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Exponentially-fitted Störmer/Verlet methods[1]

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Abstract: Exponentially-fitted Störmer/Verlet methods are constructed taking into account a six-step flow chart. It is shown that the thus constructed methods, when applied to strongly oscillating problems, are equivalent respectively to Gautschi and Deulfhard methods. As an illustration the constructed algorithms are used to solve bounded states as well as resonance states of Schrödinger equations. It is seen that all the versions are of order four but the way the error on the eigenvalues increases with the energy differs from one version to the other for the two problems considered.

Keywords: Exponetial fitting, Störmer/Verlet, oscillating problems, Schrödinger equations.

Mathematics Subject Classification: 65L05,65L12

1 Introduction

In this paper we consider systems of second order differential equations

$$y'' = f(y) \, , \tag{1}$$

where the right-hand side $f(y)$ does not depend on y'. Many problems in molecular dynamics, nuclear and atomic physics, etc. are of this form. If we choose a step size h and grid points $t_n = t_0 + nh$, the most simple and natural discretization of (1) is

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f(y_n) \, , \tag{2}$$

which determines y_{n+1} whenever y_{n-1} and y_n are known. The above method is known in the literature under various names. Especially in molecular dynamics it is often called the *Verlet method* [1]. Another name for this method is *Störmer method* of lowest order, since C. Störmer [2] used higher-order variants of it for his computations of the motion of ionised particles in the earth's magnetic field. Mainly in the context of partial differential equations of wave propagation, this method is called the *leap-frog method*. In this paper we shall construct two versions of the exponentially-fitted (EF) form of the Störmer/Verlet method by taking into account the six-step flow chart described by Ixaru and Vanden Berghe [3, 4].

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2 Construction of the EF-forms of the Störmer/Verlet algorithm

We use the six-step procedure described in [3], pp. 68–70.

Step *i*
The appropriate form of the operator $\mathcal{L}[h, \mathbf{a}]$ and the expressions of the corresponding classical moments.

A Störmer/Verlet method has the following general form

$$y_{n+1} + a_2 y_n + a_3 y_{n-1} = h^2 a_4 f(y_n) \ . \tag{3}$$

The corresponding operator reads

$$\mathcal{L}[h, \mathbf{a}]y(t) := y(t+h) + a_2 y(t) + a_3 y(t-h) - h^2 a_4 y''(t) \ , \tag{4}$$

and $\mathbf{a} := [a_2, a_3, a_4]$. $\mathcal{L}$ is dimensionless and the dimension l as described in [3] is 0. The operator applied to $1, t, t^2, t^3$ and t^4 results in

$$\begin{aligned}
\mathcal{L}[h, \mathbf{a}]1 &= 1 + a_2 + a_3 \ , \\
\mathcal{L}[h, \mathbf{a}]t &= (t+h) + a_2 t + a_3 (t-h) \ , \\
\mathcal{L}[h, \mathbf{a}]t^2 &= (t+h)^2 + a_2 t^2 + a_3 (t-h)^2 - 2h^2 a_4 \ , \\
\mathcal{L}[h, \mathbf{a}]t^3 &= (t+h)^3 + a_2 t^3 + a_3 (t-h)^3 - 6h^2 a_4 t \ , \\
\mathcal{L}[h, \mathbf{a}]t^4 &= (t+h)^4 + a_2 t^4 + a_3 (t-h)^4 - 12h^2 a_4 t^2 \ ,
\end{aligned}$$

and the corresponding classical moments defined as $L_m(h, \mathbf{a}) := \mathcal{L}[h, \mathbf{a}]t^m$ for $t = 0$ and the dimensionless moments $L_m^*(\mathbf{a}) = h^{-l-m} L_m(h, \mathbf{a})$ are respectively

$$\begin{aligned}
L_0(h, \mathbf{a}) &= 1 + a_2 + a_3 = L_0^*(\mathbf{a}) \\
L_1(h, \mathbf{a}) &= h(1 - a_3) = hL_1^*(\mathbf{a}) \\
L_2(h, \mathbf{a}) &= h^2(1 + a_3 - 2a_4) = h^2 L_2^*(\mathbf{a}) \\
L_3(h, \mathbf{a}) &= h^3(1 - a_3) = h^3 L_3^*(\mathbf{a}) \\
L_4(h, \mathbf{a}) &= h^4(1 + a_3) = h^4 L_4^*(\mathbf{a}) \ .
\end{aligned}$$

Step *ii*
Examination of the algebraic system

$$L_m^*(\mathbf{a}) = 0, \quad m = 0, 1, 2, \ldots, M-1$$

to find out the maximal M for which it is compatible.

In our case the algebraic system

$$\begin{aligned}
L_0^* &= 1 + a_2 + a_3 = 0 \\
L_1^* &= 1 - a_3 = 0 \\
L_2^* &= 1 + a_3 - 2a_4 = 0 \\
L_3^* &= 1 - a_3 = 0
\end{aligned}$$

is compatible and one finds $M = 4$ and

$$a_3 = 1, \quad a_4 = 1, \quad a_2 = -2 \,. \tag{5}$$

This results in the classical Störmer/Verlet method (2):

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f(y_n) \,.$$

Step *iii*

Construction of the formal expressions of $E_0^*(z, \mathbf{a})$, $G^{\pm}(Z, \mathbf{a})$ and $G^{\pm(p)}(Z, \mathbf{a})$.

