

The Three-Dimensional Fourier Grid Hamiltonian Method

F. Brau and C. Semay

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

E-mail: claude.semay@umh.ac.be

Received May 7, 1997; revised October 1, 1997

A method to compute the bound state eigenvalues and eigenfunctions of a Schrödinger equation or a spinless Salpeter equation with central interaction is presented. This method is the generalization to the three-dimensional case of the Fourier grid Hamiltonian method for a one-dimensional Schrödinger equation. It requires only the evaluation of the potential at equally spaced grid points and yields the radial part of the eigenfunctions at the same grid points. It can be easily extended to the case of coupled channel equations and to the case of nonlocal interactions. © 1998 Academic Press

I. INTRODUCTION

Numerous techniques have been developed to find the eigenvalues and eigenvectors of the Schrödinger and the spinless Salpeter equations. In particular, developments of the Hamiltonian in a convenient bases have been widely used (see, for instance, Refs. [1, 2]). The accuracy of the solutions depends on two parameters: The size of the basis and a characteristic length which determines the range of the basis states. Upper bounds of the true eigenvalues are computed by diagonalizing the corresponding Hamiltonian matrix. The quality of the bounds increases with the size of the basis and for a given number of basis states there exist a characteristic length which minimizes the value of a particular upper bound.

In the case of a Schrödinger equation, other methods requiring only the evaluation of the potential at equally spaced grid points yield directly the amplitude of the eigenfunctions at the same grid points [3, 4]. In particular, the Fourier grid Hamiltonian method [4, 5] appears very accurate and simple to handle. This method is variational [6] and 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.

In this paper, we show that this last method can be generalized to treat the semirelativistic kinetic energy operator, simply by developing the Fourier grid Hamiltonian method in

three-dimensional space. Consequently, we propose to call our approach, the three-dimensional Fourier grid Hamiltonian method. We focus our attention on the case of purely central local potential, but the method can also be applied if the potential is nonlocal, or if coupling exists between different channels. As explained below, the accuracy of the method depends on the number of grid points and on the maximal radial distance considered to integrate the eigenvalue equation. This last parameter is not easy to calculate without knowing *a priori* the wave function, so we propose an *ansatz* to determine it.

Our method is outlined in Section II, while Section III presents a convenient way to compute the domain on which the wave functions are calculated. Test applications of the method are described in Section IV, and a brief summary is given in Section V.

II. METHOD

A. Theory

We assume that the Hamiltonian can be written as the sum of the kinetic energy \hat{T} and a potential energy operator \hat{V} . The eigenvalue equation for a stationary state is given by

$$[\hat{T} + \hat{V}]|\Psi\rangle = E|\Psi\rangle, \quad (1)$$

where \hat{T} depends only on the square of the relative momentum \mathbf{p} between the particles, \hat{V} is a local interaction which depends on the relative distance, and E is the eigenenergy of the stationary state. This equation is a nonrelativistic Schrödinger equation if

$$\hat{T} = m_1 + m_2 + \frac{\mathbf{p}^2}{2\mu}, \quad (2)$$

where m_1 and m_2 are the masses of the particles and μ is the reduced mass of the system (we use the natural units $\hbar = c = 1$ throughout the text). Equation (1) is a spinless Salpeter equation if

$$\hat{T} = \sqrt{\mathbf{p}^2 + m_1^2} + \sqrt{\mathbf{p}^2 + m_2^2}. \quad (3)$$

In configuration space, Eq. (1) is written

$$\int [\langle \mathbf{r} | \hat{T} | \mathbf{r}' \rangle + \langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle] \langle \mathbf{r}' | \Psi \rangle d\mathbf{r}' = E \langle \mathbf{r} | \Psi \rangle. \quad (4)$$

In the following, we only consider the case of a local central potential

$$\langle \mathbf{r} | \hat{V} | \mathbf{r}' \rangle = V(r) \delta(\mathbf{r} - \mathbf{r}') \quad \text{with } r = |\mathbf{r}|. \quad (5)$$

