be achieved in the framework of the Gauss approximation, although the mathematical reasons for the high efficiency of this method are not well known yet [10].

The accuracy of the eigensolutions depends on two parameters: The number of mesh points N and the value of the scale parameter h. For a sufficiently high value of N (which can be as low as 20 or 30), the eigenvalues present a large plateau as a function of h. This is a great advantage for the Lagrange-mesh method since the nonlinear parameter must not be determined with high precision. Nevertheless, if h is too small, a significant part of the wave function is not covered by the points of the Lagrange mesh. When h is too large, all points of the mesh are located in the asymptotic tail of the wave functions, and then, it is impossible to obtain good eigenvalues. So, it is interesting to have a procedure to directly estimate a reasonable 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 last mesh points are located not too far in the asymptotic tail. So, if we choose a point $r_{\max}$ in the tail of the wave function, the value of h can be obtained by $h = r_{\max}/x_N$, where x_N is the last mesh point. A procedure to estimate $r_{\max}$ will be presented in Sec. IV.

B. Kinetic parts

Let us first look at the matrix P whose elements are $P_{ij} = \langle f_i|\vec{p}^{\,2}|f_j\rangle$. With Eq. (2), these matrix elements are given by

$$P_{ij} = \frac{1}{h^2}\left[t_{ij} + \frac{l(l+1)}{x_i^2}\delta_{ij}\right], \tag{9}$$

where l is the orbital angular momentum quantum number and where

$$t_{ij} = \int_0^\infty f_i(x)\left(-\frac{d^2}{dx^2}\right) f_j(x)dx \approx -\lambda_i^{1/2} f_j''(x_i). \tag{10}$$

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 the Appendix in Ref. [2]). However, as shown in Ref. [3], it is preferable to use the approximations (9) and (10). Then, the kinetic matrix elements are even easier to obtain and are [3]

$$t_{ij} = \begin{cases} (-)^{i-j}(x_i x_j)^{-1/2}(x_i + x_j)(x_i - x_j)^{-2} & (i \neq j), \\ \left(12x_i^2\right)^{-1}\left[4 + (4N+2)x_i - x_i^2\right] & (i = j). \end{cases} \tag{11}$$

For a nonrelativistic Hamiltonian, $T_{ij} = \frac{1}{2\mu}P_{ij}$, where μ is the reduced mass of the system. For a more general operator $T(\vec{p}^{\,2})$, as the kinetic part of a spinless Salpeter equation $2\sqrt{\vec{p}^{\,2} + m^2}$, the calculation is much more involved. The idea is to use the four-step method suggested in Ref. [15] (see also references therein) and applied in Ref. [6]:

(1) Computation of the matrix P whose elements are $P_{ij} = \langle f_i|\vec{p}^{\,2}|f_j\rangle$, given by Eqs. (9)–(11).

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

$$P = SP^DS^{-1}, \tag{12}$$

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

(3) Computation of T^D, a diagonal matrix obtained by taking the function $T(x)$ of all diagonal elements of P^D [for instance, $T(x) = 2\sqrt{x + m^2}$ for the case of a spinless Salpeter equation].

(4) Determination of the kinetic matrix T in the original basis by using the transformation (12),

$$T = ST^DS^{-1}. \tag{13}$$

The elements T_{ij} of the matrix computed with Eq. (13) are approximations of the numbers $\langle f_i|T(\vec{p}^{\,2})|f_j\rangle$. The calculation is not exact for two reasons. First, the elements T_{ij} are computed with approximate formulas (9)–(11). Second, the diagonalization is performed in the limited definition space of the trial function (6). In order to exactly compute the matrix elements of the operator $T(\vec{p}^{\,2})$, it is necessary to exactly compute all eigenvalues of the infinite matrix whose elements are $\langle T(\vec{p}^{\,2})\rangle$, again exactly computed. This is obviously not possible. In Ref. [6], it has been shown that this four-step procedure can give very good results.