By definition one has

$$E_0(h, \mu, \mathbf{a}) := \mathcal{L}[h, \mathbf{a}] \exp(\mu t)_{|t=0} = h^l E_0^*(z, \mathbf{a}) \,,$$

with $z := \mu h$. For our problem one finds

$$E_0^*(\pm z, \mathbf{a}) = \exp(\pm z) + a_2 + a_3 \exp(\mp z) - z^2 a_4$$

Write the expressions for $G^{\pm}(Z, \mathbf{a})$, where $Z := z^2$ as

$$\begin{aligned} G^+(Z, \mathbf{a}) &= \frac{1}{2}[E_0^*(z, \mathbf{a}) + E_0^*(-z, \mathbf{a})] \\ &= (1 + a_3)\frac{[\exp(z) + \exp(-z)]}{2} + a_2 - z^2 a_4 \\ G^-(Z, \mathbf{a}) &= \frac{1}{2z}[E_0^*(z, \mathbf{a}) - E_0^*(-z, \mathbf{a})] \\ &= (1 - a_3)\frac{[\exp(z) - \exp(-z)]}{2z} \end{aligned}$$

Since in further applications in this paper we shall only consider the trigonometric case, i.e. instead of $\exp(\pm\mu t)$, we shall consider sine and cosine functions, one can choose $z = \mu h = i\omega h$, i.e. $z^2 = -\omega^2 h^2 = Z$. Under this assumption one finds

$$\begin{aligned} G^+(Z, \mathbf{a}) &= (1 + a_3)\cos(\sqrt{|Z|}) + a_2 - Z a_4 \\ G^-(Z, \mathbf{a}) &= (1 - a_3)\frac{\sin(\sqrt{|Z|})}{\sqrt{|Z|}} = (1 - a_3)\,\mathrm{sinc}(\sqrt{|Z|}) \,. \end{aligned}$$

Herein $\mathrm{sinc}(x)$ is defined as

$$\mathrm{sinc}(x) = \begin{cases} \dfrac{\sin(x)}{x} & x \neq 0 \\ 1 & x = 0 \end{cases} \,.$$

As for the first order derivative of $G^{\pm}(Z, \mathbf{a})$ w.r.t. Z one obtains

$$\begin{aligned} G^{+(1)}(Z, \mathbf{a}) &= (1 + a_3)\frac{\mathrm{sinc}(\sqrt{|Z|})}{2} - a_4 \\ G^{-(1)}(Z, \mathbf{a}) &= (1 - a_3)\frac{\left[\mathrm{sinc}(\sqrt{|Z|}) - \cos(\sqrt{|Z|})\right]}{2|Z|} \end{aligned}$$

Step *iv*

Consider the reference set of M functions:

$$
\begin{aligned}
&1, t, t^2, \ldots, t^K \\
&\exp(\pm\mu t), t\exp(\pm\mu t), \ldots, t^P \exp(\pm\mu t) \\
&\text{or} \\
&1, t, t^2, \ldots, t^K \\
&\cos(\omega t), \sin(\omega t), t\sin(\omega t), t\cos(\omega t), \ldots, t^P \sin(\omega t), t^P \cos(\omega t)
\end{aligned}
$$

with $K + 2P = M - 3$.

Since for our problem $M = 4$, we have three possiblities:

- $K = 3, P = -1$, the classical case with the set $1, t, t^2, t^3$.
- $K = 1, P = 0$, the mixed case with the set $1, t, \exp(\pm\mu t)$ or $1, t, \sin(\omega t), \cos(\omega t)$.
- $K = -1, P = 1$, the pure EF case with the set $\exp(\pm\mu t), t\exp(\pm\mu t)$ or $\sin(\omega t), \cos(\omega t), t\sin(\omega t), t\cos(\omega t)$.

Step *v*

Solve the algebraic system

$$L_k^* = 0, \quad 0 \le k \le K, \qquad G^{(p)\pm}(Z, \mathbf{a}) = 0, \quad 0 \le p \le P\ .$$

In the classical case ($K = 3, P = -1$) we know already the solution, i.e. (5).
In the mixed case ($K = 1, P = 0$) one obtains

$$a_3 = 1, \quad a_2 = -2, \quad a_4 = \frac{\sin^2(\sqrt{|Z|}/2)}{|Z|/4} = \text{sinc}^2(\sqrt{|Z|}/2) = \text{sinc}^2(\omega h/2)\ .$$

This gives rise to the method

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \,\text{sinc}^2(\omega h/2) f(y_n)\ , \tag{6}$$

which is of the so-called *Gautschi* type [5]. This Gautschi type version has been studied in detail by the present authors elsewere [6, 7]. In the last mentioned paper it is shown that various interpretations can be given to that version of the Störmer/Verlet method. One can consider the two-step formulation as given here, but also a one-step formulation is possible. It can be interpreted as a composition method, a splitting method and an variational integrator. It can be extended to general partitioned problems. The method preserves geometric properties of the flow of differential equations such as reversibility, symplecticity and volume conservation. This version applied to a Hamiltonian system is symplectic and preserves linear first integrals.