It is then useful to decompose the wave function into its central and orbital parts

$$\langle \mathbf{r} | \Psi \rangle = R_l(r) Y_{lm}(\hat{r}) \quad \text{with } \hat{r} = \mathbf{r}/r. \quad (6)$$

To compute the nonlocal representation of the kinetic energy operator, we introduce the basis states $\{|k\lambda\nu\rangle\}$, which are eigenstates of the operator \mathbf{p}^2 . They are characterized by good orbital quantum numbers (λ, ν) , obey the relation

$$\hat{T}(\mathbf{p}^2) |k\lambda\nu\rangle = T(k^2) |k\lambda\nu\rangle, \quad (7)$$

and satisfy the orthogonality relation

$$\langle k'\lambda'v' | k\lambda v \rangle = \delta(k' - k)\delta_{\lambda'\lambda}\delta_{v'v}. \quad (8)$$

The representation of these states in the configuration space is given by

$$\langle \mathbf{r} | k\lambda v \rangle = \sqrt{(2k^2/\pi)} j_\lambda(kr) Y_{\lambda v}(\hat{r}), \quad (9)$$

where functions $j_l(kr)$ are spherical Bessel functions. Using the completeness relation of basis states $\{|k\lambda v\rangle\}$ and Eq. (8), we find

$$\langle \mathbf{r} | \hat{T} | \mathbf{r}' \rangle = \int_0^\infty dk \frac{2k^2}{\pi} T(k^2) \sum_{\lambda=0}^\infty \sum_{v=-\lambda}^\lambda j_\lambda(kr) j_\lambda(kr') Y_{\lambda v}(\hat{r}) Y_{\lambda v}^*(\hat{r}'). \quad (10)$$

Introducing the regularized function $u_l(r) = rR_l(r)$, Eq. (4) is written

$$\frac{2}{\pi} r \int_0^\infty dr' r' u_l(r') \int_0^\infty dk k^2 T(k^2) j_l(kr) j_l(kr') + V(r)u_l(r) = E u_l(r). \quad (11)$$

This equation is the basis of the three-dimensional Fourier grid Hamiltonian method.

B. Discretization

We now replace the continuous variable r by a grid of discrete values r_i defined by

$$r_i = i \Delta \quad \text{with } i = 0, 1, \dots, N, \quad (12)$$

where Δ is the uniform spacing between the grid points. Regularity at the origin imposes $u_l(r_0 = 0) = 0$. For bound states, we have $\lim_{r \rightarrow \infty} u_l(r) = 0$. Consequently, we choose to set $u_l(r_N = N\Delta) = 0$. Actually, this last condition is not necessary but it does not spoil the accuracy of solutions. The normalization condition for the radial wave function is

$$\int_0^\infty dr [u_l(r)]^2 = 1. \quad (13)$$

The discretization of this integral on the grid gives

$$\Delta \sum_{i=1}^{N-1} [u_l(r_i)]^2 = 1. \quad (14)$$

This corresponds to an integration by trapezoidal rule thanks to the choice of a vanishing radial wave function at $r = r_0$ and $r = r_N$.

The grid spacing Δ in the configuration space determines the grid spacing Δk in the momentum space. The maximum value of r considered being $r_N = N\Delta$, the wave function lives in a sphere of diameter $2r_N$ in the configuration space. This length determines the longest wavelength λ_{\max} and, therefore, the smallest frequency Δk which appears in the k -space is

$$\Delta k = \frac{2\pi}{\lambda_{\max}} = \frac{\pi}{N\Delta}. \quad (15)$$

We have now a grid in configuration space and a corresponding grid in momentum space

$$k_s = s \Delta k = \frac{s\pi}{N\Delta} \quad \text{with } s = 0, 1, \dots, N. \quad (16)$$