C. Mean values of radial observables

The mean value of the operator $U(r)$ for a trial state $|\psi\rangle$ is given by

$$\langle\psi|U(r)|\psi\rangle = \sum_{i,j=1}^{N} C_i C_j \langle f_i|U(r)|f_j\rangle. \tag{14}$$

Using the Lagrange condition (1) and the Gauss quadrature (2), this integral reduces to

$$\langle\psi|U(r)|\psi\rangle = \sum_{j=1}^{N} C_j^2 U(hx_j). \tag{15}$$

If U is the identity, we recover the normalization condition as expected. Very high accuracy can be obtained with this simple procedure [5,12].

III. METHOD IN MOMENTUM SPACE

A. Fourier transform

For some particular problems, it can be useful to compute the Fourier transform of a wave function in the position space in order to obtain the corresponding wave function in the momentum space. The Fourier transform $\phi^{\rm FT}(\vec{p}\,)$ of a wave function $\phi(\vec{r}\,)$ is defined by

$$\phi^{\rm FT}(\vec{p}\,) = \frac{1}{(2\pi)^{3/2}} \int \phi(\vec{r}) e^{-i\vec{p}\cdot\vec{r}}\, d\vec{r}. \tag{16}$$

Using the spherical representation of the wave function,

$$\phi(\vec{r}\,) = R_{nl}(r)\, Y_{lm}(\hat{r}), \tag{17}$$

and using the spherical expansion of the function $e^{-i\vec{p}\cdot\vec{r}}$ [16], it can be shown that

$$\phi^{\rm FT}(\vec{p}\,) = R_{nl}^{\rm FT}(p)\tilde{Y}_{lm}(\hat{p}), \tag{18}$$

where $p = |\vec{p}|$ and $\hat{p} = \vec{p}/p$, and where

$$R_{nl}^{\rm FT}(p) = (-1)^l \sqrt{\frac{2}{\pi}} \int_0^\infty R_{nl}(r)\, j_l(pr) r^2 dr, \tag{19}$$

$$\tilde{Y}_{lm}(\hat{p}) = i^l Y_{lm}(\hat{p}). \tag{20}$$

$j_l(x)$ is a spherical Bessel function [17], and $\tilde{Y}_{lm}(\hat{x})$ is called a modified spherical harmonic [16].

Using expansion (6), the radial part $R(r)$ of the trial function is given by

$$R(r) = \sum_{j=1}^{N} C_j \frac{f_j(r/h)}{\sqrt{h}r}. \tag{21}$$

The Fourier transform $R^{\rm FT}(p)$ of this radial function is defined by Eq. (19). It is tempting to use the Gauss quadrature rule (2) with the Lagrange condition (1) to perform this calculation. The problem is that spherical Bessel functions are rapidly oscillating functions. Then, it is not obvious that such a procedure could work. Actually, we have checked that the Fourier transform of a unique regularized Lagrange function, which is also a rapidly oscillating function, cannot be obtained in this way with good accuracy. Fortunately, the radial part of a wave function has a much smoother behavior. As we will see, with several examples in Sec. V, its Fourier transform can easily be obtained in the framework of the Lagrange-mesh method by taking benefit of the very special properties of the regularized Lagrange function. Using Eq. (2) with Eq. (1), the integral (19) for a given eigenfunction (21) simply reduces to

$$\bar{R}^{\rm FT}(p) = (-1)^l \sqrt{\frac{2}{\pi}} h^{3/2} \sum_{i=1}^{N} C_i \sqrt{\lambda_i} x_i\, j_l(hx_i p), \tag{22}$$

where we use the bar to indicate that this is not the exact Fourier transform $R^{\rm FT}(p)$. For a sufficiently high value of N (which can be as low as 50), $\bar{R}^{\rm FT}(p)\tilde{Y}_{lm}(\hat{p})$ can be a very good approximation of the genuine eigenstate in the momentum space for values of $p \in [0, p_{\max}]$, where $p_{\max}$ can be determined with the procedure used to compute $r_{\max}$ (see Sec. IV). For values of $p \gtrsim p_{\max}$, $\bar{R}^{\rm FT}(p)$ can present large unphysical rapid oscillations. These oscillations do not develop in $R(r)$ because they are killed by the rapid decrease in the regularized Lagrange functions. Let us note that, in order to take benefit of the Lagrange condition (1) and to obtain the simple expression (22), the mesh used to compute the integral (19) must be the same as the mesh used to solve the eigenvalue equation (8).