In the case of highly oscillating problems, i.e. problems where the right-hand side of (1) can be written as

$$f(y) = -\omega^2 y + g(y) \tag{7}$$

with $\omega \gg 1$ (6) reduces to

$$y_{n+1} - 2\cos(\omega h) y_n + y_{n-1} = h^2 \operatorname{sinc}^2(\omega h/2) g(y_n) \ .$$

In the pure EF case ($K = -1, P = 1$) one obtains

$$a_3 = 1, \quad a_2 = -(2\cos(\sqrt{|Z|}) + \sqrt{|Z|}\sin(\sqrt{|Z|})), \quad a_4 = \operatorname{sinc}(\sqrt{|Z|})$$

or

$$a_3 = 1, \quad a_2 = -(2\cos(\omega h) + \omega h \sin(\omega h)), \quad a_4 = \operatorname{sinc}(\omega h) \ ,$$

giving rise to the equation

$$y_{n+1} - (2\cos(\omega h) + \omega h \sin(\omega h)) y_n + y_{n-1} = h^2 \operatorname{sinc}(\omega h) f(y_n) \ . \tag{8}$$

In case $f(y)$ is given by (7) the relation (8) reduces to

$$y_{n+1} - 2\cos(\omega h) y_n + y_{n-1} = h^2 \operatorname{sinc}(\omega h) g(y_n) \ ,$$

which is known as the *Deuflhard* formula [8].

Step *vi*

The leading term of the error of the formula obtained in this way reads [3]

$$lte_{ef} = (-1)^{P+1} h^{l+M} \ \frac{L^*_{K+1}(\mathbf{a})}{(K+1)! Z^{P+1}} \ D^{K+1}(D^2 - \mu^2)^{P+1} y(t_n), \tag{9}$$

whereby $\mu = i\ \omega$. For the three methods constructed one finds the following results:

- $K = 3, P = -1$

$$lte_{ef} = \frac{h^4}{12} y^{(4)}(t_n) \ . \tag{10}$$

- $K = 1, P = 0$

$$lte_{ef} = -h^4 \ \frac{|Z| - 4\sin^2(\sqrt{|Z|}/2)}{|Z|^2} (\omega^2 y^{(2)}(t_n) + y^{(4)}(t_n)) \ . \tag{11}$$

- $K = -1, P = 1$

$$lte_{ef} = h^4 \ \frac{2 - (2\cos(\sqrt{|Z|}) + \sqrt{|Z|}\sin(\sqrt{|Z|}))}{|Z|^2} (\omega^4 y(t_n) + 2\omega^2 y^{(2)}(t_n) + y^{(4)}(t_n)) \ . \tag{12}$$

3 The Störmer/Verlet methods applied to Schrödinger equations

3.1 The bounded states problem

In the past there has been much interest in problems requiring efficient and accurate computation of a large number of eigenvalues of regular Sturm-Liouville problems and/or Schrödinger problems, which can be written without loss of generality as

$$-y"(t) + q(t) y(t) = \lambda y(t) \ , \tag{13}$$

with boundary condtions of the type

$$y(0) = y(\pi) = 0 \ .$$

When finite difference methods are used to approximate the eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \ldots$ of (13) by the eigenvalues $\lambda_1^{(n)} < \lambda_2^{(n)} < \lambda_3^{(n)} < \ldots$ of an algebraic eigenvalue problem of order n, the error $|\lambda_k^{(n)} - \lambda_k|$, $(k = 1, 2, \ldots, n)$ is known to increase rapidly with k [11]. Much efforts have been devoted to finding more uniformly valid approximations by either using so-called asymptotic corrections [11]–[14] or by introducing finite difference schemes with frequency-dependent coefficients [6, 15], methods which are equivalent to the EF algorithms of the present paper.

It is well known [16] that for general $q(t)$ the exact eigenvalues of (13) are given by

$$\lambda_l = l^2 + \frac{1}{\pi}\int_0^\pi q(t)dt + \mathcal{O}(l^{-2}), \quad (l = 1, 2, 3, \ldots) \ .$$

Without loss of generality one can assume that

$$\int_0^\pi q(t)dt = 0$$

since it imposes the same constant translation on each of the λ_l and on each of the numerical determined eigenvalues. Under this assumption, it follows that

$$\lambda_l = l^2 + \mathcal{O}(l^{-2}), \quad l = 1, 2, 3 \ldots . \tag{14}$$

Paine et *al.* [11] also proved that (for $q \neq 0$) the general eigenfunction of (13) corresponding to λ_l is given by

$$y_l(t) = C_l \sin(lt) + \frac{1}{l}\int_0^t (l^2 - \lambda_l - q(x)) \sin(l(t - x))y(x)dx, \quad (l = 1, 2, 3, \ldots) \ , \tag{15}$$

where, since y_l is arbitrary up to a scalar multiple, we can set $C_l = 1 \quad (l = 1, 2, 3, \ldots)$. Taking this remark in account one can write the eigenvalue as

$$y_l(t) = \sin(lt) + e_l(t) \ , \tag{16}$$

where e_l is the integral defined in (15). Since

$$e_l^{(j)}(x) = \mathcal{O}(l^{j-1}), (j = 0, 1, 2, \ldots) \ , \tag{17}$$

the sine function is a first order approximation for $y(t)$.

