Lagrange-mesh calculations and Fourier transform

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The Lagrange-mesh method is a very accurate procedure to compute eigenvalues and eigenfunctions of a two-body quantum equation. The method requires only the evaluation of the potential at some mesh points in the configuration space. It is shown that the eigenfunctions can be easily computed in the momentum space by a Fourier transform using the properties of the basis functions. Observables in this space can also be easily obtained.

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I. INTRODUCTION

The Lagrange-mesh method is a very accurate procedure to compute 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 a great accuracy can nevertheless 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 non-orthogonal bases has also been developed [11]. Even if we only focus on two-body systems in this paper, it is worth mentioning that 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. [12]).

At the beginning, this method was developed in the position space. As we will 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 be also 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 type of data very efficiently and very easily, using the fundamental properties of the Lagrange functions.

The Lagrange-mesh methods in configuration space is described in Sec. II, while Sec. III presents some results in momentum space. An ansatz to compute easily the only non-linear 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 are respectively the abscissae and the weights of a Gauss quadrature formula

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

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As we work with the radial part of wavefunctions, 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 a high precision with 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 origin, so it is preferable to use the regularized Lagrange functions whose explicit form is given by

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

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 it is often the case) to the determination of eigensolutions of a given matrix. Let us consider the eigenvalue equation

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

where $T(\vec{p}^{\,2})$ is the kinetic energy term of the Hamiltonian and $V(r)$ the potential which depends only on the radial coordinate $r = |\vec{r}|$. In the following, we will always work in natural units: $\hbar = c = 1$. A trial state $|\psi\rangle$, 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 non-linear parameter aimed at adjusting the mesh to the domain of physical interest. Contrary to some other mesh methods, the wavefunction is also defined between mesh points by (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

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

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. Their computation will be explained in the next section. With (6) and (7), the variational method applied to (5) provides a system of N mesh equations

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

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, a very high accuracy can be achieved in the framework of the Gauss approximation, though 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 non-linear parameter must not be determined with a high precision. Nevertheless, if h is too small, a significant part of the wavefunction

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 wavefunctions and it is then impossible to obtain good eigenvalues. So, it is interesting to have a procedure to estimate directly 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 wavefunction, 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 (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 appendix in Ref. [2]). However, as shown in Ref. [3], it is preferable to use the approximation (9)-(10). The kinetic matrix elements are then even easier to obtain and read [3]

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

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 a 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 (9)-(11).
2. Diagonalization of the matrix P. If P^D is the diagonal matrix formed by the eigenvalues of P, we have
$$P = S\, P^D\, S^{-1}, \tag{12}$$
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)
$$T = S\, T^D\, S^{-1}. \tag{13}$$

The elements T_{ij} of the matrix computed with (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 an approximate formula (9)-(11). 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 $T(\vec{p}^2)$, it is necessary to compute exactly all eigenvalues of the infinite matrix whose elements are $\langle T(\vec{p}^2)\rangle$, again exactly computed. This is obviously not possible. It has been shown in Ref. [6], 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. A 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 wavefunction in the position space in order to obtain the corresponding wavefunction in the momentum space. The Fourier transform $\phi^{\rm FT}(\vec{p})$ of a wavefunction $\phi(\vec{r})$ is defined by

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

Using the spherical representation of the wavefunction

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

and using the spherical expansion of the function $e^{-i\vec{p}.\vec{r}}$ [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

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

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

$j_l(x)$ 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 (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. It is then 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 a good accuracy. Fortunately, the radial part of a wavefunction has a much smoother behavior. As we will see on several examples in Sec. V, its Fourier transform can be easily obtained in the framework of the Lagrange-mesh method by taking benefit of the very special properties of the regularized Lagrange function. Using (2) with (1), the integral (19) simply reduces to

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

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 $p \in [0, p_{\rm max}]$, where $p_{\rm max}$ can be determined with the procedure used to compute $r_{\rm max}$ (see Sec. IV). For values of $p \gtrsim p_{\rm max}$, $\bar{R}^{\rm FT}(p)$ can present large unphysical rapid oscillations. These oscillations do not develop in $R(r)$, because they are killed by the rapid decreasing of the regularized Lagrange functions.

