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A New Variable Step Method for the Numerical Integration of the One-Dimensional Schrödinger Equation

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The numerical integration of the one-dimensional Schrödinger equation is considered. A new variable step method is presented within the "Canonical Functions" scheme, characterized namely by: (i) the replacement of the Schrödinger equation by the "equivalent" integral equation; (ii) the representation of the wavefunction by a superposition of simple integrals; (iii) the definition of "Taylor Series like" difference equations. At each interval, an estimate of the step-size h is determined in order to obtain the desired local accuracy. For the practical case of a given potential function with polynomial interpolations, the step-size h is directly given by a simple formula depending on: (i) the potential function in the interval; (ii) the "initial values" of the wavefunction at the origin of the interval. This variable step method is applied to the Morse potential function used for the recent Raptis and Cash method (*Comput. Phys. Commun.* **36**, 113 (1985)). For this application, the present method presents some advantages over the previous one.

1. INTRODUCTION

In the diatomic vibrational–rotational eigenvalue problem (as in other similar problems), one has to consider the numerical integration of the one-dimensional Schrödinger equation [1].

According to the widely used Cooley method [2], the problem is reduced to the integration of the equation

$$y''(r) = (U(r) - E)\, y(r) = f(r)\, y(r) \tag{1}$$

for a given potential function $U(r)$ (where r is the internuclear distance), and a succession of trial values $\tilde{E}$ of E in order to obtain a solution $y(r)$ obeying

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(i) the boundary conditions

$$y(0)=0 \tag{2}$$

$$\lim_{r\to\infty} y(r)=0 \tag{2'}$$

(ii) the continuity condition for $y(r)$ and $y'(r)$ at any arbitrary point r_0 $(0<r_0<\infty)$.

For each trial value $\tilde{E}$ of E, many trial values of the "initial values" y_0, y'_0 (at $r\sim 0$ or at $r\sim\infty$) are sucessively used in order to assure the continuity of $y(r)$ at a given point r_0. Then other trial values $\tilde{E}$ are successively used in order to assure the continuity of $y'(r)$ at r_0. In summary, the Cooley method is reduced to a sucession of one "elementary" operations, i.e., the integration of Eq. (1) for a given $U(r)$, with a given E and given initial values y_0 and y'_0 at a given point r_0.

While this method has been known for two decades and proved to be efficient in many practical applications, many papers still appear every year dealing with some details of the method [3], or looking to new other schemes [4–7].

One of the last schemes presented (the "Canonical Functions" method [7]) has the advantage of dissociating the determination of the eigenvalue E from that of the eigenfunction $y(r)$, by defining an "eigenvalue-function" $F(E)$ related to the given potential function $U(r)$, E being a variable parameter. The successive roots of the equation $F(E)=0$ are the successive eigenvalues related to $U(r)$.

This method eliminates the explicit use of the eigencfunction (and the "initial values" problem), but makes use of the canonical functions $\alpha(r)$ and $\beta(r)$ which are particular solutions of Eq. (1) with well-defined initial values. We deduce that the "canonical functions" method is reduced to the determination of $\alpha(r)$ and $\beta(r)$ for several values of E, i.e., to the integration of Eq. (1) for a given $U(r)$ with a given E and given initial values (at an initial point r_0).

This overview of the Schooting method and the canonical functions method can be extended to many other methods; it neglects many important details, but it underlines the importance of the choice of a convenient difference equation for the numerical integration of the Schrödinger equation.

Among the large variety of difference equations, the Numerov difference equation [8] is the most used in diatomic problems. Yet in some specific cases, Runge–Kutta formulae [9], or other alternatives [10] are used.

In this trend to improve the accuracy of the numerical integration of the one-dimensional Schrödinger equation, we point out the recent important work of Raptis and Cash [11] who obtained good results by using a variable step method in order to reduce the "local truncation error" within pre-defined limits.

The present work is inspired from the previous one. We present a variable step method along with a difference equation usually not used for the diatomic eigenvalue problem, yet efficient and highly accurate. This method makes use of the "canonical functions" approach.

2. The Difference Equation

2.1. We know that the Schrödinger equation (Eq. (1)) is equivalent to the integral equation [12]

$$y(r) = y(r_0) + (r - r_0)\, y'(r_0) + \int_{r_0}^{r} (r - t)\, f(t)\, y(t)\, dt \tag{3}$$

in the sense that any solution of the one is a solution of the other and vice versa; r_0 being an arbitrary origin $(0 < r_0 < \infty)$.