By considering the three versions of the Störmer/Verlet method (2), (6) and (8) and a uniform mesh length $h := \pi/(n + 1), \lambda_1, \ldots, \lambda_n$ are approximated by the eigenvalues $\sigma_1^{(n)}(K, P) < \ldots < \sigma_n^{(n)}(K, P)$ of the generalized algebraic eigenvalue problem

$$-A(K, P)\mathbf{v} + B(K, P) \ Q\mathbf{v} = \sigma(K, P)B(K, P)\mathbf{v} \tag{18}$$

where

$$Q := \mathrm{diag}(q(t_1), \ldots, q(t_n)) \text{ with } t_j := jh, (j = 1, \ldots, n) \ .$$

$B(K, P)$ are diagonal matrices and the $A(K, P) := (a_{ij}(K, P))$ are symmetric tridiagonal with

- $K = 3, P = -1$

$$a_{ii}(3,-1) = -\frac{2}{h^2}, (i = 1, \ldots, n) \quad a_{ii\pm 1}(3,-1) = \frac{1}{h^2}, (i = 1, \ldots, n-1) \ ,$$

$$B(3,-1) := \mathrm{diag}(1, 1, \ldots, 1) \ ,$$

- $K = 1, P = 0$

$$a_{ii}(1,0) = -\frac{2}{h^2}, (i = 1, \ldots, n) \quad a_{ii\pm 1}(1,0) = \frac{1}{h^2}, (i = 1, \ldots, n-1) \ ,$$

$$B(1,0) := \mathrm{diag}(\mathrm{sinc}^2(\omega h/2), \mathrm{sinc}^2(\omega h/2), \ldots, \mathrm{sinc}^2(\omega h/2)) = \mathrm{sinc}^2(\omega h/2)\mathrm{diag}(1, 1, \ldots, 1) \ ,$$

- $K = -1, P = 1$

$$\begin{aligned} a_{ii}(-1,1) &= -\frac{2\cos(\omega h) + \omega h \sin(\omega h)}{h^2}, \quad (i = 1, \ldots, n) \\ a_{ii\pm 1}(-1,1) &= \frac{1}{h^2}, (i = 1, \ldots, n-1) \ , \end{aligned} \tag{19}$$

$$B(-1,1) := \mathrm{diag}(\mathrm{sinc}(\omega h)\,\mathrm{sinc}(\omega h), \ldots, \mathrm{sinc}(\omega h)) = \mathrm{sinc}(\omega h)\mathrm{diag}(1, 1, \ldots, 1) \ . \tag{20}$$

When $q \equiv 0$ the corresponding algebraic eigenvalues (i.e. the eigenvalues of $(-B(-1,1)^{-1}A(-1,1))$ (the case $(K, P) = (1, 0)$ has been treated in [6]) are given by

$$\mu_s^{(n)} = \frac{\omega}{h \sin(\omega h)} \left[2\cos(\omega h) + \omega h \sin(\omega h) - 2\cos(sh)\right] \ , \quad (s = 1, 2, \ldots, n) \tag{21}$$

The corresponding eigenvectors are

$$w_s^{(n)} = (\sin(st_1), \ldots, \sin(st_k))^T, \quad (s = 1, 2, \ldots, n) \ . \tag{22}$$

It is clear that by choosing $\omega = s, (s = 1, 2, \ldots, n), \mu_s^{(n)}$ coincides with the exact eigenvalues $\lambda_s = s^2$ of (13).

Since as well the mixed Störmer/Verlet as the pure EF Störmer/Verlet integrates $\sin(\omega t)$, ω arbitrary and real, exactly, one can expect that (18) for the cases $K = 1, P = 0$ and $K = -1, P = 1$ respectively, yields satisfactory approximations for the l-th eigenvalue λ_l when we choose

$$\omega = l, \quad (l = 1, 2, 3, \ldots\ .)$$

Let us remark that with this choice for each eigenvalue a system (18) has to be solved. This substantially increases the amount of computation needed if many eigenvalues are wanted. The classical case has been previously discussed in [11] and the mixed case is studied in detail in [6].

In order to facilitate comparison with the results of [11] and [6], we choose the same function q in (13) for our numerical example, i.e. $q(t) = e^t$. In table 1 we compare for that potential function for $n = 39$ the errors on the eigenvalues $\sigma_l^{(39)}(K, P)$ for the methods considered for $l = 1, 2, \ldots, 20$.

As one can observe the error is increasing drastically for the classical method and is equivalent for the two EF version of the Störmer/Verlet method. For $\sigma(1, 0)$ we have proved in [6] that for $\omega = l$

$$|\sigma_l^{(n)}(1,0) - \lambda_l| \leq cl^2h^3/\sin(lh)$$

where c is a constant depending only on q. Based on the results obtained in our numerical experiment we can expect that the eigenvalues obtained by the pure EF version also follow this same pattern. A proof is given in the Appendix. On the other hand Paine *et al.* have shown that the error related to the classical approach is growing as $\mathcal{O}(l^4h^2)$, a fact which clearly illustrates the rapid growth of the error as a function of l.