B. Mean values of momentum dependent observables

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

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

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 the accuracy cannot be always guaranteed. This is the case when the observable grows rapidly with p and needs a very good quality of the asymptotic tail of the wavefunction in the momentum space. Actually, it is easier and much more efficient to compute directly

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

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): $K = S\,K^D\,S^{-1}$. As we will see below, a very good accuracy can be reached for the mean values $\langle K(p)\rangle$.

IV. SCALE PARAMETER

An estimation of $r_{\rm max}$ 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]:

- $\kappa\,r^p$ with $\kappa > 0$ and $p > 0$;
- $-\kappa/r^p$ with $\kappa > 0$ and $0 < p \leq 1$;
- 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) and $u_\lambda(r) \propto r^{l+1}\,e^{-\lambda\,r}$ (hydrogen-like state), depending on $V_\infty(r)$. If the quantum number n is not zero, an effective value of l is used (see Ref. [18]). In a third step, the optimal value of λ is determined by the usual 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 complicated T function, the following approximation can be used

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

In particular, we have

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

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

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 which satisfies the following condition

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

where ϵ (typically in the range 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 whose details are given in Ref. [18].

Note that equation (36) in Ref. [18] has an analytical solution given by (x_N is replaced here by s_ϵ in order to match the present notations and to avoid a confusion with the last Lagrange-mesh point)

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

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 corresponds approximately 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. It has been shown in Ref. [6] 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 must not be known with a 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 $u_\lambda(s = \lambda\, r)$:

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

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

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 hydrogen-like state, the situation is different since $u_\lambda^{\rm FT}(s)$ decreases much more 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 it will be 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 wavefunctions 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 more precisely the quality of the Fourier transform (22), we define a "quality factor" $Q(p_*)$

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

where $\bar{u}^{\rm FT}(p)/p = \bar{R}_{nl}^{\rm FT}(p)$ given by (22) and $u^{\rm FT}(p)/p = R^{\rm FT}(p)$ is the exact solution in momentum space.

A. Confining semirelativistic Hamiltonian

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

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

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 of variable, this Hamiltonian can be recast into the form of a nonrelativistic Hamiltonian with a linear interaction [20], for which solutions are known for 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]

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

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

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

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

To perform the following calculations, we have set $a = 0.25$. The units of the results are given in powers of the unit chosen for the only energy scale of the system $a^{1/3}$. 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 wavefunction, it is necessary to use more points. As we can see on Fig. 1, the agreement can be very good for the main part of $u^{\mathrm{FT}}(p)$. 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 till $2p_{\max}$. In these 3 cases, for which $\epsilon = 10^{-8}$, we have respectively $Q(p_{\max}) = 0.034$, 0.0042, 0.0052. The quality factor first decreases rapidly due to the improvement of the wavefunction for large values of p, and then stabilizes because the quality of the wavefunction 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}.

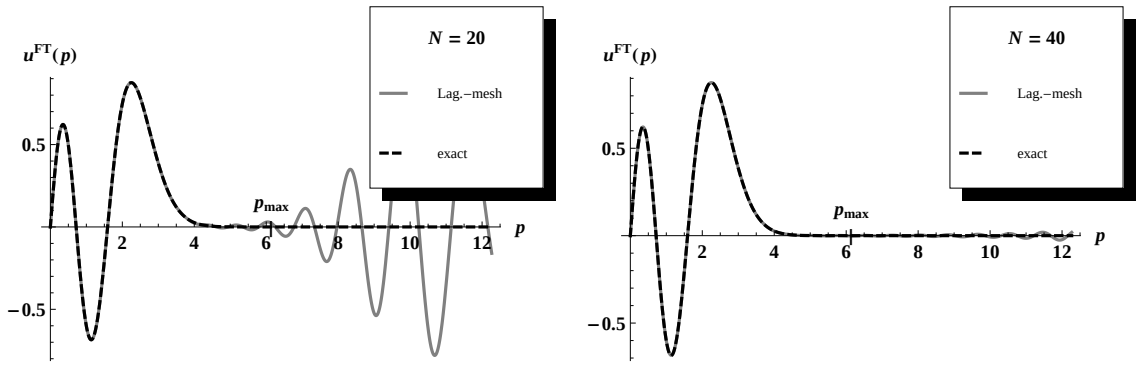

FIG. 1: The exact solution (36) with $a = 0.25$ for $n = 2$ is compared with the corresponding approximation given by formula (22) for $0 \le p \le 2p_{\max}$. The value of $p_{\max}$ is determined with the procedure presented in Sec. IV with $\epsilon = 10^{-8}$.