B. Mean values of momentum-dependent observables

The mean value of the operator $K(p)$ for a trial state $|\psi\rangle$ is given by

$$\langle\psi|K(p)|\psi\rangle = \int_0^\infty K(p)[R^{\rm FT}(p)]^2 p^2 dp, \tag{23}$$

where the angular part is already integrated. In this formula, the function $R^{\rm FT}(p)$ can be replaced by $\bar{R}^{\rm FT}(p)$. Good results can sometimes be obtained, but accuracy cannot always be guaranteed. This is the case when the observable grows rapidly with p and needs very good quality for the asymptotic tail of the wave function in the momentum space. Actually, it is easier and much more efficient to directly compute

$$\langle\psi|K(p)|\psi\rangle = \sum_{i,j=1}^{N} C_i C_j \langle f_i|K(p)|f_j\rangle. \tag{24}$$

The matrix elements $\langle f_i|K(p)|f_j\rangle$ can be determined by a procedure identical to the one used to compute $\langle f_i|T(\vec{p}^{\,2})|f_j\rangle$. An intermediate step is the calculation of the matrix K^D, a diagonal matrix obtained by taking the function $K(\sqrt{x})$ of all diagonal elements of P^D (remember that P is linked to the matrix elements of $\vec{p}^{\,2}$, not p). The numbers $\langle f_i|K(p)|f_j\rangle$ are well approximated by the elements of the matrix K obtained by using the transformation (12): $K = SK^DS^{-1}$. As we see

below, very good accuracy can be reached for the mean values $\langle K(p)\rangle$.

IV. SCALE PARAMETER

An estimation of $r_{\max}$ can be computed using the technique developed in Ref. [18]. The first step is to find a potential $V_\infty(r)$, which matches, at best, the potential $V(r)$ for $r \to \infty$. Three cases are considered in Ref. [18]:

(1) $\kappa\, r^p$ with $\kappa > 0$ and $p > 0$;
(2) $-\kappa/r^p$ with $\kappa > 0$ and $0 < p \leqslant 1$;
(3) a square well.

The second step is to choose a trial state $|\lambda\rangle$, which depends on one parameter λ, taken as the inverse of a distance. Two cases are considered in Ref. [18]: $u_\lambda(r) \propto r^{l+1}e^{-\lambda^2 r^2/2}$ (harmonic oscillator state) for $V_\infty(r) = \kappa r^p$; $u_\lambda(r) \propto r^{l+1}e^{-\lambda r}$ (hydrogenlike state) for $V_\infty(r) = -\kappa/r^p$ or a square well. If the quantum number n is not zero, an effective value of l is used: $l \to 2n + l$ if $u_\lambda(r)$ is a harmonic oscillator state; $l \to n + l$ if $u_\lambda(r)$ is a hydrogenlike state (see Ref. [18]). In a third step, the optimal value of λ is determined by the variational condition

$$\frac{\partial}{\partial\lambda}\langle\lambda|T + V_\infty(r)|\lambda\rangle = 0, \tag{25}$$

where T is the kinetic part of the Hamiltonian considered. In the case of the complicated T function, the following approximation can be used:

$$\langle T(\vec{p}^{\,2})\rangle \to T(\langle\vec{p}^{\,2}\rangle). \tag{26}$$

In particular, we have

$$\langle\sqrt{\vec{p}^{\,2} + m^2}\rangle \leqslant \sqrt{\langle\vec{p}^{\,2}\rangle + m^2}. \tag{27}$$

Various expressions for the optimal parameter λ are given in Ref. [18].

By introducing the dimensionless variable $s = \lambda r$, the regularized radial part $u_\lambda(s)$ of the trial state $|\lambda\rangle$ is then analyzed to find the value of s_ϵ that satisfies the following condition:

$$\frac{u_\lambda(s_\epsilon)}{\max\limits_{s\in[0,\infty]}[u_\lambda(s)]} = \epsilon, \tag{28}$$

where ϵ (typically in the range of 10^{-4}–10^{-8}) is a number small enough to neglect the contribution of $u_\lambda(s)$ for values of s greater than s_ϵ. This is the last step of the procedure, which is very fast, and the details of which are given in Ref. [18]. The dimensionless quantity s_ϵ is the solution of the transcendental equation (36) in Ref. [18] (x_N is replaced here by s_ϵ in order to match the present notations and to avoid confusion with the last Lagrange-mesh point). Note that this equation has an analytical solution given by

$$s_\epsilon = \left[-(l+1)W_{-1}\left(-\frac{\epsilon^{m/(l+1)}}{e}\right)\right]^{1/m}, \tag{29}$$

where W_{-1} is the Lambert function [19] and $m = 1$ or 2 depending on the trial function $u_\lambda(r)$.