Table 1: The errors ($\times 10^{+3}$) for the three algorithms considered for $q(t) = e^t$.

k	λ_k	$(\lambda_k - \sigma_k(3,-1))10^3$	$(\lambda_k - \sigma_k(1,0))10^3$	$(\lambda_k - \sigma_k(-1,1))10^3$
1	4.8966694	2.8791	1.9266	1.4879
2	10.045190	17.2560	7.1767	5.3158
3	16.019267	54.6275	11.8128	10.5744
4	23.266271	143.6155	13.8125	15.1944
5	32.263707	330.8462	14.3727	17.5289
6	43.220020	672.01264	14.5907	18.4305
7	56.181594	1232.5636	14.7911	18.8204
8	71.152998	2088.9558	15.0412	19.0678
9	88.132119	3328.2918	15.3513	19.2906
10	107.11668	5047.1548	15.7307	19.5348
11	128.10502	7353.7473	16.1686	19.8019
12	151.09604	10361.6595	16.6816	20.1113
13	176.08900	14194.7289	17.2825	20.4748
14	203.08337	18983.4539	17.9591	20.8762
15	232.07881	24864.8114	18.7363	21.3369
16	263.07507	31981.3651	19.6288	21.8633
17	296.07196	40480.3908	20.6448	22.4559
18	331.06934	50512.9812	21.7987	23.1187
19	368.06713	62233.1409	23.1357	23.8838
20	407.06524	75796.7785	24.6735	24.7522

3.2 The resonance problem

For a resonance problem one observes the difference between the three versions of the Störmer/Verlet method very good. We consider the case of the one-dimensional Schrödinger equation

$$y"(t) + (E - V(t))y(t) = 0, \quad t > 0 \, ,$$

where $\lim_{t\to\infty} V(t) = 0$, with the conditions $y(0) = 0$ and $y(t)$ is finite for any $t > 0$. As explained in [3] the knowledge of the potential function $V(t)$ and of the energy E is sufficient to get reasonable approximations for frequencies: the integration domain $[a, b]$ is divided in subintervals and on each of them the function $V(t)$ is approximated by a constant $\bar{V}$. On all steps in such a subinterval one and the same μ^2 is used, $\mu^2 = \bar{V} - E$.

The order of each of the constructed Störmer/Verlet versions remains two but the errors will be very different when big values of the energy are involved. To see this let us express the higher order derivatives of y in terms of y, y' and the derivatives of $V(x)$, for example $y''(x) = (V(x) - E)y(x)$, $y^{(3)}(x) = V'(x)y(x) + (V(x) - E)y'(x)$ etc., and finally introduce them in the expressions of the last factors in the *lte*, which will be denoted $\Delta_i(t_n)$, $i = 0, 1, 2$. The expression of each $\Delta_i(t_n)$ resulting from such a treatment will consist in a sum of y and y' with coefficients which depend on E and on the derivatives of $V(x)$.

If $E \gg \bar{V}$, μ^2 becomes negative and we are working in the trigonometric regime, where as above $\mu = i\,\omega$. In that case $|\omega^2|$ has a big value and then the ω^2 dependence of $\Delta_i(t_n)$ will become dominating; the approximation $\omega^2 \approx E$ will hold as well. To compare the errors it is then sufficient to organize the coefficients of y and of y' as polynomials in E and to retain only the terms with the highest power. This gives:

$$\Delta_0(t_n) = (E^2 - 2EV + V^{(2)} + V^2)y + 2V'y' \approx E^2y - 2EVy + 2V'y' ,$$

$$\Delta_1(t_n) = (V^{(2)} + \omega^2(V - E) + (V - E)^2)y + 2V'y'$$
$$\approx (-EV + V^{(2)} + V^2)y + 2V'y' \approx -EVy + 2V'y' ,$$

$$\Delta_2(t_n) = (V^{(2)} + 2\omega^2(V - E) + (V - E)^2 + \omega^4)y + 2V'y'$$
$$\approx (V^{(2)} + V^2)y + 2V'y' \approx 2V'y' .$$

Since in the discussed range of energies the solution is of oscillatory type with almost constant coefficients, the amplitude of the first derivative is bigger by a factor $E^{1/2}$ than that of the solution itself and then the error from the three schemes increases with E as E^2, E and $E^{1/2}$, respectively.

For illustration we take the sum of the Woods–Saxon potential and its first derivative (see for example [10]), that is

$$V(x) = v_0/(1 + t) + v_1t/(1 + t)^2, \ t = \exp[(x - x_0)/a],$$

where $v_0 = -50$, $x_0 = 7$, $a = 0.6$ and $v_1 = -v_0/a$. Its shape is such that only two values for $\bar{V}$ are sufficient: $\bar{V} = -50$ for $0 \leq x \leq 6.5$ and $\bar{V} = 0$ for $x \geq 6.5$ (see figure 1).

