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APPLICATION OF THE EXPONENTIAL PROPAGATION MATRIX METHOD TO THE NUMERICAL SOLUTION OF THE SCHRDINGER EQUATION

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We propose a numerical method for obtaining the eigenvalues and eigenfunctions of the one-dimensional time-independent Schrödinger equation. The eigenvalue problem is transformed into a system of two first-order ordinary linear differential equations for the wavefunction and its first derivative. The propagation matrix for the solution is written as the exponential of a traceless matrix which is then approximated by the Magnus expansion. The bound-state eigenvalues and eigenfunctions are obtained from the boundary conditions. We investigate the analytical properties of the method and show that algorithms proposed by other authors are particular cases of the present one. We test the accuracy of the results by means of exactly solvable eigenvalue problems and discuss the application of the method to the calculation of vibrational-rotational energies of diatomic molecules.

I. INTRODUCTION

Although the one-dimensional time-independent Schrödinger equation can be accurately solved in many different ways there is still a great interest in developing simpler and more accurate algorithms that can be run in small personal computers [1]. The most general and widely used algorithms are based on the finite-difference

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approach. Among them we mention the Numerov-Cooley [2,3] method and its improvements [4–8]. A simpler and powerful integration formula has been derived by the use of perturbation theory [9]. There are also methods based on the transformation of the linear eigenvalue problem into a nonlinear ordinary differential equation such as Milne's [10] or Riccati's [11].

Here, we are interested in the numerical algorithms based on the propagation matrix method. Light and co-workers proved that it is useful in treating potential [12], inelastic [13–15], and reactive [16] scattering. Devries [17] resorted to an approximate sum of the Taylor expansion of the propagation matrix to obtain resonant eigenvalues. Ixaru [18] proposed an efficient perturbative approach to the propagation matrix for the calculation of resonant and bound-state eigenvalues. A power series expansion for the propagation matrix proves to be simpler and accurate in the calculation of eigenvalues when the potential can be easily expanded in a Taylor series [19].

As far as we know, the exponential form of the propagation matrix [12–16] and the Magnus expansion [20] have not been used in the calculation of bound state eigenvalues and eigenfunctions. The purpose of the present article is to explore such an application. We develop the method and discuss some of its properties in Sec. II. The accuracy of the eigenvalues and eigenfunctions is tested in Sec. III by means of exactly solvable models. There we also consider the performance of the method in the calculation of vibrational-rotational energies of diatomic molecules. The use of approximation schemes other than the Magnus expansion is outlined.

II. THE EXPONENTIAL PROPAGATION MATRIX METHOD

The time-independent Schrödinger equation for one-dimensional and central-field models can be written

$$\psi''(x) = q(x)\psi(x), \qquad q(x) = V(x) - E, \tag{1}$$

where E is the energy eigenvalue and units are chosen so that $\hbar = m = 1$. The boundary conditions will be considered later on along with the examples. Eq. (1) can be transformed into a system of two first-order linear ordinary differential equations as follows:

$$\Phi'(x) = H(x)\Phi(x), \tag{2a}$$

where

$$\Phi(x) = \begin{bmatrix} \psi(x) \\ \psi'(x) \end{bmatrix}, \qquad H(x) = \begin{bmatrix} 0 & 1 \\ q(x) & 0 \end{bmatrix} \tag{2b}$$

The propagation matrix $U(x', x)$ enables one to obtain $\Phi(x')$ from $\Phi(x)$ according to

$$\Phi(x') = U(x', x)\Phi(x). \tag{3}$$

On differentiating this last equation with respect to x' and using Eq. (1) we find that $U(x', x)$ satisfies

$$\frac{\mathrm{d}}{\mathrm{d}x'}U(x', x) = H(x')U(x', x), \tag{4}$$

where according to (3) $U(x, x) = I$ is the 2×2 identity matrix.

It follows from (4) that the propagation matrix can be written

$$U(x', x) = \begin{bmatrix} u(x', x) & v(x', x) \\ \frac{\partial u(x', x)}{\partial x'} & \frac{\partial v(x', x)}{\partial x'} \end{bmatrix}, \tag{5}$$

where $u(x', x)$ and $v(x', s)$ are two linearly independent solutions of $\partial^2 w(x')/\partial x'^2 = q(x')w(x')$ with the initial conditions

$$u(x, x) = \frac{\partial v}{\partial x'}(x', x)|_{x'=x} = 1 \text{ and } v(x, x) = \frac{\partial u}{\partial x'}(x', x)|_{x'=x} = 0.$$

This form of the propagation matrix has been used by Ixaru [18] and Fernández et al. [19] and is the basis of the canonical functions method [23] which has recently [24] been proved to be numerically and formally equivalent to the Numerov-Cooley algorithm [2,3].