If we note $V_i = V(r_i)$, the discretization procedure replaces the continuous Eq. (11) by an eigenvalue matrix problem

$$\sum_{j=1}^{N-1} H_{ij} \phi_j^n = e_n \phi_i^n \quad \text{for } i = 1, \dots, N-1, \quad (17)$$

where

$$H_{ij} = \frac{2\pi^2}{N^3} ij \sum_{s=1}^N s^2 T \left(\left(\frac{\pi s}{N\Delta} \right)^2 \right) j_i \left(\frac{\pi s}{N} si \right) j_l \left(\frac{\pi}{N} sj \right) + V_i \delta_{ij}. \quad (18)$$

The $(N-1)$ eigenvalues e_n of Eq. (17) correspond approximately to the first $(N-1)$ eigenvalues of Eq. (11). In the case of a potential which possesses a continuum spectra, only eigenvalues below the dissociation energy are relevant. Other eigenvalues, which form a discrete spectrum of positive energies, are spurious and correspond to standing wave solutions satisfying $u(r) = 0$ at $r = 0$ and $r = N\Delta$. The eigenvector ϕ_i^n gives approximately the values of the radial part of the n th solution of Eq. (11) at the grid points. The eigenvectors ϕ_i^n must be normalized according to Eq. (14) in order that $\phi_i^n \simeq u_i^n(r_i)$.

This method can also be used in the case of a nonlocal potential. If the interaction depends only on the radial variable, then the discretization of the action of the potential on the wave function gives

$$\int_0^\infty dr' W(r, r') u(r') \rightarrow \Delta \sum_{j=1}^{N-1} W(r_i, r_j) u(r_j) \quad \text{for } i = 1, \dots, N-1. \quad (19)$$

This corresponds also to an integration by trapezoidal rule thanks to the choice of a vanishing radial wave function at $r = r_0$ and $r = r_N$.

Coupled channels calculations can also be performed with this method. For instance, let us consider the coupled equations

$$\begin{aligned} \hat{H}^{(1)} |\phi^{(1)}\rangle + \hat{W} |\phi^{(2)}\rangle &= E |\phi^{(1)}\rangle \\ \hat{W} |\phi^{(1)}\rangle + \hat{H}^{(2)} |\phi^{(2)}\rangle &= E |\phi^{(2)}\rangle. \end{aligned} \quad (20)$$

The corresponding discretized equations are

$$\begin{aligned} \sum_{j=1}^{N-1} [H_{ij}^{(1)} \phi_j^{(1)} + W_{ij} \phi_j^{(2)}] &= E \phi_i^{(1)} \\ \sum_{j=1}^{N-1} [W_{ij} \phi_j^{(2)} + H_{ij}^{(1)} \phi_j^{(1)}] &= E \phi_i^{(2)}, \end{aligned} \quad (21)$$

where $H_{ij}^{(1,2)}$ and W_{ij} are the three-dimensional Fourier grid representation of the interaction

operators $\hat{H}^{(1,2)}$ and \hat{W} , respectively; $\phi_i^{(1,2)}$ are approximately the values of the radial part of the eigenstates $|\phi^{(1,2)}\rangle$ at grid points $r_i = i\Delta$ for $i = 1, \dots, N-1$.

C. Relevance of Discretization

As shown in Section IIA, the three-dimensional Fourier grid Hamiltonian method relies on the relation

$$\frac{2}{\pi}xx' \int_0^\infty j_l(kx)j_l(kx')k^2 dk = \delta(x-x'). \quad (22)$$

The equivalent discrete orthogonality relation on our grid of points is

$$\frac{2\pi^2}{N^3}ij \sum_{s=1}^N s^2 j_l\left(\frac{\pi}{N}si\right) j_l\left(\frac{\pi}{N}s j\right) = \Delta_{ij}^{(N,l)}. \quad (23)$$

One can thus expect that $\Delta_{ij}^{(N,l)} = \delta_{ij}$ for all values of N and l . Actually, the situation is less favorable. As shown in the Appendix for $l=0$ we have

$$\Delta_{ij}^{(N,l=0)} = \delta_{ij} \quad \forall N. \quad (24)$$

For $l=1$, $\Delta_{ij}^{(N,l=1)} \neq \delta_{ij}$, but we have verified numerically that

$$\lim_{N \rightarrow \infty} \Delta_{ij}^{(N,l=1)} = \delta_{ij}. \quad (25)$$

For values of l larger than 1, formula (25) is only approximately correct for small values of i and j . Consequently, the accuracy of this method becomes poorer when l increases; nevertheless for a large enough number of grid points, very good results can be obtained.