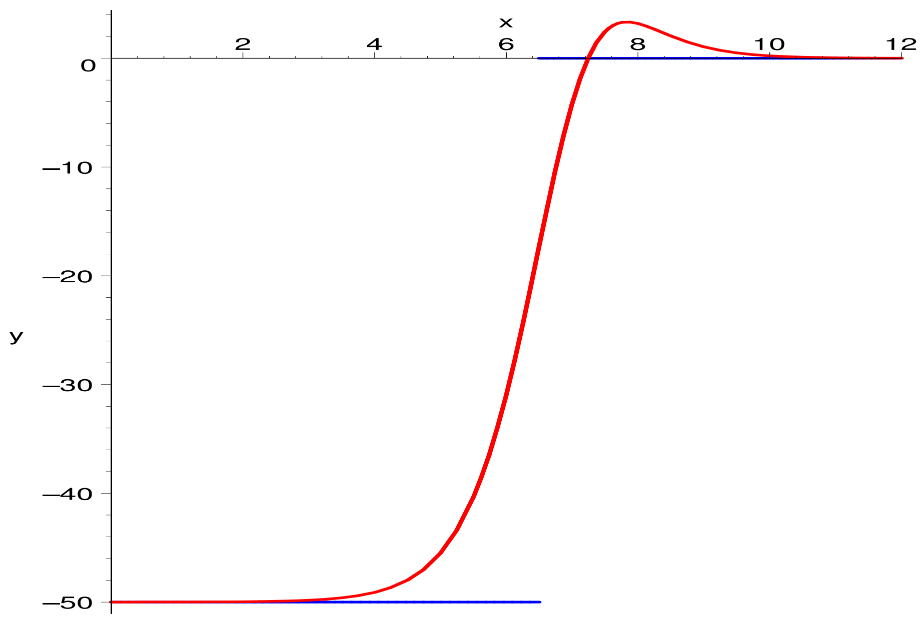

Figure 1: The Woods-Saxon potential and the values of $\bar{V}$.

We solve the resonance problem which consists in the determination of the positive eigenvalues corresponding to the boundary conditions

$$y(0) = 0, \quad y(x) = \cos(E^{1/2}x) \text{ for big } x.$$

The physical interval $x \geq 0$ is cut at $b = 20$ and the eigenvalues are obtained by shooting at $x_c = 6.5$. For any given E the solution is propagated forwards with the starting values $y(0) = 0$, $y(h) = h$ or $y(h) = -h$ up to $x_c + h$, and backwards with the starting conditions $y(b) = \cos(E^{1/2}b)$, $y(b - h) =$

$\cos(E^{1/2}(b-h))$ up to x_c. If E is an eigenvalue the forward and backward solutions are proportional and then the numerical values of quantities as the logarithmic derivatives $y^{f'}(x_c)/y^f(x_c)$ and $y^{b'}(x_c)/y^b(x_c)$, or as the products $y^f(x_c+h)y^b(x_c)$ and $y^b(x_c+h)y^f(x_c)$, must coincide. However, since the Störmer/Verlet method does not compute the derivatives of the solution, the latter has to be adopted. If so, the resonance eigenenergies searched for are the roots of the mismatch function

$$\Delta(E) = y^f(x_c+h)y^b(x_c) - y^b(x_c+h)y^f(x_c),$$

which can be evaluated directly on the basis of the available data. The error in the eigenvalues will then reflect directly the quality of the solvers for the initial value problem used for the determination of the solution $y(x)$.

In Table 2 we list the absolute errors in three such eigenvalues for all three schemes of the Störmer/Verlet method; reference values, which are exact in the written figures, have been generated in a separate run with the method CPM(2) from [9] at $h = 1/16$. It is seen that, as expected, all these versions are of order two but the way in which the error increases with the energy differs from one version to another.

Table 2: Absolute errors $E_{exact} - E_{comput}$ in 10^{-6} units of the three schemes of the Störmer/Verlet method for the resonance eigenenergy problem of the Schrödinger equation in the Woods–Saxon potential. The empty areas indicate that the corresponding errors are bigger than the format adopted in the table.

h	S_0	S_1	S_2
$E_{exact} = 53.588852$			
1/32	475055	−8923	2391
1/64	105697	−2181	585
1/128	25663	−539	145
1/256	6378	−134	36
$E_{exact} = 163.215298$			
1/32		−51015	5582
1/64	2118308	−12435	1382
1/128	433611	−3095	338
1/256	103806	−786	71
$E_{exact} = 341.495796$			
1/32		203090	−11578
1/64		48959	−2802
1/128		12114	−657
1/256		3086	−170

Appendix

From here on, for reason of simplicity of notation we omit the (K, P) in the A, B and σ-objects. The following theorem is written down for the case $(K, P) = (-1, 1)$.

Theorem

If $q \in \mathbb{C}^2[0, \pi]$ there exists a constant c depending only on q such that for all $m \in \mathbb{N}, k = 1, 2, \ldots, m$ and $\omega = k$

$$|\sigma_k^{(n)} - \lambda_k| \leq ckh^2, \quad 1 \leq k \leq \alpha n. \tag{23}$$

Proof of the theorem (we have been inspired for the proof by [6])

Since A and B are symmetric, commuting, invertible matrices

$$AB^{-1} = B^{-1}A = \left(B^{-1}A\right)^T \ .$$

Hence by (18)

$$-\mathbf{v}^T B^{-1} A + \mathbf{v}^T Q = \sigma \mathbf{v}^T$$

Then by (13)

$$\begin{aligned} \sigma \mathbf{v}^T \mathbf{y} + \mathbf{v}^T B^{-1} A \mathbf{y} &= \mathbf{v}^T Q \mathbf{y} \\ &= \lambda \mathbf{v}^T \mathbf{y} + \mathbf{v}^T \mathbf{y}'' \ . \end{aligned}$$

that is

$$(\sigma - \lambda)\, \mathbf{v}^T \mathbf{y} = \mathbf{v}^T \left(\mathbf{y}'' - B^{-1} A \mathbf{y}\right) \ . \tag{24}$$