At this stage, the ratio s_ϵ/λ approximately corresponds to a radial distance in the asymptotic tail of an eigenstate of the Hamiltonian $T + V_\infty(r)$. The idea is to identify this distance with the value of $r_{\max}$ for the genuine Hamiltonian considered. In Ref. [6], it has been shown that this procedure works quite well and can give a value of the scale parameter h ($h = r_{\max}/x_N$) in the plateau mentioned above. The efficiency of this ansatz is due to the fact that the value of h need not be known with great accuracy in the Lagrange-mesh method. So, a crude determination of $r_{\max}$ is sufficient, and it is not necessary to go beyond the use of the very simple trial functions $u_\lambda(r)$ mentioned above and the approximation (26) for the computation of the kinetic contribution.

To determine an estimation of $p_{\max}$, let us look at the Fourier transform $u_\lambda^{\rm FT}(s = p/\lambda)$ of the trial states considered $u_\lambda(s = \lambda r)$, where s is a dimensionless variable,

$$u_\lambda(s) \propto s^{l+1}e^{-s^2/2} \quad\Rightarrow\quad u_\lambda^{\rm FT}(s) \propto s^{l+1}e^{-s^2/2}, \tag{30}$$

$$u_\lambda(s) \propto s^{l+1}e^{-s} \quad\Rightarrow\quad u_\lambda^{\rm FT}(s) \propto \frac{s^{l+1}}{(s^2+1)^{l+2}}. \tag{31}$$

If $u_\lambda(s)$ is a harmonic oscillator state, $u_\lambda^{\rm FT}(s)$ has the same form. So it seems quite natural to set $p_{\max} = \lambda s_\epsilon$, since both functions present the same ratio (28) at the same value of their dimensionless argument. If the trial state is a hydrogenlike state, the situation is different since $u_\lambda^{\rm FT}(s)$ decreases much faster than $u_\lambda(s)$ for large (but not too large) values of s. Nevertheless, the simple choice $p_{\max} = \lambda s_\epsilon$ works quite well also, as shown below. So, finally, we have

$$r_{\max} = s_\epsilon/\lambda \quad\text{and}\quad p_{\max} = \lambda s_\epsilon, \tag{32}$$

with s_ϵ and λ determined by the procedure described above.

V. NUMERICAL TESTS

In this section, several tests will be performed for the Lagrange-mesh method with both nonrelativistic and semirelativistic kinematics. We will focus on the quality of wave functions and observables in the momentum space since the efficiency of the method in the position space has already been demonstrated elsewhere [1–9]. In order to estimate the quality of the Fourier transform (22) more precisely, we define a quality factor $Q(p_*)$,

$$Q(p_*) = \max_{p\in[0,p_*]}\left|\frac{\bar{u}^{\rm FT}(p) - u^{\rm FT}(p)}{\max\limits_{p\in[0,p_*]}|u^{\rm FT}(p)|}\right|, \tag{33}$$

where $\bar{u}^{\rm FT}(p)/p = \bar{R}_{nl}^{\rm FT}(p)$ given by Eq. (22) and $u^{\rm FT}(p)/p = R^{\rm FT}(p)$ is the exact solution in momentum space (p_* is not necessarily identical to $p_{\max}$). For the two simple cases considered here, $V_\infty(r) = V(r)$.