III. DOMAIN OF INTEGRATION

The accuracy of the eigenvalues and eigenfunctions depends on two parameters: The value of N and the value of r_N . Obviously, for a given value of r_N the accuracy increases with N . A proper choice for the domain of integration is not evident. If r_N is too small, incorrect solutions will be found. If this parameter is too large, a great number of grid points will be necessary to obtain stable eigenvalues. In this section, we propose an *ansatz* to compute a suitable value of r_N . The idea is to find the radial distance r_ϵ for which the radial part $R(r)$ of the eigenfunction considered is such that

$$\frac{r_\epsilon R(r_\epsilon)}{\max[rR(r)]} \leq \epsilon, \quad (26)$$

where ϵ is a number small enough to neglect the contribution of $R(r)$ for values of r greater than r_ϵ . The eigenfunction considered being *a priori* unknown, we propose to use a trial wave function matching at best the true eigenfunction, at least for the large r behavior. The value of r satisfying the condition (26) for the trial wave function will be the value r_N used for the numerical computation.

The first step is to find a potential $V_\infty(r)$ which matches at best the potential $V(r)$ for $r \rightarrow \infty$. In the following, we will consider three different types:

$$V_\infty(r) = \kappa r^p \quad \text{with } \kappa > 0; p > 0, \quad (27a)$$

$$V_\infty(r) = -\frac{\kappa}{r^p} \quad \text{with } \kappa > 0; 0 < p \leq 1, \quad (27b)$$

$$V_\infty(r) = -V_0 \theta(a - r) \quad \text{with } V_0 > 0; a > 0. \quad (27c)$$

The second step is to choose a trial state $|\lambda\rangle$ which depends on one parameter λ , taken here as the inverse of a distance. This trial state and the eigenstate considered are characterized by similar behaviors for $r \rightarrow 0$ and $r \rightarrow \infty$. The best matching between this state and the trial state is obtained by means of the variational principle. The average value,

$$\langle \lambda | \hat{H}_\infty | \lambda \rangle = \langle \lambda | \hat{T} + V_\infty(r) | \lambda \rangle, \quad (28)$$

is then computed and the value of λ is determined by the usual condition,

$$\frac{\partial \langle \lambda | \hat{H}_\infty | \lambda \rangle}{\partial \lambda} = 0. \quad (29)$$

In the case of the spinless Salpeter equation, the variational solution is computed using the fundamental inequality

$$\langle \sqrt{\mathbf{p}^2 + m^2} \rangle \leq \sqrt{\langle \mathbf{p}^2 \rangle + m^2}. \quad (30)$$

The radial part $R(r)$ of the trial state is then analyzed to find the value of r which satisfies the condition (26).

We have remarked that with $\epsilon = 10^{-4}$ it is possible to reach a relative accuracy better than 10^{-5} on eigenvalues, provided N is large enough ($N \gtrsim 50 - 100$). A relative accuracy on eigenvalues better than ϵ can be achieved because the mean value of an observable is computed using the square of the function $rR(r)$.

A. Ground States

We first consider the case of ground states, that is to say states without vibrational excitation. In the case of a potential with a large r behavior given by Eq. (27a), we use harmonic oscillator wave functions as trial states. The radial part is given by

$$R(r) = \sqrt{\left(2\lambda^{2l+3}/\Gamma\left(l + \frac{3}{2}\right)\right)} r^l \exp(-\lambda^2 r^2/2). \quad (31)$$

Using procedures (28), (29) and Eq. (30) for the spinless Salpeter equation with potential (27a), we find

$$\lambda = \left[p\kappa \frac{\Gamma(l + (p+3)/2)}{\Gamma(l + \frac{5}{2})} \left(\frac{1}{\sqrt{(l + \frac{3}{2})\lambda^2 + m_1^2}} + \frac{1}{\sqrt{(l + \frac{3}{2})\lambda^2 + m_2^2}} \right)^{-1} \right]^{1/(p+2)}. \quad (32)$$

The corresponding relation for the case of nonrelativistic kinematics is obtained with a vanishing value for the parameter λ in the right-hand side of the above formula. The reduced mass of the system appears naturally and the equation is no longer a transcendental equation.