Due to (16) with $l = k$, (l=1,2,...) one has

$$y_k''(t) = -k^2 \sin(kt) + e_k''(t) = -k^2 w_k(t) + e_k''(t), \quad (k = 1, 2, \dots) \ , \tag{25}$$

and from (21) and (22), for $s = k$ and $\omega = k$ one finds

$$-B^{-1} A \mathbf{w}_k^{(n)} = k^2 \mathbf{w}_k^{(n)}, \quad (k = 1, 2, \dots) \ . \tag{26}$$

It follows from (16) and (24)–(26) that

$$(\sigma_k - \lambda_k)\, \mathbf{v}_k^T \mathbf{y}_k = \mathbf{v}_k^T \left(-k^2 \mathbf{w}_k + \mathbf{e}_k'' - B^{-1} A \mathbf{e}_k + k^2 \mathbf{w}_k\right)$$

or

$$\begin{aligned} (\sigma_k - \lambda_k)\, \mathbf{v}_k^T \mathbf{y}_k &= \mathbf{v}_k^T \left(\mathbf{e}_k'' - B^{-1} A \mathbf{e}_k\right) \\ &= \epsilon_k^T \left(\mathbf{e}_k'' - B^{-1} A \mathbf{e}_k\right) + \mathbf{w}_k^T \left(\mathbf{e}_k'' - B^{-1} A \mathbf{e}_k\right) , \\ &\quad (k = 1, 2, \dots), \end{aligned} \tag{27}$$

where

$$\epsilon_k = \mathbf{v}_k - \mathbf{w}_k \ . \tag{28}$$

The following lemmas enable us to estimate the two terms in (27). We assume $\mathbf{y}_k$ normalized as in [11], with analogous normalization of $\mathbf{v}_k$. From here on, for reason of simplicity of notation we omit the subscript k in all vectors.

Lemma 1.

$$||\epsilon||_\infty \le \frac{\pi}{k} ||q||_\infty ||\mathbf{v}||_\infty \ .$$

Proof. Subtracting $k^2 B\mathbf{v} + Q\mathbf{v}$ from both sides of (18) yields

$$-A\mathbf{v} - k^2 B \mathbf{v} = (\sigma_k - k^2) B \mathbf{v} - BQ\mathbf{v} \ ,$$

or

$$v_{j-1} - 2\cos(kh) v_j + v_{j+1} = h^2 \,\mathrm{sinc}(kh) (k^2 - \sigma_k + q_j) v_j, \quad (j = 1, \dots, n).$$

¿From Lemma 2.3 of [11] it follows that

$$\epsilon_j = \frac{h}{k} \sum_{i=1}^{j-1} \sin[k(x_j - x_i)](k^2 - \sigma_k + q_i) v_i \ . \tag{29}$$

Since $B^{-1}A$ and Q are real symmetric matrices it follows from (18) and (21) and standard perturbation theory that

$$|k^2 - \sigma_k| \le ||\mathbf{Q}||_\infty = ||\mathbf{q}||_\infty \ .$$

Hence by (29) and the triangle inequality

$$\begin{aligned} |\epsilon_j| &\le (j-1)\frac{h}{k} \max_i (|k^2 - \sigma_k + q_i|\,|v_i|) \\ &\le \frac{\pi}{k} ||\mathbf{q}||_\infty ||\mathbf{v}||_\infty \end{aligned}$$

since $h(j-1) \le \pi$. □

Lemma 2. *Let*

$$f := (k^2 - \lambda_k + q)y \ ,$$

$$\alpha(x,h) := \int_x^{x+h} f(t) \sin[(x-h-t)]dt \ , \tag{30}$$

$$E_j := \alpha(x_j, h) + \alpha(x_j, -h) \ , \tag{31}$$

then

$$A\mathbf{e} - B\mathbf{e}'' = \frac{\mathbf{E}}{h^2 k} - \frac{\sin kh}{kh}\mathbf{f} \ . \tag{32}$$

Proof. Due to the definition of $e(x)$ (see (15),(16))

$$e'' = f - k^2 e$$

and hence

$$B\mathbf{e}'' = B\mathbf{f} - k^2 B\mathbf{e} = \frac{\sin(kh)}{kh}(\mathbf{f} - k^2\mathbf{e}) \ . \tag{33}$$

Also by (19),(15),(16) and (31)

$$\begin{aligned} hk^2(A\mathbf{e})_j &= k(e_{j+1} - (2\cos(kh) + kh\sin(kh))e_j + e_{j-1}) \\ &= \int_0^{x_j} f(t)\,[\sin[(k(x_{j+1} - t)] - (2\cos(kh) + kh\sin(kh))\sin[k(x_j - t)] \\ &\quad + \sin[k(x_{j-1} - t)]]\,dt + E_j \\ &= -kh\sin(kh)\int_0^{x_j} f(t)\sin[(k(x_j - t)]dt + E_j \\ &= -k^2 h \sin(kh) e_j + E_j \ . \end{aligned}$$

Hence

$$A\mathbf{e} = -\frac{k}{h}\sin(kh)\mathbf{e} + \frac{\mathbf{E}}{kh^2} \ . \tag{34}$$