A. Confining semirelativistic Hamiltonian

Let us consider the ultrarelativistic two-body system with a quadratic potential,

$$H = 2\sqrt{\vec{p}^{\,2}} + ar^2. \tag{34}$$

This Hamiltonian is particularly interesting because it is probably the only one with a semirelativistic kinematics, which is (partly) analytically solvable. With an appropriate change in variable, this Hamiltonian can be recast into the form of a nonrelativistic Hamiltonian with a linear interaction [20], for

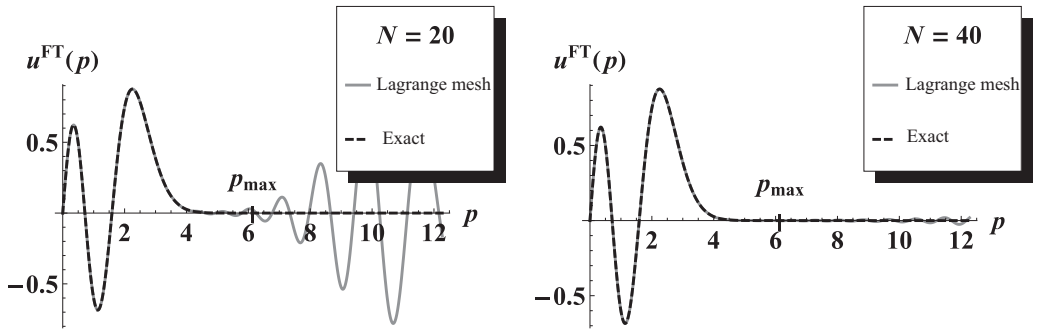

FIG. 1. The exact solution (36) with $a = 0.25$ for $n = 2$ is compared with the corresponding approximation given by formula (22) for $0 \leqslant p \leqslant 2p_{max}$. The values of $r_{max} = 8.76$ and $p_{max} = 6.13$ are determined with the procedure presented in Sec. IV with $\epsilon = 10^{-8}$.

which solutions are known for the S states. The eigenvalues for $l = 0$ are given by

$$E_{n0} = (4a)^{1/3}|\alpha_n|, \tag{35}$$

where α_n is the $(n+1)$th zero of the Airy function (Ai) [17]. The corresponding regularized eigenfunctions are obtained directly in the momentum space [21],

$$u^{FT}_{n0}(p) = pR_{n0}(p) = \frac{1}{\mathrm{Ai}'(\alpha_n)}\left(\frac{2}{a}\right)^{1/6}\mathrm{Ai}\left[\left(\frac{2}{a}\right)^{1/3}p + \alpha_n\right]. \tag{36}$$

Let us note that $\int_{\alpha_n}^{\infty}\mathrm{Ai}^2(s)ds = \mathrm{Ai}'^2(\alpha_n)$, where Ai′ is the derivative of Ai. Using the generalized virial theorem [22], it can be shown that $\langle n0|\sqrt{\vec{p}^{\,2}}|n0\rangle = \langle n0|ar^2|n0\rangle$ where $|n0\rangle$ is an S eigenstate. Moreover, all powers of p can be computed exactly [23]. So, we have

$$\langle n0|\sqrt{\vec{p}^{\,2}}|n0\rangle = \frac{E_{n0}}{3}, \tag{37}$$

$$\langle n0|\vec{p}^{\,4}|n0\rangle = \left(\frac{a}{2}\right)^{4/3}\frac{16}{315}(8|\alpha_n|^4 + 25|\alpha_n|). \tag{38}$$

The only energy scale of the problem is given by $a^{1/3}$. So, all physical quantities considered are given in powers of the unit chosen for $a^{1/3}$. For instance, all results are given in powers of GeV in hadronic problems for which a is given in GeV^3. To perform the following calculations, we have set $a = 0.25$. Using the Lagrange-mesh method with $N = 10$ and $\epsilon = 10^{-4}$, the eigenvalues (35) can already be obtained with a relative error smaller than 1%. But, to obtain a good Fourier transform of the wave function, it is necessary to use more points. As we can see in Fig. 1, the agreement can be very good for the main part of $u^{FT}(p)$. With $N = 20$, unphysical oscillations appear just before p_{max}. With $N = 40$, they develop halfway between p_{max} and $2p_{max}$. With $N = 80$ (not presented here), the asymptotic behavior is correct until $2p_{max}$. In these three cases, for which $\epsilon = 10^{-8}$, we have $Q(p_{max}) = 0.034, 0.0042, 0.0052$, respectively. The quality factor first decreases rapidly due to the improvement in the wave function for large values of p and then stabilizes because the quality of the wave function stays constant in the low-p part. It is possible to improve the quality factor by decreasing the value of ϵ (increasing the value of p_{max}). For $N = 40$, the value of $Q(p_{max})$ decreases from 0.015 to 0.0020 when ϵ varies from 10^{-4} to 10^{-12}.