Magnus [20] showed that $U(x', x)$ can be written

$$U(x', x) = \exp A(x', x), \qquad A(x, x) = 0, \tag{6}$$

provided $|x' - x|$ is small enough, and that the exponent $A(x', x)$ can be approached by a series

$$A(x', x) = A_1(x', x) + A_2(x', x) + \cdots, \tag{7}$$

the first terms of which are

$$A_1(x', x) = \int_x^{x'} H(s)\mathrm{d}s, \tag{8a}$$

$$A_2(x', x) = \frac{1}{2}\int_x^{x'} \left[H(s), \int_x^s H(t)\mathrm{d}t\right] \mathrm{d}s \tag{8b}$$

$$A_3(x', x) = \frac{1}{4}\int_x^{x'} \left[H(s), \int_x^s \left[H(t), \int_x^t H(u)\mathrm{d}u\right] \mathrm{d}t\right] \mathrm{d}s + \frac{1}{12}\int_x^{x'} \left[\left[H(s), \int_x^s H(t), \mathrm{d}t\right], \int_x^s H(t)\mathrm{d}t\right] \mathrm{d}s, \tag{8c}$$

$$A_4(x', x) = \frac{1}{8}\int_x^{x'} \left[H(s), \int_x^s \left[H(t), \int_x^t \left[H(u), \int_x^u H(v)\mathrm{d}v\right] \mathrm{d}u\right] \mathrm{d}t\right] \mathrm{d}s + \frac{1}{24}\int_x^{x'} \left[H(s), \int_x^s \left[\left[H(t), \int_x^t H(u)\mathrm{d}u\right], \int_x^t H(v)\mathrm{d}v\right] \mathrm{d}t\right] \mathrm{d}s + \frac{1}{24}\int_x^{x'} \left[\left[H(s), \int_x^s \left[H(t), \int_x^t H(u)\mathrm{d}u\right] \mathrm{d}t\right], \int_x^s H(v)\mathrm{d}v\right] \mathrm{d}s + \frac{1}{24}\int_x^{x'} \left[\left[H(s), \int_x^s H(t)\mathrm{d}t\right], \int_x^s \left[H(t), \int_x^s H(u)\mathrm{d}u\right] \mathrm{d}t\right] \mathrm{d}s. \tag{8d}$$

This expansion provides a systematic way of improving the propagation matrix.

In order to simplify the discussion of the properties of the propagation matrix we introduce the matrices

$$M_0 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad M_+ = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad M_- = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \tag{9}$$

which span the split 3-dimensional simple Lie algebra [21] as follows from the commutation relations

$$[M_0, M_\pm] = \pm 2M_\pm, \qquad [M_+, M_-] = M_0. \tag{10}$$

Because $H(x)$ belongs to the algebra:

$$H(x) = M_+ + q(x)M_-, \tag{11}$$

then $A(x', x)$ belongs to it too and can be written [21,22]

$$A(x', x) = a_0(x', x)M_0 + a_+(x', x)M_+ + a_-(x', x)M_-, \tag{12}$$

where $a_0(x, x) = a_+(x, x) = a_-(x, x) = 0$. One can easily write the propagation matrix in terms of the eigenvalues $\pm a$, $a = (a_0^2 + a_+a_-)^{1/2}$ of the traceless matrix $A(x', x)$:

$$U = I \cdot \cosh a + A \cdot \sinh a/a, \tag{13}$$

where $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$. When $a_0^2 + a_+a_- < 0$ then we replace $\cosh a$ and $\sinh a/a$ by $\cos\alpha$ and $\sin\alpha/\alpha$, respectively, with $\alpha^2 = -a^2$. According to [13] the determinant of U equals unity as expected from the fact that this determinant is the Wronskian of the functions u and v mentioned before. It is a remarkable property of the Magnus expansion that its truncation at any order preserves the value of the Wronskian.