Furthermore, we know that the solution of Eq. (3) is given by a "superposition of integrals" of the form

$$y(r) = \sum_{n=0}^{\infty} H_n(r), \tag{4}$$

with

$$H_n(r) = \int_{r_0}^{r} (r - t)\, f(t)\, H_{n-1}(t)\, dt \tag{5}$$

$$H_0(r) = y(r_0) + (r - r_0)\, y'(r_0), \tag{6}$$

where the series (4) is proved to be absolutely and uniformly convergent [13].

This expression of $y(r)$ can lead to the following difference equations:

$$y_1 = y_0 + h y'_0 + \sum_{n=1}^{\infty} H_n(h) \tag{7}$$

$$y'_1 = y'_0 + \sum_{n=1}^{\infty} H'_n(h), \tag{7'}$$

with

$$y_0 = y(r_0); \qquad y'_0 = y'(r_0)$$

$$y_1 = y(r_0 + h); \qquad y'_1 = y'(r_0 + h)$$

$$H_n(x) = \int_0^{x} (x - t)\, f(t)\, H_{n-1}(t)\, dt \tag{8}$$

$$H_0(x) = y_0 + x y'_0 \tag{9}$$

$$x = r - r_0; \qquad 0 \leqslant x \leqslant h$$

and

$$H'_n(x) = \int_0^{x} f(t)\, H_{n-1}(t)\, dt. \tag{10}$$

2.2. These difference equations cannot be considered of interest for numerical applications unless: (i) the potential $U(x)$ (on the interval $(0, h)$) is given by a "convenient" function, for which the integral sign in $H_n(x)$ (Eq. (8)) is eliminated ($U(x)$ is given, for example, by a combination of x^m, or of $\sin ax$, or e^{ax}, or others...); (ii) the series in Eq. (7) (resp. Eq. (7′)) is "quickly" convergent, so one may replace Eqs. (7) and (7′) by

$$y_1 \simeq y_0 + hy'_0 + \sum_{n=1}^{N} H_n(h) \tag{11}$$

$$y'_1 \simeq y'_0 + \sum_{n=1}^{N} H'_n(h), \tag{11'}$$

where N is a positive integer related to the required precision.

Fortunately, in the diatomic eigenvalue problem, the potential may be given by an analytical function (Morse, Lennard–Jones, Dunham, ...) or by a numerical table of the *RKR*-type (determined by the *RKR* method [14] or by a recent quantum method [15]). This *RKR* potential is usually determined by the coordinates of some points (turning points and/or others), with suitable interpolations and extrapolations, which usually are (or can be reduced to) polynomials. For these potentials, as well as for some well-known analytical potentials (Dunham, Morse, Lennard–Jones, ...), we can write on the interval $(0, h)$

$$U(x) = \sum_{n=0}^{M} \gamma_n x^n; \qquad 0 \leqslant x \leqslant h, \tag{12}$$

where M is the degree of the given polynomial interpolation.

In this case, the difference equations (Eqs. (11) and (11′)) are greatly simplified; they become

$$y_1 \simeq y_0 + hy'_0 + \sum_{n=2}^{N} c_n h^n \tag{13}$$

$$y'_1 \simeq y'_0 + \sum_{n=2}^{N} nc_n h^{n-1}, \tag{13'}$$

where the coefficients c_n are given by the recursion formula

$$(n+2)(n+1)\, c_{n+2} = -Ec_n + \sum_{m=0}^{n} c_m \gamma_{n-m} \tag{14}$$

with $c_0 = y_0$; $c_1 = y'_0$. (For obvious reasons, we must always take $N \geqslant M$.)

2.3. As we mentioned above, the difference equation (13) is the special case of Eq. (11) suitable for a potential with polynomial interpolations and extrapolations. Other forms of the general difference equation (11) can be derived for other types of interpolations.

For the present special case, one can notice that the difference equation (13) is nothing but the well-known Taylor series expansion of the solution of Eq. (1). To our knowledge, this expansion is not used for the diatomic eigenvalue problem. One may find many applications to some *RKR* potentials as well as to many Morse and Lennard–Jones functions [16].