Some observables for a particular eigenstate, $l = 0$ and $n = 2$, computed with formula (24) are presented in Table I and compared with the exact values. Similar results are obtained for other eigenstates. A very good accuracy can be obtained with a quite small number of points. Actually, it appears that the precision does not automatically increases 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 of the kinetic part which requires a supplementary approximation than 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 plateau in the behavior of this observable as a function of N for a given value of ϵ. In the next section, we will see on an example that accuracy increases with N for a nonrelativistic system.

B. Hydrogen atom Hamiltonian

We consider now a completely different case, the hydrogen atom: the kinematics is nonrelativistic and the Coulomb potential, $-\alpha/r$, is non-confining. The eigensolutions in the position space are well known and their Fourier transform

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 $a^{1/3}$.

		$\left\langle \sqrt{\vec{p}^2} \right\rangle$	$\langle \vec{p}^4 \rangle$	$\left\langle \exp(-\vec{p}^2/a^{2/3}) \right\rangle$
Exact		1.84019[(a)]	24.0273[(b)]	0.109740[(c)]
$\epsilon = 10^{-6}$	$N = 10$	1.84198	23.6260	0.108562
	20	1.84265	24.0735	0.109299
	40	1.84399	24.0982	0.108892
$\epsilon = 10^{-8}$	$N = 10$	1.81901	23.6006	0.112181
	20	1.84163	24.0545	0.109512
	40	1.84236	24.0680	0.109359

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

can be expressed in term of the Appell Hypergeometric function F_2 [24]. As these special functions are difficult and lengthy to obtain accurately, it is more convenient to work with numerically computed eigensolutions in momentum space. Particular momentum dependent observables can be exactly computed [23]:

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

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

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

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

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		1.54414[(a)]	11.9218[(b)]	0.786997[(c)]
$\epsilon = 10^{-6}$	$N = 10$	1.54417	11.9225	0.787043
	20	1.54414	11.9218	0.786995
	40	1.54414	11.9218	0.786994
$\epsilon = 10^{-8}$	$N = 10$	1.54711	11.9471	0.787255
	20	1.54414	11.9218	0.786997
	40	1.54414	11.9218	0.786997

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

A good Fourier transform of the main part of the wavefunction $u^{\mathrm{FT}}(p)$ can be obtained with a small number of points, around $N = 20$-40. But, to obtain a good asymptotic tail, it is necessary to use more points, as we can see on Fig. 2. 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 respectively $Q(p_{\max}) = 0.504$, 0.097, 0.00028, 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 wavefunction. It is also possible to improve the quality factor by decreasing the value of ϵ (increasing the value of $p_{\max}$).

