REGULARIZATION APPLIED TO THE RECOVERY OF PIECEWISE CONSTANT STURM–LIOUVILLE POTENTIALS

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ABSTRACT

In a recent paper [3] a method was proposed for solving the inverse Sturm–Liouville problem by finding a piecewise constant potential whose leading eigenvalues agree with the specified eigenvalues. The numerical evidence presented there indicated that the method worked well, but that the recovered solution was sensitive to perturbations in the specified eigenvalues. In this note the sensitivity of the recovered potential with respect to errors in the eigenvalues is investigated and a regularization technique for reducing the influence of such errors is proposed.

1. Introduction

In this note attention will be restricted to the simplest form of the inverse Sturm–Liouville problem:

> *Find the function* $q \in L^2[0,\pi]$ *for which*
>
> $$-u'' + qu = \lambda u \quad u(0) = 0 = u(\pi) \tag{1.1}$$
>
> *has the specified eigenvalues* $\{\lambda_k\}_{k=1}^{\infty}$, *and which satisfies the symmetry condition* $q(x) = q(\pi - x)$.

It is well known [1] that this problem has a unique solution. More general problems, including conditions for existence and uniqueness of solutions, can be found in [2].

In [3] a method was proposed for approximating the solution of the inverse Sturm–Liouville problem by finding a piecewise constant potential which has

the first N of the specified eigenvalues as the leading part of its spectrum. With the following assumptions and notation

(1) the N specified eigenvalues satisfy $\lambda_1 < \lambda_2 < \ldots < \lambda_N$

(2) the function $\tilde{q}$ is a piecewise constant functions defined on $[0, \pi]$, constant on each of the subintervals of the uniform partition with stepsize $h = \pi/2N$.

(3) $\lambda_k(\tilde{q})$ denotes the $k\,th$ eigenvalue of (1.1) with q replaced by $\tilde{q}$

and with the assumption that all functions used are symmetric about $\pi/2$, the inverse Sturm–Liouville problem posed above is replaced by the simpler problem of finding the function $\tilde{q}^*$ for which

$$\lambda_k(\tilde{q}^*) = \lambda_k \quad k = 1, \ldots, N\,.$$

The solution of this problem reduces to that of finding a solution to the non–linear system :

$$\mathbf{f}(\tilde{q}^*) := \begin{bmatrix} \lambda_1(\tilde{q}^*) - \lambda_1 \\ \vdots \\ \lambda_N(\tilde{q}^*) - \lambda_N \end{bmatrix} = \mathbf{0}$$

for which the Newton iteration takes the form

$$\mathbf{J}(\tilde{q}^\nu)(\tilde{\mathbf{q}}^{\nu+1} - \tilde{\mathbf{q}}^\nu) = -\mathbf{f}(\tilde{q}^\nu) \tag{1.2}$$

where $\tilde{\mathbf{q}}$ is an N component vector with $j\,th$ component $\tilde{q}_j$ which is the value of the $j\,th$ constant piece of $\tilde{q}$, and the $(i,j)\,th$ element of $\mathbf{J}(\tilde{q})$ is given by

$$J_{i,j}(\tilde{q}) = 2\int_{x_j}^{x_{j+1}} u_i^2\,dx$$

where u_i is the normalized eigenfunction corresponding to the eigenvalue $\lambda_i(\tilde{q})$. It should be noted that $\mathbf{J}(\tilde{q})$ can be readily evaluated because of the simple form of the function $\tilde{q}$, and so this iteration can be easily implemented.