If the potential, at great distances, is similar to the potentials given by Eqs. (27b)–(27c), the trial states used are the bound state Coulomb wave functions. The radial part is written

$$R(r) = \sqrt{((2\lambda)^{2l+3}/\Gamma(2l+3))} r^l \exp(-\lambda r). \quad (33)$$

The variational calculation for the spinless Salpeter equation with potential (27b) gives

$$\lambda = \left[p\kappa 2^p \frac{\Gamma(2l+3-p)}{\Gamma(2l+3)} \left(\frac{1}{\sqrt{\lambda^2 + m_1^2}} + \frac{1}{\sqrt{\lambda^2 + m_2^2}} \right)^{-1} \right]^{1/(2-p)}. \quad (34)$$

With the potential (27c), we obtain

$$\lambda = \frac{1}{2a} \left[(2l+1) \ln(2\lambda a) - \ln \left(\frac{\Gamma(2l+3)}{4a^2 V_0} \left(\frac{1}{\sqrt{\lambda^2 + m_1^2}} + \frac{1}{\sqrt{\lambda^2 + m_2^2}} \right) \right) \right]. \quad (35)$$

Again, the corresponding relations for the case of nonrelativistic kinematics is obtained with a vanishing value for the parameter λ under the square roots in the right-hand side of the above formulas. The reduced mass of the system appears naturally, but Eq. (35) remains a transcendental equation.

Once λ is found, it is easy to find r_N . Let us introduce a dimensionless variable $x_N = \lambda r_N$. Using condition (26) with Eqs. (31) and (33), x_N is given by the transcendental equation

$$x_N = \left[(l+1) \left(\ln \frac{x_N^m}{l+1} + 1 \right) - \ln \epsilon^m \right]^{1/m}, \quad (36)$$

with $m = 2$ in the case of Eq. (31) and $m = 1$ in the case of Eq. (33).

B. Vibrational Excited States

When the eigenstate considered is characterized by a vibrational excitation v different from 0, we can use, in principle, the $(v+1)$ th harmonic oscillator or Coulomb wave function as a trial wave function. But such a procedure makes analytical calculation of the optimal λ much more complicated. One knows that the polynomial multiplying the exponential term in the $(v+1)$ th wave function has degree $(v+l)$ in the Coulomb case and $(2v+l)$ in the harmonic oscillator case. So we can use a trial state with the value of l replaced by an effective orbital angular momentum l_{eff} which take into account the highest degree of the polynomial part of the radial trial state. We have verified that for potentials with large distance behavior of type (27a), it is a good approximation to take $l_{\text{eff}} = 2v+l$. In the case of potentials with large distance behavior of types (27b) or (27c), it is better to use $l_{\text{eff}} = v+l$.

IV. NUMERICAL IMPLEMENTATION

We have tested the accuracy of our method with different models found in the literature [1, 2, 7]. In particular, we have find the same results as those of Ref. [1], in which a

Schrödinger equation and a spinless Salpeter equation are used with a potential containing a Coulomb part and a linear part. In this section, we only present the results for a Schrödinger equation with a linear potential and for a spinless Salpeter equation with the Coulomb potential.