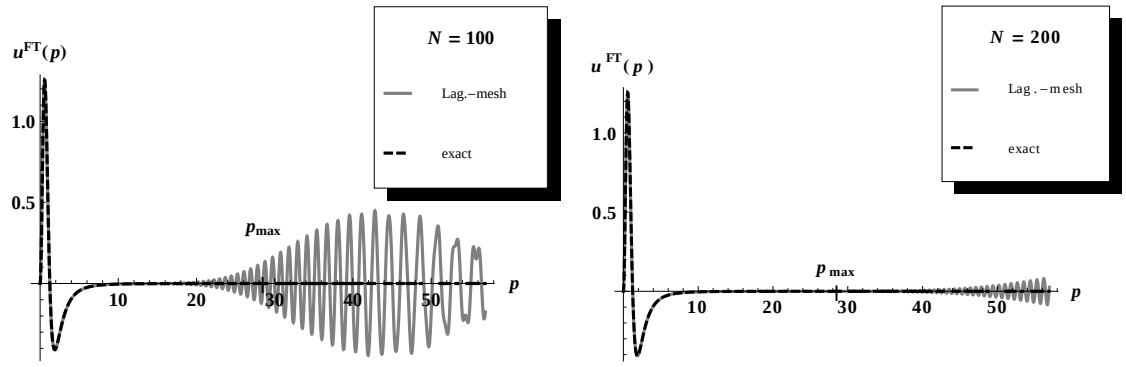

FIG. 2: The accurate numerically computed (exact) Fourier transform of the hydrogen atom wavefunction for $l = 1$ and $n = 1$ is compared with the corresponding approximation given by formula (22) for $0 \leq p \leq 2p_{\max}$. The value of $p_{\max}$ is determined with the procedure presented in Sec.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

VI. CONCLUDING REMARKS

The Lagrange-mesh method is a procedure to compute eigenvalues and eigenfunctions of quantum equations. It is very simple to implement and can yield very accurate results for a lot of observables, specially for nonrelativistic kinematics. At the origin, the method has been developed in the position space since the evaluation of potential matrix elements requires only 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 wavefunction in the momentum space by the Fourier transform of the wavefunction in the position space can be easily performed with a very good accuracy. Moreover, mean values of momentum dependent operators can also be easily and accurately calculated using a technique similar to the one used to compute the semirelativistic kinetic matrix elements. This shows again the great efficiency of the Lagrange-mesh method which can yield very accurate results for a minimal computational effort. We can wonder if this technique could also be used directly in the momentum space, for instance in the case where the interaction is only known as a function of the relative momentum. This question will be addressed in a subsequent paper.

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[1] D. Baye and P.-H. Heenen, J. Phys. A **19**, 2041 (1986).
[2] M. Vincke, L. Malegat, and D. Baye, J. Phys. B **26**, 811 (1993).
[3] D. Baye, J. Phys. B **28**, 4399 (1995).
[4] D. Baye, Phys. Stat. Sol. (b) **243**, 1095 (2006).
[5] D. Baye and K. D. Sen, Phys. Rev. E **78**, 026701 (2008).
[6] C. Semay, D. Baye, M. Hesse, and B. Silvestre-Brac, Phys. Rev. E **64**, 016703 (2001).
[7] F. Brau and C. Semay, J. Phys. G: Nucl. Part. Phys. **28**, 2771 (2002).
[8] F. Buisseret and C. Semay, Phys. Rev. E **71**, 026705 (2005).
[9] F. Buisseret and C. Semay, Phys. Rev. E **75**, 026705 (2007).
[10] D. Baye, M. Hesse, and M. Vincke, Phys. Rev. E **65**, 026701 (2002).
[11] D. Baye and M. Vincke, Phys. Rev. E **59**, 7195 (1999).
[12] M. Hesse and D. Baye, J. Phys. B **32**, 5605 (1999).
[13] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes* (Cambridge University Press, 2007).
[14] G. H. Golub and J. H. Welsch, Math. Comput. **23**, 221 (1969).
[15] L. P. Fulcher, Phys. Rev. D **50**, 447 (1994).

[16] D. A. Varshalovich, A. N. Moskalev, and V. K. Khersonskii, *Quantum Theory of Angular Momentum* (World Scientific, Singapore, 1988).
[17] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
[18] F. Brau and C. Semay, J. Comput. Phys. **139**, 127 (1998).
[19] R. M. Corless, G. H. Gonnet, D. E. G. Hare, D. J. Jeffrey, and D. E. Knuth, Adv. Comput. Math., 329 (1996).
[20] W. Lucha, F. F. Schöberl, and D. Gromes, Phys. Rep. **200**, 127 (1991).
[21] C. Semay, B. Silvestre-Brac, and I. M. Narodetskii, Phys. Rev. D **69**, 014003 (2004).
[22] W. Lucha, Mod. Phys. Lett. A **5**, 2473 (1990).
[23] C. Semay and B. Silvestre-Brac, J. Phys. A: Math. Theor. **43**, 265302 (2010).
[24] A.W. Niukkanen, Int. J. Quantum. Chem. **25**, 941 (1984).