When $\tilde{q} \equiv 0$ the (i,j) element of $\mathbf{J} := \mathbf{J}(0)$ is given by

$$J_{i,j} = \frac{h}{\pi}(1 - \frac{\sin ih}{ih}\cos(2ix_{j-\frac{1}{2}}))\,.$$

Thus $\mathbf{J}$ can be written in the form

$$\mathbf{J} = \frac{h}{\pi}\left(\mathbf{u}\mathbf{v}^{\mathrm{T}} - \mathbf{D}\mathbf{F}\right)$$

where $\mathbf{u}^{\mathrm{T}} = (1, 1, \ldots, 1, 0)$, $\mathbf{v}^{\mathrm{T}} = (1, 1, \ldots, 1, 1)$

$$\mathbf{D} = diag\{\frac{\sin h}{h}, \frac{\sin 2h}{2h}, \ldots, \frac{\sin Nh}{Nh}\}$$

and

$$\mathbf{F} = \begin{bmatrix} \cos 2x_{\frac{1}{2}} & \cos 2x_{\frac{3}{2}} & \ldots & \cos 2x_{N-\frac{1}{2}} \\ \cos 4x_{\frac{1}{2}} & \ldots & \ldots & \cos 4x_{N-\frac{1}{2}} \\ \vdots & & & \vdots \\ \cos 2(N-1)x_{\frac{1}{2}} & \ldots & \ldots & \cos 2(N-1)x_{N-\frac{1}{2}} \\ -\frac{\pi}{2} & \ldots & \ldots & -\frac{\pi}{2} \end{bmatrix}$$

Since the matrix $\mathbf{D}$ is clearly non–singular and the matrix $\mathbf{F}$ is closely related in form to a discrete Fourier transform, it is not difficult to establish that $\mathbf{F}$ is non–singular and also that

$$\mathbf{J}^{-1} = -\frac{\pi}{h}\mathbf{F}^{-1}\mathbf{D}^{-1}\mathbf{V}$$

where

$$\mathbf{V} = \begin{bmatrix} 1 & & & -1 \\ & 1 & & -1 \\ & & \ddots & \vdots \\ & & 1 & -1 \\ & & & 1 \end{bmatrix}$$

In [3] it was shown that the condition number of the matrix $\mathbf{J}$ satisfies $cond(\mathbf{J}) < 3N$, thus indicating that errors in the specified eigenvalues would be substantially amplified in the recovered solution. Numerical results confirmed that this was indeed the case, and also indicated that the errors in the recovered solution showed a regular oscillatory behaviour and were highly dependant on the error in the largest eigenvalue used.

Once again an examination of the structure of $\mathbf{J}^{-1}$ given above provides an indication of the reasons for these observed properties of the error. If ε denotes the vector of errors in the specified eigenvalues, and $\mathbf{e}$ the error in the recovered potential, then when the specified eigenvalues are close to those of the zero potential we have

$$\begin{aligned} \mathbf{e} &\approx \mathbf{J}^{-1}\varepsilon \\ &= -\frac{\pi}{h}\mathbf{F}^{-1}\mathbf{D}^{-1}\left(\varepsilon + \varepsilon_N \mathbf{u}\right) \end{aligned}$$

where ε_N is the $N\,th$ component of ε. A simple calculation shows that

$$\left\| \frac{\pi}{h} \mathbf{F}^{-1} \mathbf{D}^{-1} \right\|_2 \leq \pi \sqrt{2N}$$

and so the contribution of the eigenvalue errors due to the first term in brackets above behaves like $N^{1/2} \|\varepsilon\|_2$. The second term however contributes a factor of the form $N|\varepsilon_N|$ to the error, and so the last component of the eigenvalue error vector (unless it is zero or relatively small) contributes as much as all the other components combined to the error in the potential.

Indeed, an examination of the elements of $\mathbf{J}^{-1}$ shows that the size of the elements in the first $N-1$ columns grows only slowly with N, but the elements of the last column are large in magnitude, oscillate in sign and increase proportionately with N. Of course this observation is not highly significant in itself, but this structure is at least consistent with results of the numerical experiments so far conducted. It is also clear that even if the largest eigenvalue contains no error, the recovered potential will still contain errors, but the implication of this observed structure is that large errors in the recovered potential will tend to be oscillatory (excluding those due to large uniform perturbations of the eigenvalues).

The practical import of these observations is that regularization techniques can usefully be applied to improve the recovered potential by moderating the oscillation of the solution when such oscillations are most likely to be due to the errors in the eigenvalues rather than an inherent property of the required potential.