Light and co-workers [12–15] showed that the Magnus expansion provides a good approximation to $A(x', x)$. In what follows we discuss some appealing properties of the first order approach, namely $A(x', x) \cong A_1(x', x)$. In this case

$$a_0 = 0, \quad a_+ = x' - x = h, \quad a_- = \int_x^{x'} q(s)ds, \tag{14}$$

In the neighborhood of a classical turning point, $q(x) = 0$, one has $a_- \cong q'(x)h^2/2$, $a^2 \cong q'(x)h^3/2$, $\cosh a \cong 1$, and $\sinh a/a \cong 1$ provided $|h| \ll 1$. Therefore, the approximate eigenfunction propagates in the correct way: $\psi(x') \cong \psi(x) + (x' - x)\psi'(x)$ [25].

When the form of the potential does not allow to calculate the integral in Eq. (14) analytically one may either solve it numerically or use an appropriate reference potential [25]. If we choose a constant reference potential $\bar{q}$ then $a_- = \bar{q}h$

and the present algorithm reduces to those proposed, by Canosa and Oliveira [26] and Papageorgiou and Raptis [27]. The latter, based on the equations of the transmission-line theory, yields remarkably accurate eigenvalues. It is therefore sensible to expect even better results when the integral in Eq. (14) is exactly or more accurately calculated.

From a practical point of view one replaces a boundary condition at infinity $\psi(x \to \infty) = 0$ by $\psi(x^*) = 0$ for a large enough x^* values. Therefore, if $h = x' - x \ll 1$ and we choose $x' = x^*$ so that $ha_- \gg 1$, then $\cosh[(ha_-)^{1/2}] \cong \sinh[(ha_-)^{1/2}] \cong \exp(ha_-)^{1/2}$ and $a_- \cong q(x)h$ which leads to the proper large $-x$ behavior $\psi'(x)/\psi(x) \cong -q(x)^{1/2}$.

In addition to this, we expect the first-order approach to be remarkably accurate for large x values when $V(x \to \infty) = 0$ because $H(x)$ approaches a constant matrix and the commutators in Eqs. (8b)–(8d) vanish in that limit. For this reason the exponential propagation matrix method described here may be successful in treating internuclear potential of diatomic molecules.

When $V(x)$ is a relatively simple function of the coordinate as in the case of polynomial and exponential potentials, one can easily calculate many terms in the Magnus expansion. Because of the form of $H(x)$ and the commutation relations (10) the odd- and even-order terms contribute only to the off-diagonal and diagonal elements of $A(x', x)$, respectively. The series for $A = A_1$ is accurate up to terms that are of second order in h. A straightforward but tedious calculation shows that when $A = A_1 + A_2 + \cdots + A_{2k}$, $k > 1$, the series $\psi(x') = \psi(x) + \psi'(x)h + q(x)\psi(x)h^2/2 + \cdots$ is exactly reproduced up to terms of order h^{2k+2}. For the sake of brevity the propagation matrices obtained from $A = A_1$, $A = A_1 + A_2$ and $A = A_1 + A_2 + A_3 + A_4$ will be denoted FOPM, SOPM, and TOPM, (first-, second-, and third-order propagation matrix), respectively.

III. RESULTS AND DISCUSSION

According to what we showed in the previous section, the Magnus expansion serves with a remarkable approximation to the propagation matrix $U(x', x)$ provided $|x' - x|$ is small enough. The propagation matrix for large intervals is easily constructed by successive application of the rule $U(x'', x) = U(x'', x')U(x', x)$.

For the sake of concreteness in what follows we assume that the boundary conditions are $\psi(-\infty) = \psi(\infty) = 0$, which for practical purpose are replaced by $\psi(x_L) = \psi(x_R) = 0$, where $x_L \ll 0 \ll x_R$. We choose an appropriate coordinate value x_0 within the interval (x_L, x_R) and integrate the Schrödinger equation from x_L to x_0 and from x_R to x_0 along the lattice x_L, $x_L + h, \ldots, x_L + mh = x_0$, $x_0 + h, \ldots, x_0 + nh = x_R$ by means of the propagation matrices

$$U(x_0, x_R) = \prod_{j=1}^{n} U(x_R - jh, x_R - jh + h), \tag{15a}$$

$$U(x_0, x_L) = \prod_{j=1}^{m} U(x_L + jh, x_L + jh - h), \tag{15b}$$

Because of the boundary conditions and that $\Phi(x_0) = U(x_0, x_L)\Phi(x_L) = U(x_0, x_R)\Phi(x_R)$ it follows that