In the model of Ref. [7], the masses of some meson states are simply given by a nonrelativistic Hamiltonian with a confinement linear potential

$$H = m_1 + m_2 + \frac{\mathbf{p}^2}{2\mu} + ar + C. \quad (37)$$

The regularized radial part $u^n(r)$ of the n th zero orbital angular momentum eigenfunction of this Hamiltonian can be written in terms of the Airy function [8]

$$u^n(r) = (2\mu a)^{1/6} \frac{\text{Ai}((2\mu a)^{1/3}r + x_n)}{\sqrt{\int_{x_n}^{\infty} \text{Ai}^2(x) dx}}, \quad (38)$$

where x_n is the n th zero of the airy function. In Fig. 1, we show the eighth S-wave eigenfunction of Hamiltonian (37) for parameters values: $m_1 = m_2 = 0.300$ GeV, $a = 0.1677$ GeV², and $C = -0.892$ GeV, found in Ref. [7] (this corresponds to the seventh excitation of the ρ -meson). On this figure, the exact function is obtained with formula (38) and the numerical one has been computed with a value of r_N calculated with the procedure described in Section III for $\epsilon = 10^{-4}$ and with a number of grid points $N = 30$. In these conditions, the eighth eigenvalue is found with a relative accuracy better than 10^{-4} . This error can be reduced by a factor 10 or more by increasing N . The numerical solution is indistinguishable from the analytical solution to the resolution of the figure. If the wave function must be used to compute mean values of observables, a greater number of points is obviously necessary.

None analytical solution of the spinless Salpeter equation with Coulomb potential is known. But this equation has been extensively studied and it is possible to compare the

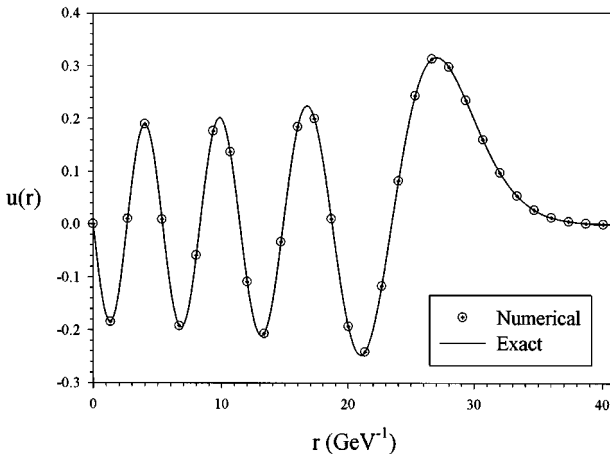


FIG. 1. Comparison of exact (solid curve) and numerically computed (crosses surrounded by circles) eigenfunctions for the seventh excitation of the ρ -meson for the quark–antiquark Hamiltonian of Ref. [7]. Our computation is carried out with $N = 30$ and an integration domain determined by the procedure given in Section III for $\epsilon = 10^{-4}$. See the text for further details.

TABLE 1

Energy Eigenvalues of the Spinless Salpeter Equation with Coulomb Potential $V(r) = -\kappa/r$ for the Parameter values $m_1 = m_2 = 1$ GeV and $\kappa = 0.456$

| State | $N = 100$ | $N = 200$ | $N = 300$ | Ref. [1] | Ref. [2] |
|-------|-----------|-----------|-----------|----------|----------|
| 1S | 1.9460 | 1.9453 | 1.9451 | 1.9450 | 1.9450 |
| 2S | 1.9870 | 1.9867 | 1.9866 | 1.9865 | 1.9868 |
| 3S | 1.9944 | 1.9942 | 1.9941 | 1.9941 | 2.0015 |
| 4S | 1.9969 | 1.9968 | 1.9967 | 1.9967 | 2.0238 |
| 1P | 1.9869 | 1.9869 | 1.9869 | 1.9869 | 1.9875 |

Note. Our results, for three values of N with a value of r_N calculated with the procedure described in Section III for $\epsilon = 10^{-4}$, are given with the upper bounds obtained by the variational methods described in Refs. [1, 2].

results of our method with results from other works. In Table 1, we show some eigenvalues of the semirelativistic Hamiltonian

$$H = \sqrt{\mathbf{p}^2 + m_1^2} + \sqrt{\mathbf{p}^2 + m_2^2} - \frac{\kappa}{r}, \quad (39)$$

with the parameter values: $m_1 = m_2 = 1$ GeV and $\kappa = 0.456$. The accuracy of our results are similar to those of Refs. [1, 2], even better for excited states found in Ref. [2] (the purpose of the work in Ref. [2] was not to reach the greatest possible accuracy, but to demonstrate the feasibility of a method). We have remarked that a greater number of grid points is necessary for the spinless Salpeter equation than for the Schrödinger equation to reach a similar accuracy.