2. Regularization

The basic principle of regularization is to modify the objective function to be minimized by adding a term which penalizes "rough" solutions. Thus the solution which minimizes the modified objective function will represent a trade–off between accuracy and smoothness. In the context of the inverse problem being examined here, perhaps the most natural measure for the roughness of $\tilde{q}$ is

$$r(\tilde{q}) := \sum_{i=1}^{N} \left(\frac{\tilde{q}_{i+1} - \tilde{q}_i}{h} \right)^2$$

The modified objective function which is to be minimized is then

$$E_\alpha(\tilde{q}) := \|\mathbf{f}(\tilde{q})\|_2^2 + \alpha^2 r(\tilde{q})$$

where α is a parameter which is to be chosen to balance the accuracy and smoothness requirements.

This is once again a non–linear problem for which the objective function E is a continuously differentiable function of $\tilde{q}$ and so E will be minimized at $\tilde{q}^*$ if

$$\mathbf{J}^{\mathrm{T}}(\tilde{q}^*)\mathbf{f}(\tilde{q}^*) + \mathbf{T}\tilde{\mathbf{q}}^* = \mathbf{0}$$

where

$$\mathbf{T} = \left(\frac{\alpha}{h}\right)^2 \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 1 \end{bmatrix}$$

If the current estimate of the solution is $\tilde{q}^\nu$, then the Newton iteration for finding a solution to this system can readily be shown to be

$$\left(\mathbf{J}^{\mathrm{T}}(\tilde{q}^\nu)\mathbf{J}(\tilde{q}^\nu) + \mathbf{T}\right)\left(\tilde{\mathbf{q}}^{\nu+1} - \tilde{\mathbf{q}}^\nu\right) = -\mathbf{J}^{\mathrm{T}}(\tilde{q}^\nu)\mathbf{f}(\tilde{q}^\nu) - \mathbf{T}\tilde{\mathbf{q}}^\nu$$

If this iteration converges, the regularized problem can thus be solved in much the same way as the original problem, the only extra expense being the calculation of $\mathbf{J}^{\mathrm{T}}(\tilde{q}^\nu)\mathbf{J}(\tilde{q}^\nu)$ and $\mathbf{J}^{\mathrm{T}}(\tilde{q}^\nu)\mathbf{f}(\tilde{q}^\nu)$.

3. Numerical Experiments

Once again the obvious potential to use to investigate the effectiveness of the regularization technique is the Mathieu potential $6\cos 2x$. The error in the recovered potential using the first sixteen exact eigenvalues is displayed in Figure 1 along with the error when the $k\,th$ exact eigenvalue is perturbed by $.1(-1)^k$. Also displayed in Figure 1 is the error in the recovered potential using regularization with $\alpha^2 = .001$. The large oscillatory error caused by the perturbations of the eigenvalues has obviously been greatly reduced by the regularization, though the error is still substantially greater than when the exact eigenvalues are used.

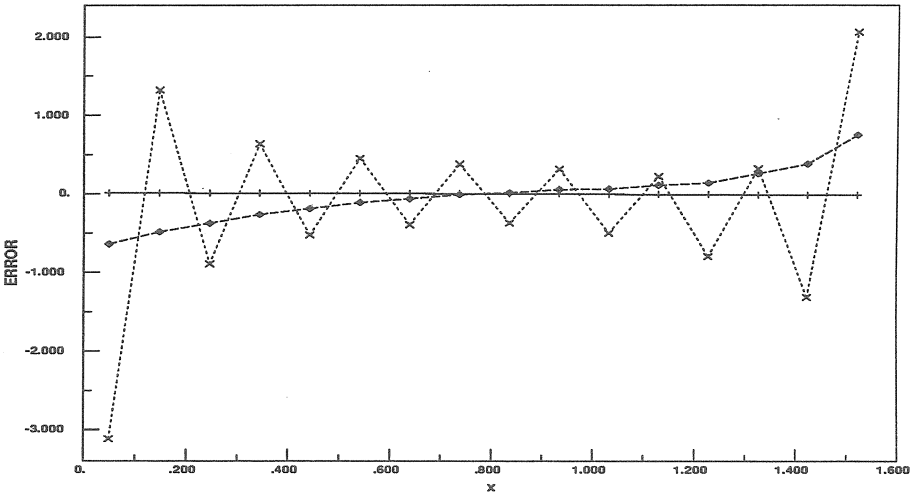

Figure 1. Errors in reconstructed Mathieu potential using sixteen eigenvalues. Exact eigenvalues : ——— , perturbed eigenvalues : ····· , regularized solution : ------ .