$$[v(x, x_R)\partial v(x, x_L)/\partial x - v(x, x_L)\partial v(x, x_R)/\partial x]_{x=x_0} = 0, \tag{16}$$

where $v(x, x_R)$, $\partial v(x, x_R)/\partial x$, $v(x, x_L)$, and $\partial v(x, x_L)/\partial x$ are elements of $U(x, x_R)$ and $U(x, x_L)$ as shown in Eqs. (5). The roots of Eq. (16) are the eigenvalues of the Schrödinger equation. If $\psi(x)$ is normalized so that $\psi(x_0) = 1$, then $\psi'(x_R) = 1/v(x_0, x_R)$, $\psi'(x_L) = 1/v(x_0, x_L)$ and $\psi(x) = v(x, x_R)/v(x_0, x_R) = v(x, x_L)/v(x_0, x_L)$.

Since the physical solution is minimal with respect to the outward integration scheme and dominant for the inward one, the latter is chosen because it is stable at every point [28]. Both procedures yield accurate eigenvalues but only the inward integration provides acceptable eigenfunctions which are necessary for the calculation of expectation values, matrix elements, etc..

The calculation is much easier when $V(x)$ is parity invariant because as the eigenfunctions are even or odd functions of the coordinate the propagation from x_R

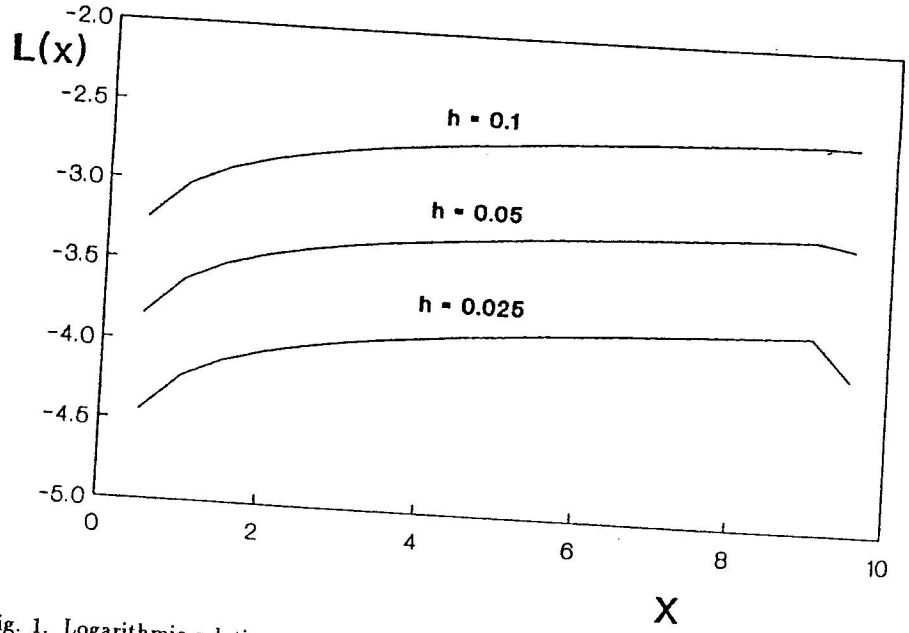

Fig. 1. Logarithmic relative error $L(x) = \log|[\psi(x) - \psi_{app}(x)]/\psi_{app}(x)|$ for the ground-state wavefunction of the harmonic oscillator calculated with the first order propagation matrix and several h values.