Subtracting (33) from (34) gives (32). □

Lemma 3. *For all $q \in \mathbb{C}^2[0,\pi]$ there exists a constant c such that*

$$|\epsilon^T[B^{-1}A\mathbf{e} - \mathbf{e}'']| \leq chk, \quad (k = 1, 2, \dots n).$$

Proof. By (31) and (30)

$$E_j = \int_{x_j}^{x_{j+1}} f(t)\sin[k(x_{j+1}-t)]dt + \int_{x_j}^{x_{j+1}} f(t)\sin[(x_{j-1}-t)]dt \, .$$

Expanding f about x_j by Taylor's theorem in both integrals and integrating by parts shows that

$$\frac{\mathbf{E}}{h^2k} = \frac{2}{k^2h^2}(1-\cos(kh))\mathbf{f} + \left[\frac{1}{k^2} - \frac{2}{k^4h^2}(1-\cos(kh))\right]\mathbf{f}'' + \mathcal{O}(h^4||f^{(4)}||_\infty) \, .$$

Combining (32) with this result, yields

$$\frac{\mathbf{E}}{h^2K} = \frac{2}{k^2h^2}\left[2 - 2\cos(kh) - kh\sin(kh)\right]\mathbf{f} + \left[\frac{1}{k^2} - \frac{2}{k^4h^2}(1-\cos(kh))\right]\mathbf{f}'' + \mathcal{O}(h^4||f^{(4)}||_\infty) \, . \quad (35)$$

Since it can be easily verified that

$$\frac{2}{k^2h^2}\left[2 - 2\cos(kh) - kh\sin(kh)\right] = \mathcal{O}(h^2k^2) \text{ and } \left[\frac{1}{k^2} - \frac{2}{k^4h^2}(1-\cos(kh))\right] = \mathcal{O}(h^2)$$

(35) results in

$$A\mathbf{e} - B\mathbf{e}'' = \mathcal{O}(h^2k^2) + \mathcal{O}(h^2||\mathbf{f}''||_\infty) = \mathcal{O}(h^2k^2) \, , \quad (36)$$

since $\mathcal{O}(||f^{(p)}||_\infty) = \mathcal{O}(k^p)$ [14]. Since also

$$|\epsilon^T(B^{-1}A\mathbf{e} - \mathbf{e}'')| \leq n||\epsilon||_\infty||B^{-1}||_\infty||A\mathbf{e} - B\mathbf{e}''||_\infty$$

and

$$n = \mathcal{O}\left(\frac{1}{h}\right), \qquad ||B^{-1}||_\infty = \mathcal{O}(1),$$

the results follows from (35) and Lemma 1 and Lemma 2. □

It is easy to verify that due to (15), (16), $\omega = s = k, (k = 1, \dots, n)$

$$\mathbf{w}^T(\mathbf{e}'' - B^{-1}A\mathbf{e}) = \mathbf{w}^T(\mathbf{e}'' + k^2\mathbf{e}) \, . \quad (37)$$

Lemma 4.

$$\mathbf{w}^T(\mathbf{e}'' + k^2\mathbf{e}) = \mathcal{O}(kh + (n-k)^{-2}h^{-1})$$

or

$$\mathbf{w}^T(\mathbf{e}'' + k^2\mathbf{e}) \leq c'kh \, . \quad (38)$$

For the proof we refer to [11]. □

By Lemma 1 and (17), $||\mathbf{v} - \mathbf{w}||_\infty$ and $||\mathbf{y} - \mathbf{w}||_\infty$ are both $\mathcal{O}(k^{-1})$ for large k. Hence, since $(\mathbf{w}^T\mathbf{w})^{-1} = \mathcal{O}(h)$, there exist positive constants k_0 and c'' such that

$$\mathbf{v}^T\mathbf{y} \geq c''/h, \qquad \forall\, k \geq k_0 \, . \quad (39)$$

Combining (27) and (39) with the results of Lemma 3 and 4 proves the theorem for $k \geq k_0$.

For $k < k_0$ we have (12) to state that the i-th component of $(-A + BQ - \lambda_k B)\mathbf{y}$ is

$$h^2\ \frac{2-(2\cos(kh)+kh\sin(kh))}{k^4h^4}(k^4y(\eta_p)+k^2y^{(2)}(\eta_p)+y^{(4)}(\eta_p))\ . \tag{40}$$

where $|\eta_p - t_p| < h, (p = 1, \ldots, n)$. One can easily prove that

$$(-A + BQ - \lambda_k B)\mathbf{y} = \mathcal{O}(h^2k^4||\mathbf{y}||_\infty)$$

since

$$h^2\ \frac{2-(2\cos(kh)+kh\sin(kh))}{k^4h^4} = \mathcal{O}(h^2)$$

and

$$(k^4y(\eta_p)+k^2y^{(2)}(\eta_p)+y^{(4)}(\eta_p)) = \mathcal{O}(k^4||y||_\infty)\ .$$

By $||B^{-1}||_\infty = \mathcal{O}(1)$ and an analysis similar to that in [17] (pp 133-134), one can show that

$$|\sigma_k^n - \lambda_k| = \mathcal{O}(h^2k^4)\ .$$

This result implies that there exists a constant c''' such that for k, k_0

$$|\sigma_k^{(n)} - \lambda_k| \le c'''h^2k^4 \le c'''k_0^3kh^2\ .$$

□

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