3. THE NEW VARIABLE STEP METHOD

In the difference equation (13) derived in the previous section, a truncation error R_N is omitted. According to the general formulation, we write

$$y_1 = y_0 + hy'_0 + \sum_{n=2}^{N-1} c_n h^n + R_N \tag{15}$$

with

$$R_N = \sum_{n=N}^{\infty} c_n H^n. \tag{16}$$

If the step-size h is constant (or pre-determined), the choice of the integer N can be determined by the condition

$$|c_N h^N| \leqslant \varepsilon, \tag{17}$$

where ε is a chosen "tolerance."

Conversely, N may be fixed a priori, and h may be determined in order to have

$$|R_N| \leqslant \varepsilon. \tag{18}$$

According to this condition, and to the convergence of the series (7), we obviously have

$$R_{N+1} \leqslant \varepsilon$$

and furthermore

$$|(R_N - R_{N+1})/R_N| = |c_N h^N/R_N| \leqslant \varepsilon$$

which leads to

$$|c_N h^N| \leqslant \varepsilon^2$$

and finally

$$h \leqslant (\varepsilon^2/|c_N|)^{1/N}. \tag{19}$$

For a given N and a given ε, h is a function of the coefficient c_N, i.e., of the initial values y_0, y'_0 on one hand, and of the potential function $U(r)$ and the given value of E on the other hand (see the recursion formula (14)). The step-size h will therefore vary from one interval to another.

Since we may take ε as small as we desire, the variable step h can be given by

$$h = (\varepsilon^2/|c_N|)^{1/N}. \tag{20}$$

This value assures that R_N obeys condition (18).

4. THE NUMERICAL APPLICATION

4.1. In order to test the validity of the present method, we choose to present the application to the Morse potential

$$U(r) = D(1 - \exp(-a(r - r_e)))^2 - D$$

with $r_e = 1.9975$, $a = 0.711248$, and $D = 188.4355$, in a.u.

The main reason for this choice is the possibility of comparison of our results with those of Raptis and Cash [11] who used the same potential in their numerical applications.

The other reasons for this choice are:

(i) The exact vibrational eigenvalues E_v^M for the Morse potential are known, and one can compare the computed eigenvalue E_v^c with the exact one for each vibrational level v.

(ii) The exact value of the logarithmic derivative of the vibrational Morse wavefunction is known at r_e: $l_v^M = y'_v(r_e)/y_v(r_e)$ [17]. This offers a severe test of the computation of the canonical functions α and β proper to the canonical functions method.

(iii) The exact value of the vibrational Morse wavefunction $y_v^M(r)$ is also known. This offers a direct test of the difference equations and the variable step method [18].

The vibrational eigenvalues E_v are computed by using the variable step method described here along with the canonical functions scheme outlined in the Appendix.

Within this frame, one has to compute the canonical functions $\alpha(E; r)$ and $\beta(E; r)$ (for a given value E) at several points r_i^+ (for $r > r_0$) and r_i^- (for $r < r_0$).

At the starting point r_0, one has to calculate the mesh-size h_1 from Eq. (20) and can deduce $r_1 = r_0 + h_1$ as well as $\alpha(E; r_1)$, $\beta(E; r_1)$, $\alpha'(E; r_1)$, and $\beta'(E; r_1)$. This procedure is repeated at r_1, where h_2 is calculated, then at $r_2 = r_1 + h_2$, etc.

At each point r_i, the determination of h from Eq. (20) implies that of c_N for a given ε and a given N; the choice of ε and N will be discussed below. To determine c_N, one has to make use of Eq. (14), i.e., to know $c_0 = y(r_i)$ and $c_1 = y'(r_i)$. In the present application, we use α for $y(r)$; so at r_0, we have $c_0 = 1$ and $c_1 = 0$ (see the Appendix for the initial values of α); at r_1, we take $c_0 = \alpha(E; r_1)$ and $c_1 = \alpha'(E; r_1)$; and so on. We notice that one may use β instead of α in order to determine the step-sizes h_i.

In spite of this pre-determination of the step-size h at each interval, the present application follows the standard canonical functions scheme [7] outlined in the Appendix. We notice here that the determination of h, and that of α and β, is done simultaneously, in the same "run." So the program gives, for any potential, the eigenvalues E_0, $E_1, ..., E_v, ...$, along with the wavefunction logarithmic derivative $l(E_v) = y'(E_v; r_0)/y(E_v; r_0)$; the same program may be easily adapted to compute the wavefunction $y(E_v; r)$.