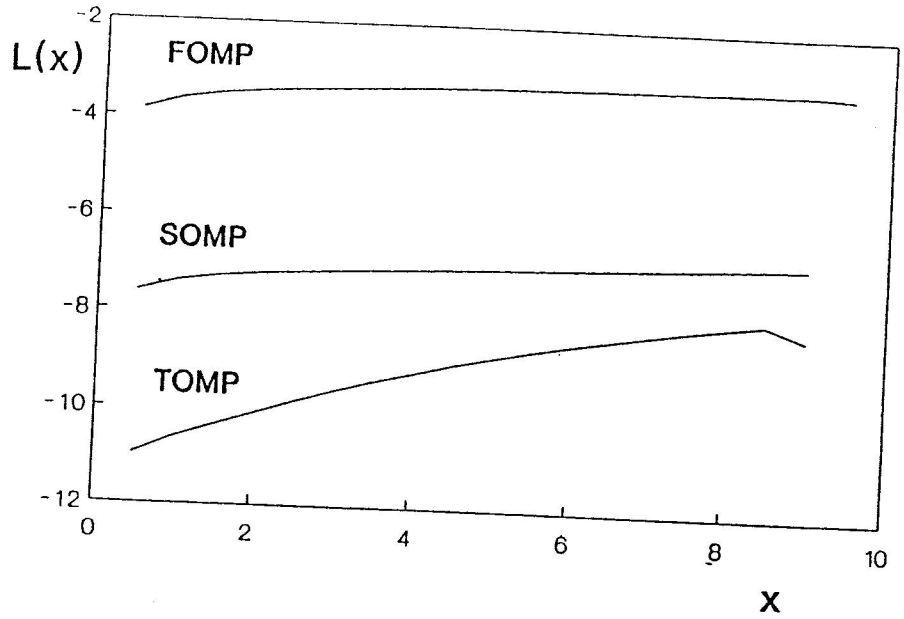

Fig. 2. Logarithmic relative error $L(x) = \log|[\psi(x) - \psi_{app}(x)]/\psi_{app}(x)|$ for the ground-state wavefunction of the harmonic oscillator calculated with the first, second and third order propagation Matrices and $h = 0.05$.

to $x_0 = 0$ is sufficient. Furthermore, the eigenvalues are determined by the roots of

$$v(0, x_R)[\partial v(x, x_R)/\partial x]_{x=0} = 0. \tag{17}$$

If we normalize the even and odd states so that $\psi(0) = 1$ and $\psi'(0) = 1$, respectively, then we can write them in terms of the elements of the propagation matrix as $\psi(x) = v(x, x_R)/v(0, x_R)$ and $\psi(x) = v(x, x_R)/[\partial v(x, x_R)/\partial x]_{x=0}$, respectively.

Among the exactly solvable models we choose the harmonic oscillator to test the method because its potential, $V(x) = x^2$, is simple enough to allow the calculation of several terms of the Magnus expansion analytically. In figures 1 and 2 we compare the ground-state eigenfunction obtained approximatelly with the boundary condition $\psi_{app}(0) = 1$ and $E = 1$, and the exact eigenfunction $\psi(x) = \exp(-x^2/2)$. The plots of the logarithmic relative deviation $\log|[\psi(x) - \psi_{app}(x)]/\psi(x)|$ show that the accuracy of the numerically computed eigenfunction increases as h decreases (Fig. 1) or the number of terms in the Magnus expansion increases (Fig. 2). The agreement is remarkable even for the FOPM. In the light of these results we conclude that the matrix propagation method and the Magnus expansion may prove useful in the calculation of physical observables.

Table 1 shows the ground-state eigenvalue calculated by the FOPM for sev-

Table 1
Ground-state eigenvalue of the harmonic oscillator calculated with the first-order propagation matrix and different h and x_R values.

x_R	$h = 0.1$	$h = 0.05$	$h = 0.025$
3.0	1.0021076573921	1.0010057197181	1.0007834086428
4.0	1.0016668366891	1.0004173145352	1.0001049742361
5.0	1.0016663882838	1.0004166493890	1.0001041657014
6.0	1.0016663882268	1.0004166492952	1.0001041655814
7.0	1.0016663882268	1.0004166492952	1.0001041655814

eral values of h and x_R. We notice that the difference between the approximate eigenvalue and the exact one, $E = 1$, is of order h^2 and that the accuracy is not noticeably improved by increasing x_R beynod $x_R = 5$. Clearly, for larger eigenvalues one has to consider larger values of x_R.

In Table 2 we show the first six eigenvalues calculated with $x_R = 10$. One can verify that the difference between the approximate eigenvalues obtained by means of the kth-order Magnus expansion and the exact ones, $E_n = 2n + 1$, is of order h^{2k}. We also notice that the FOPM error is energy independent. However, other model potentials do not exhibit such a nice feature.