Some observables for the particular eigenstate $l = 0$ and $n = 2$ computed with formula (24) are presented in Table I and are compared with the exact values. Similar results are obtained for other eigenstates. Very good accuracy can be obtained with quite a small number of points. Actually, it appears that the precision does not automatically increase with N. On the contrary, for a given value of ϵ, the accuracy is optimal for a given number of points. This behavior is typical of semirelativistic Hamiltonians. This is due to the computation

TABLE I. Some observables with $a = 0.25$ for the eigenstate $l = 0$ and $n = 2$ computed with formula (24) and compared with the exact values. Results are given in powers of the unit for $a^{1/3}$.

		$\langle\sqrt{\vec{p}^{\,2}}\rangle$	$\langle\vec{p}^{\,4}\rangle$	$\langle\exp(-\vec{p}^{\,2}/a^{2/3})\rangle$
Exact		1.840 19[a]	24.0273[b]	0.109 740[c]
$\epsilon = 10^{-6}$	$N = 10$	1.841 98	23.6260	0.108 562
	20	1.842 65	24.0735	0.109 299
	40	1.843 99	24.0982	0.108 892
$\epsilon = 10^{-8}$	$N = 10$	1.819 01	23.6006	0.112 181
	20	1.841 63	24.0545	0.109 512
	40	1.842 36	24.0680	0.109 359

[a]Computed with Eq. (37).
[b]Computed with Eq. (38).
[c]Computed with the quadrature using Eq. (36).

TABLE II. Some observables for the hydrogen atom eigenstate $l = 1$ and $n = 1$ computed with formula (24) and compared with the exact values. Results are given in powers of keV.

		$\langle\vec{p}^{\,2}\rangle$	$\langle\vec{p}^{\,4}\rangle$	$\langle\exp(-p/\eta)\rangle$
Exact		1.544 14[a]	11.9218[b]	0.786 997[c]
$\epsilon = 10^{-6}$	$N = 10$	1.544 17	11.9225	0.787 043
	20	1.544 14	11.9218	0.786 995
	40	1.544 14	11.9218	0.786 994
$\epsilon = 10^{-8}$	$N = 10$	1.547 11	11.9471	0.787 255
	20	1.544 14	11.9218	0.786 997
	40	1.544 14	11.9218	0.786 997

[a]Computed with Eq. (39).
[b]Computed with Eq. (40).
[c]Computed with the quadrature of the numerical Fourier transform of the wave function in position space.

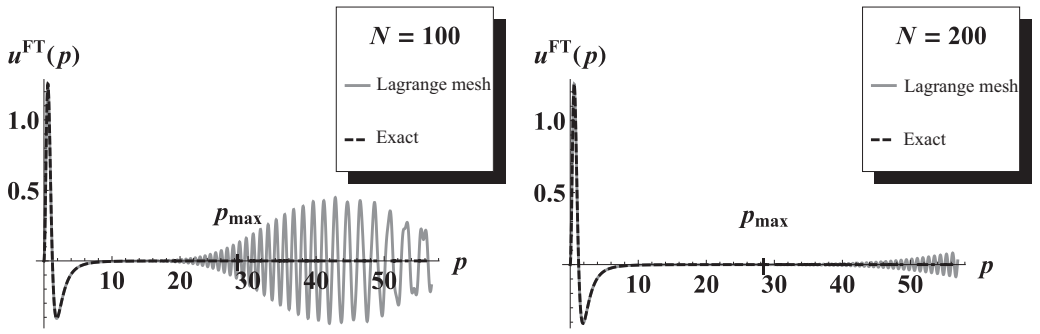

FIG. 2. The accurate numerically computed (exact) Fourier transform of the hydrogen atom wave function for $l = 1$ and $n = 1$ is compared with the corresponding approximation given by formula (22) for $0 \leqslant p \leqslant 2p_{max}$. The values of $r_{max} = 18.44$ and $p_{max} = 28.48$ are determined with the procedure presented in Sec. IV with $\epsilon = 10^{-6}$.

of the kinetic part, which requires a supplementary approximation to the use of the Gauss quadrature rule (see Sec. II B). Our experience is that an optimal value for an observable can be found by looking at extrema or plateaus in the behavior of this observable as a function of N for a given value of ϵ. In the next section, in an example, we will see that the accuracy increases with N for a nonrelativistic system.