V. SUMMARY

The three-dimensional Fourier grid Hamiltonian method, formulated and tested in this paper, appears as a convenient method to find the eigenvalues and the eigenvectors of a Schrödinger or a spinless Salpeter equation. It has the advantage of simplicity over all the other techniques. In particular, it requires only the evaluation of the potential at some grid points and not the calculation of matrix elements in a given basis. The method generates directly the values of the radial part of the wave function at grid points; they are not given as a linear combination of basis functions. Moreover, the extension of the method to the cases of nonlocal interaction or coupled channel equations is trivial.

It is worth noting that the method, based on the expansion of the wave function in basis functions, can present some interesting features. In some cases, all the matrix elements can be generated from analytic expressions. Further, the size of the matrices required can be considerably smaller (about 20×20 or 40×40) [1].

The accuracy of the solutions of the three-dimensional Fourier grid Hamiltonian method can easily be controlled since it depends only on two parameters: The number of grid points and the largest value of the radial distance considered to perform the calculation. A very good estimation of this last parameter can be easily determined by using the procedure described above, and the number of grid points can be automatically increased until a convergence is reached for the eigenvalues. The reliability of the method is also ensured by its variational character.

The method involves the use of matrices of order $((N - 1) \times (N - 1))$, where N is the number of grid points. Generally, the most time-consuming part of the method is the diagonalization of the Hamiltonian matrices. This is not a problem for modern computers, even for PC stations. Moreover, several powerful techniques for finding eigenvalues and/or eigenvectors exist and can be used at the best convenience. A demonstration program is available via anonymous FTP on umhsp02.umh.ac.be/pub/ftp_pnt/.

APPENDIX: ORTHOGONALITY CONDITION FOR S-WAVE STATE

Using the development of spherical Bessel functions in terms of sine and cosine functions, we have

$$\Delta_{ij}^{(N,l=0)} = \frac{2}{N} \sum_{s=1}^N \sin\left(\frac{\pi}{N}si\right) \sin\left(\frac{\pi}{N}sj\right). \quad (A1)$$

Replacing the sine function in terms of exponential functions and using $\sin(0) = \sin(\pi) = 0$, the formula above becomes

$$\Delta_{ij}^{(N,l=0)} = -\frac{1}{2N} \sum_{s=0}^{N-1} (e^{i(\pi/N)si} - e^{-i(\pi/N)si})(e^{i(\pi/N)sj} - e^{-i(\pi/N)sj}). \quad (A2)$$

Distributing and using the well-known relation

$$\sum_{s=0}^{N-1} e^{i(\pi/N)sj} = \frac{1 - e^{i\pi j}}{1 - e^{i(\pi/N)j}}, \quad (A3)$$

one can obtain Eq. (24).

ACKNOWLEDGMENTS

We thank Professor R. Ceuleneer, Dr. F. Michel, and Dr. Y. Brihaye for useful discussions. One of us (C.S.) is grateful to Professor C. Gignoux for providing useful references.

REFERENCES

1. L. P. Fulcher, *Phys. Rev. D* **50**, 447 (1994).
2. W. Lucha and F. F. Schöberl, *Phys. Rev. A* **56**, 139 (1997).
3. P. J. Cooney, E. P. Kanter, and Z. Vager, *Am. J. Phys.* **49**, 76 (1981).
4. C. C. Marston and G. G. Balint-Kurti, *J. Chem. Phys.* **91**, 3571 (1989).
5. G. G. Balint-Kurti, C. L. Ward, and C. C. Marston, *Comput. Phys. Commun.* **67**, 285 (1991).
6. J. C. Light, I. P. Hamilton, and J. V. Lill, *J. Chem. Phys.* **82**, 1400 (1985).
7. W. H. Blask *et al.*, *Z. Phys. A* **337**, 327 (1990).
8. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).