In order to evaluate the performance of the propagation matrix method in the study of vibrational-rotational energies of diatomic molecules we apply it to the Morse oscillator. The radial part of the Schrödinger equation can be written $\psi''(x) = q(x)\psi(x)$ in which $q(x) = U(x) - E$. The bound states satisfy the boundary conditions $\psi(0) = \psi(\infty) = 0$ and can therefore be treated as discussed before. For comparison purpose we write the effective potential $U(x)$ as

$$U(x) = \frac{J(J+1)}{x^2} + D\left[e^{-2b(x-x_e)} - 2e^{-b(x-x_e)}\right], \qquad (18)$$

so that the Bohr radius a_B and $\hbar^2/(2\mu a_B^2)$ are respectively the units of length and energy. We also choose the parameters $D = 188.4355$, $x_e = 1.9975$ and $b = 0.711248$ in these units which correspond to the state B of the hydrogen-ion molecule. In Table 3 we display the lowest vibrational-rotational energies obtained by means of the procedure described in the previous section with $x_0 = x_e$, $x_L = 0.2$, $x_R = 8.0$, and $h = 0.01$. The agreement between the results of our calculation and the exact eigenvalues, available for $J = 0$, is remarkable. We expect that the accuracy of the eigenvalues with non zero rotational quantum number is similar because we used the same convergence criterion (i.e. stability when one increases x_R or decreases x_0 or h). In accordance with the argument of the previous section our FOPM results agree exactly with those of Papageorgiou and Raptis [27]. Our SOPM energies are approximately as accurate as those of Kobeissi [23], one order of magnitude more accurate than those of Hajj et al. [4] and two orders of magnitude more accurate than those of Cooley [2]. Finally our TOPM results are in better agreement with the exact eigenvalues than those mentioned above.

Table 2
Lowest eingenvalues of the harmonic oscillator calculated with the first-, second- and third- order propagation matrices for $x_0 = 0$, $x_R = 10$, and different values of h.

h	FOMP	SOMP	TOMP
		$n = 0$	
0.100	1.001666388226746	1.000001112299251	1.000000001667552
0.050	1.000416649295219	1.000000069463037	1.000000000026109
0.025	1.000104165581436	1.000000004340568	1.000000000000408
		$n = 1$	
0.100	3.001665832139755	3.000003333986899	3.000000004834050
0.050	3.000416614564720	3.000000208343637	3.000000000075681
0.025	3.000104163411168	3.000000013020995	3.000000000001183
		$n = 2$	
0.100	5.001665275521265	5.000005555143052	5.000000011178325
0.050	5.000416579825945	5.000000347215961	5.000000000174868
0.025	5.000104161240770	5.000000021701292	5.000000000002733
		$n = 3$	
0.100	7.001664718369674	7.000007775766107	7.000000020702477
0.050	7.000416545078887	7.000000486080002	7.000000000323679
0.025	7.000104159070244	7.000000030381460	7.000000000005058
		$n = 4$	
0.100	9.001664160683368	9.000009995854451	9.000000033408599
0.050	9.000416510323541	9.000000624935754	9.000000000522122
0.025	9.000104156899588	9.000000039061498	9.000000000008159
		$n = 5$	
0.100	11.001663602460729	11.000012215406464	11.000000049298775
0.050	11.000416475559899	11.000000763783211	11.000000000770205
0.025	11.000104154728803	11.000000047741408	11.000000000012034

Numerical calculation of the integrals in the terms of the Magnus expansion makes the algorithm remarkably lengthier and slower. For this reason, if a model potential is too complicated to allow the calculation of those integrals in analytic closed form one may keep just the first term in the Magnus expansion and use the constant reference potential $V(x+h/2)$ within the interval $(x, x+h)$. The resulting exponent $A(x+h, x)$ will be given by Eqs. (12) and (14) with $a_- = hq(x+h/2)$. Although this approach requires the use of smaller step sizes it commonly proves preferable.

Throughout this paper we have shown that the exponential propagation matrix method and the Magnus expansion form a simple, highly accurate algorithm to calculate eigenvalues and eigenfunctions of the Schrödinger equation for one-dimensional and central-field models. The calculation can be performed on a microcomputer. In fact, the results we present here have been obtained by means of a program written in Turbo Pascal on a PC XT. In principle one can improve

Table 3

Eigenvalues for the Morse potential for several values of the vibrational (v) and rotational (J) quantum numbers. The numbers of terms in the Magnus expansion is N.