4.2. We give in Table I the eigenvalue E_v computed by the present method for the first 14 vibrational levels considered by Raptis and Cash [11]. For each v, the Morse eigenvalues $E_v^M = w_e(v + 1/2) - w_e x_e(v + 1/2)^2$ (with $w_e = 2a\sqrt{D}$, $w_e x_e = a^2/19/)$ are given along with the discrepancy $\Delta E_v = |E_v - E_v^M|$, for the "present method" (ΔE_v^{PM}) and for the results of Raptis and Cash (ΔE_v^{RC}). The total number of steps I is also given for each level, along with the greatest step-size h.

These computations were done on a personal computer (NewBrain AD) giving eight significant figures; so we took $\varepsilon = 10^{-8}$ for the determination of h for all the considered levels.

TABLE I

Computed Eigenvalues E_v for the Vibrational Levels of the Morse Potential

v	E_v^M	ΔE_v^{PM}	ΔE_v^{RC}	I^{PM}	I^{RC}	h^{PM}	h^{RC}
0	−178.798 538	2	0	13	238	0.428	0.08
1	−160.283 406	4	1	14	238	0.375	0.08
2	−142.780 060	0	2	15	238	0.351	0.08
3	−126.288 442	2	3	17	238	0.365	0.08
4	−110.808 572	2	6	19	238	0.349	0.08
5	−96.340 449	0	7	21	238	0.355	0.08
6	−82.884 074	0	10	22	238	0.377	0.08
7	−70.439 445	0	11	23	238	0.416	0.08
8	−59.006 565	0	14	25	237	0.407	0.08
9	−48.585 432	0	38	27	165	0.417	0.08
10	−39.176 046	0	22	28	176	0.466	0.08
11	−30.778 407	0	45	30	166	0.464	0.08
12	−23.392 520[a]	0	35	31	170	0.535	0.08
13	−17.018 372	0	36	33	173	0.617	0.08

[a] This value is different from that given in Ref. [11].

Note. For each level v, the Morse eigenvalue E_v^M is given (in a.u.) along with $\Delta E_v = E_v - E_v^M$ (in 10^{-6} a.u.) for the present method (ΔE_v^{PM}) and for that of Raptis and Cash [11] (ΔE_v^{RC}). The number of steps I and the greatest step-size h are also given for both methods.

On each interval, one has to compute the coefficients c_n used first to determine h, then used in the difference equations (13) (to determine α and β). According to the recursion formula (14), c_n depend on E and on the coefficients γ_n of the potential U (see Eq. (12)).

4.3. For the Morse potential function used in the present application, the coefficients γ_n (on the interval (r_i, r_{i+1})) are deduced from those of the expansion in Taylor series of some other functions. We write for the chosen interval

(i) $r = r_i + x \qquad (0 \leqslant x \leqslant h = r_{i+1} - r_i)$

(ii) $U(x) = DZ^2(x)$

$Z(x) = 1 - Az(x)$

$z(x) = \exp(-ax)$

with $A = \exp(-ar_i)$.

The function $z(x)$ is expanded in the Taylor series

$$z(x) = \sum_{n=0}^{\infty} \delta_n x^n,$$

where $\delta_{n+1} = -a\delta_n/(n+1)$ with $\delta_0 = 1$.

The function $Z(x)$ can be written

$$Z(x) = \sum_{n=0}^{\infty} \Delta_n x^n,$$

where $\Delta_0 = 1 - A\delta_0$, and $\Delta_n = -A\delta_n$.

Then the coefficients γ_n of the function $U(x) = \sum_{n=0}^{\infty} \gamma_n x^n$ are deduced from Δ_n by the relation $\gamma_n = D \sum_{m=0}^{n} \Delta_m \Delta_{n-m}$.

5. DISCUSSION

5.1. The results presented in Table I show that:

(i) The eigenvalues E_v^{PM} computed by the present method are equal to the Morse eigenvalues E_v^M within the computer precision (to eight significant figures). Those of Raptis and Cash E_v^{RC} are less precise.

(ii) The number of intervals I^{PM} used in the present method, increases with v (from $I = 13$ for $v = 0$ to $I = 33$ for $v = 13$); yet it stays clearly inferior—for every level— than that I^{RC} of Raptis and Cash.