B. Hydrogen atom Hamiltonian

Now, we consider a completely different case, the hydrogen atom: The kinematics is nonrelativistic, and the Coulomb potential $-\alpha/r$ is nonconfining. The eigensolutions in the position space are well known, and their Fourier transforms can be expressed in terms of the Appell hypergeometric function F_2 [24]. As these special functions are difficult and lengthy to accurately obtain, it is more convenient to work with numerically computed eigensolutions in momentum space. Particular momentum-dependent observables can exactly be computed [23] as

$$\langle \vec{p}^{\,2} \rangle = \frac{\eta^2}{(n+l+1)^2}, \tag{39}$$

$$\langle \vec{p}^{\,4} \rangle = \eta^4 \frac{8n+2l+5}{(2l+1)(n+l+1)^4}, \tag{40}$$

where $\eta = \mu\alpha$, with μ as the reduced mass.

To perform the following calculations, we have set $m_1 = 940$ MeV, $m_2 = 511$ KeV, and $\alpha = 1/137$. The units of the results are given in powers of keV. Some observables for the particular eigenstate $l = 1$ and $n = 1$, computed with formula (24), are presented in Table II and are compared with the exact values. Similar results are obtained for other eigenstates. Again, very good accuracy can be obtained with quite a small number of points. This time, the accuracy always increases with N for a given value of ϵ, as already found in previous papers [2,10].

Although good accuracy can be obtained with quite a small number of mesh points for the eigenvalues, the eigenfunctions in configuration space, and some momentum-dependent observables, it is necessary to use many more points to obtain a good Fourier transform of a wave function in the physical momentum domain. For instance, a relative error as small as 10^{-6} can be reached for the lowest eigenvalues with only $N = 10$. But, as can be seen in Fig. 2, the situation is very different for the Fourier transform. With $N = 100$, unphysical oscillations appear before p_{max}. With $N = 200$, they develop halfway between p_{max} and $2p_{max}$. For $\epsilon = 10^{-6}$, we have $Q(p_{max}) = 0.504, 0.097, 0.000\,28$, respectively, for $N = 50, 100, 200$. Nevertheless, the quality factor $Q(p_*)$ can be as small as 10^{-6} if p_* is in the main part of the wave function. It is also possible to improve the quality factor by decreasing the value of ϵ (increasing the value of p_{max}). In several examples, we have checked that the necessity to use a large number of mesh points to compute a good Fourier transform of the wave function is common for potentials that present a singularity at the origin as $-1/r$ or $\ln r$.

VI. CONCLUDING REMARKS

The Lagrange-mesh method is a procedure for computing eigenvalues and eigenfunctions of quantum equations. It is very simple to implement and can yield very accurate results for many observables, especially for nonrelativistic kinematics. At the origin, the method was developed in the position space since the evaluation of potential matrix elements only requires the computation of the interaction at some mesh points. This is due to the use of a Gauss quadrature rule with the fact that the basis functions satisfy the Lagrange conditions, that is to say, they vanish at all mesh points except one. Using this very special property, we have shown that the computation of the wave function in the momentum space by the Fourier transform of the wave function in the configuration space can easily be performed with very good accuracy, although it seems necessary to use a larger number of mesh points for potentials that present a singularity at the origin. Moreover, mean values of momentum-dependent operators can also easily and accurately be calculated using a technique similar to the one used to compute the semirelativistic kinetic matrix elements. Again, this shows the great efficiency of the Lagrange-mesh method, which can yield very accurate results for a minimal computational effort.

If the interaction considered is only known as a function of the relative momentum, it could be interesting to work directly in the momentum space. In this case, the eigenvalue equation appears as an integral equation in this space. The Lagrange-mesh method could then be applied by considering

a mesh of points to discretize the module of the relative momentum and by computing the integrals with the associated Gauss quadrature rule. This problem will be addressed in a subsequent paper.

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