N	$v=0$	$J=0$	$J=1$
1		−178.797764588577943	−178.305284925476544
2		−178.798538263551342	−178.306057346579050
3		−178.798538351031139	−178.306057433805927
exact		−178.79853835103135	
	$v=1$		
1		−160.282693070230953	−159.807412114368549
2		−160.283425366433451	−159.808143277319149
3		−160.283425629321983	−159.808143539451210
exact		−160.28342562935005	
	$v=2$		
1		−142.779368978548474	−142.322221347803915
2		−142.780059933044415	−142.322911278602185
3		−142.780060342604629	−142.322911686955199
exact		−142.78006034267675	
	$v=3$		
1		−126.287792314811521	−125.849707749928826
2		−126.288441962582927	−125.850356471043171
3		−126.288442490885826	−125.850356997793219
exact		−126.28844249101145	
	$v=4$		
1		−110.807963079963385	−110.389863575645176
2		−110.808571453909974	−110.390471106177972
3		−110.808572074171305	−110.390471724530183
exact		−110.80857207435415	
	$v=5$		
1		−96.339881273700874	−95.942678471062490
2		−96.340448404640197	−95.943244826946290
3		−96.340449092465841	−95.943245512547490
exact		−96.34044909270485	
	$v=6$		
1		−82.883546896484921	−82.508139887978412
2		−82.884072813152286	−82.508665082198600
3		−82.884073545773321	−82.508665812334915
exact		−82.88407354606355	
	$v=7$		
1		−70.438959949112103	−70.086233694882317
2		−70.439444678160498	−70.086717737720646
3		−70.439445434096805	−70.086718490916164
exact		−70.43944543443025	

Table 3 (Cont.)

N	$v=0$	$J=2$	$J=3$
1		−177.324343077462638	−175.862844315222742
2		−177.325112977160980	−175.863610400705706
3		−177.325113063846190	−175.863610486606128
	$v=1$		
1		−158.861012919805932	−157.451673688588836
2		−158.861741795528077	−157.452399084639656
3		−158.861742056143295	−157.452399342998815
	$v=2$		
1		−141.412215136104537	−140.057763901599275
2		−141.412902991747627	−140.058448579122801
3		−141.412903397728808	−140.058448981503592
	$v=3$		
1		−124.977933107718840	−123.681076113324522
2		−124.978579940938608	−123.681720033362405
3		−124.978580464559739	−123.681720552234221
	$v=4$		
1		−109.558141827448123	−108.321555385382127
2		−109.558747630162724	−108.322158500139055
3		−109.558748244697432	−108.322159108943331
	$v=5$		
1		−95.152808748758670	−93.979132568992602
2		−95.153373507738873	−93.979694823016627
3		−95.153374188884343	−93.979695497461006
	$v=6$		
1		−81.761895095920529	−80.653727126298957
2		−81.762418793452762	−80.654248457787434
3		−81.762419518573245	−80.654249175356335
	$v=7$		
1		−69.385357776970358	−68.345251184298163
2		−69.385840391574348	−68.345731526490861
3		−69.385841139323821	−68.345732265991193

the method by means of appropriate transformations that diagonalize $H(x)$ [12–16]. However, if one is mainly interested in bound states this modification seems unnecessary.

There are other approaches that lead to a propagation matrix with a determinant of one. For instance, we can write the propagation matrix as an infinite product of exponential matrices as shown by Fer [29] and Wilcox [30]. The for-

mer approach is more accurate but the latter is much simpler [31]. An alternative strategy is based on the fact that the propagation matrix can be exactly written as

$$U(x',x) = \exp[b_0(x',x)M_0]\exp[b_+(x',x)M_+]\exp[b_-(x',x)M_-], \qquad (19)$$

where b_0, b_+ and b_- are solutions of a system of first-order nonlinear ordinary equations [21]. A straight forward calculation shows that

$$b_0(x',x) = -\ln[\partial v(x',x)/\partial x'],\ b_+(x',x) = v(x',x)\partial v(x',x)/\partial x'$$
$$b_-(x',x) = [\partial u(x',x)/\partial x']/[\partial v(x',x)/\partial x'], \qquad (20)$$

from which it follows that the product form (18) can be used provided $\partial v(x',x)/\partial x' > 0$. This condition is always met if $h = |x'-x|$ is small enough because as $\partial v(x',x)/\partial x' = 1$ at $x' = x$ then this derivative should be positive in a neighborhood of that point.

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