(iii) The maximum step-size h (for each level) varies with v for the present method, while it is constant for that of Raptis and Cash. h^{PM} is always superior to h^{RC} for all the levels.

Yet a weakness appears in the present method. Looking at the expression of h (Eq. (20)), one notices the dependence of h on ε and N. While ε must be taken, according to the theory, as small as possible, there is no theoretical indication for the choice of N.

In the present numerical application, we took $N = 25$ (guided by some previous applications of the canonical functions used with constant h). We did then some tests (for few levels) by making N vary from 10 to 60 (with a given value of E). We noticed that

(i) The values of α and β, and of $l = \lim - \alpha/\beta$ do not vary with N.

(ii) When N increases, h increases and the number I of intervals decreases.

(iii) The time t of one "run" (the integration of Eq. (1) with given E and given initial values) is practically independent from N, except when N is small ($N = 15, 10, \ldots$) or big ($N = 50, 60, \ldots$) where t is increased by a fraction of t.

This point, concerning the pre-determination of N, is still under study.

5.2. Another test is presented in Table II, where we give the values $l^+(E) = -\lim_{r\to 0} \alpha(E; r)/\beta(E; r)$ and $l^-(E) = -\lim_{r\to 0} \alpha(E; r)/\beta(E; r)$, for two values of E: $E = E_v^{PM}$ (eigenvalue of the level v computed by the present method)

TABLE II

Computed Wavefunction Logarithmic Derivative $l_v = y'(r_e)/y(r_e)$ at the Minimum r_e of a Morse Potential

		$E = E^{PM}$		$E = E^{RC}$	
v	l^M	$l^+ - l^M$	$l^- - l^M$	$l^+ - l^M$	$l^- - l^M$
0	0.355 624 00	0[a]	0	0	0
1	−12.660 309	0	0	+3	−3
2	7.970 771 3	0	0	+41	−18
3	−1.154 689 4	0	0	+32	−15
4	−15.838 390	0	0	−3	+1
5	28.462 311	0	0	−111	+36
6	5.413 083 3	0	0	−248	+71
7	−2.289 492 9	0	0	−259	+70
8	−12.540 568	0	0	−82	+20
9	−67.286 859	0	0	−3934	+814
10	35.841 979	0	0	−776	+135
11	12.869 458	0	0	−402	+59
12	5.576 495 3	0	0	−2168	+273
13	1.005 265 4	0	0	−2296	+246

[a] The deviation of l from l^M at the eighth significant figure.

Note. The two limits $l^+ = -\lim_{r\to\infty} \alpha(r)/\beta(r)$ and $l^- = -\lim_{r\to 0} \alpha(r)/\beta(r)$ are compared to the Morse value l^M for two different values of E: $E = E^{PM}$ (for the present method), and $E = E^{RC}$ (for that of Raptis and Cash [11]).

and $E = E_v^{RC}$ (corresponding value found by Raptis and Cash). The values of l^+ and l^- are then compared (for each v) to the Morse value l^M (logarithmic derivative of the Morse wavefunction [17]). This comparison is done when $r_0 = r_e$.

From this table, one may notice that for $E = E^{PM}$, we have $l^+ = l^- = l^M$, or $\lim_{r \to \infty} -\alpha/\beta = \lim_{r \to 0} -\alpha/\beta = y'(r_e)/y(r_e)$ which is theoretically true (see the Appendix). This result confirms the validity of the computed E_v^{PM}.

The previous remark may be considered as follows: since $E^{PM} = E^M$, the differences $l^+ - l^M$ and $l^- - l^M$ "measure" the error introduced by the computation of l^+ (and l^-), i.e., the error caused by the difference equations used in the computations of α and β, and any error in the determination of E_v. The excellent agreement between l^+, l^-, and l^M (for $E = E^{PM}$) and the rather less good agreement between l^+, l^-, and l^M(for $E = E^{RC}$) give an advantage to the present method over that of Raptis and Cash.

5.3. The test of the wavefunction described in Ref. [18], was also applied and showed an excellent agreement between the Morse wavefunction and that computed by the present method (by integrating Eq. (1) with E_v^{PM} and the initial values deduced from $l(E_v^{PM})$).

5.4. Finally, the following practical remarks should be made concerning the computer program:

(i) The programming effort is reduced practically to that of the recursion formula (Eq. (14)) used to determine the step-size on one side, and the canonical functions α and β (then their limits l^+ and l^-) on the other side; the program is quite simple (and available from the authors upon request).

(ii) The same canonical functions algorithm was used with the present variable-step method along with other difference equations (Numerov [8]; Runge–Kutta [9]) in order to evaluate the efficiency of the present method.

The consumption in computer time for the present method exceeds (slightly) that for the Numerov difference equation, but it is roughly half the time used with the Runge–Kutta difference equations. This result is similar to that obtained with the conventional constant-step method (see The Appendix).

(iii) The method used here to compute the eigenvalues of a bound state is adaptable to that of the eigenfunctions.

(iv) This same method was already used to compute the phase shift of an elastic collision; yet this last application presents some particularities related to the boundary conditions of the solution and not to the used difference equation (with or without local control error). This application will be the subject of a forthcoming paper.

6. CONCLUSION

A new variable-step method for the numerical integration of the one-dimensional Schrödinger equation was presented. In its general formulation, the new method is inscribed within the "Canonical Functions" scheme usually used for the diatomic problem.

Special emphasis was made on the practical case of diatomic potential function with polynomial interpolations (and extrapolations). The step-size h is given by a simple expression depending, for a given interval, on the potential function on this interval, and on the "initial values" of the wavefunction at the origin of the interval.

This method was applied to the Morse potential function already used by Raptis and Cash. The computed eigenvalue (for all the vibrational levels) is equal to the exact one, up to eight significant figures (the computer precision).

APPENDIX:

OUTLINE OF THE "CANONICAL FUNCTIONS" APPROACH TO THE DIATOMIC EIGENVALUE PROBLEM

For a given potential $U(r)$ and a given value of the "parameter" E, the canonical functions $\alpha(E; r)$ and $\beta(E; r)$ are particular solutions of Eq. (1) with the initial values [7]

$$\alpha(E; r_0) = 1; \qquad \alpha'(E; r_0) = 0$$

$$\beta(E; r_0) = 0; \qquad \beta'(E; r_0) = 1$$

with $0 < r_0 < \infty$.

The general solution of Eq. (1) is

$$y(E; r) = y(E; r_0)\,\alpha(E; r) + y'(E; r_0)\,\beta(E; r).$$

This solution is the eigenfunction if it obeys the boundary conditions (Eq. (2)): $y(E; 0) = y(E; \infty) = 0$.

For an arbitrary value of E, one may consider the two "limits"

$$l^+(E) = \lim_{r \to \infty} -\alpha(E; r)/\beta(E; r)$$

$$l^-(E) = \lim_{r \to 0} -\alpha(E; r)/\beta(E; r)$$

and the "eigenvalue function" $F(E)$ defined by

$$F(E) = l^+(E) - l^-(E).$$

When $E = E_v$ (eigenvalue), we have

$$l^+(E_v) = l^-(E_v) = y'(E_v; r_0)/y(E_v; r_0).$$

So $F(E)=0$ is the "eigenvalue-equation" having for successive solutions (when E varies from zero to the dissociation D) the successive eigenvalues $E_0, E_1, E_2, \ldots$.

This treatment is explicitly independent of the wavefunction and implies numerically the computation of $\alpha(E; r)$ and $\beta(E; r)$, i.e., the numerical integration of Eq. (1) for a given $U(r)$ and a given E, with given initial values at r_0.

This numerical integration starts at $r=r_0$, with $r>r_0$. It computes α, β, and $-\alpha/\beta$. It is stopped when $-\alpha/\beta$ reaches the constant limit $l^+(E)$. It is then repeated for $r<r_0$ and stopped when $-\alpha/\beta$ reaches the constant limit $l^-(E)$. Then it looks for the zeros of the function $F(E)=l^+(E)-l^-(E)$. The details of this numerical scheme are given in Ref. [7].

This canonical functions approach for the eigenvalue problem was already used with different types of difference equations: The Runge–Kutta equations [9], the Numerov equation [8], and the Taylor series expansion Eqs. (13) and (14) (limited to the case defined in Eq. (12)). While the latter is highly accurate [16], its consumption in computer time is much less than that of the first one (Runge–Kutta), but slightly exceeds that of Numerov's [7].

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