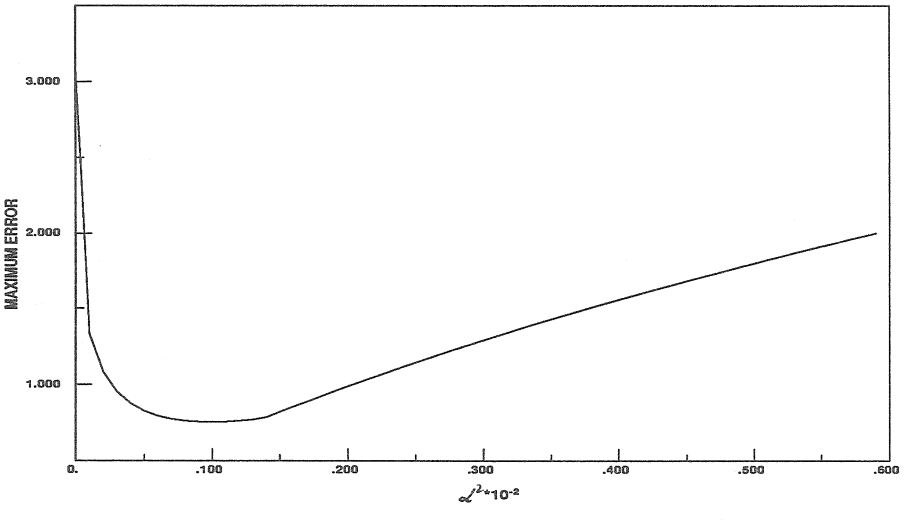

Figure 2. Dependance of the maximum error in regularized solution on the regularization parameter α^2.

In Figure 2 the behaviour of the maximum error in the recovered potential as a function of the regularizing parameter α^2 is displayed for the eigenvalue

perturbations defined above. The dependence of the maximum error on the regularization parameter is essentially as expected. The minimum is achieved near $\alpha^2 = .001$, and the error is reasonably flat there and only increases slowly as α^2 increases, so it would appear that the use of the optimal α^2 is not critical.

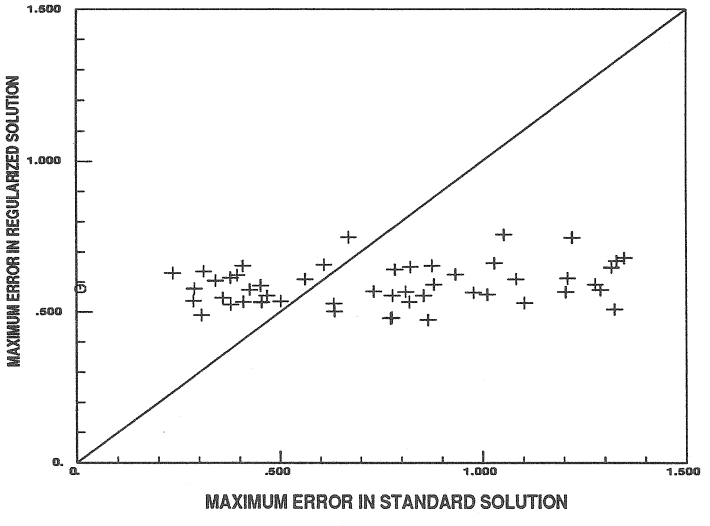

Figure 3. Scatter plot of maximum errors in standard and regularized solutions using fifty sets of randomly perturbed eigenvalues.
○ denotes solution using exact eigenvalues.

The form of perturbation used above is of course rather structured and so the errors in the recovered potential are not necessarily representative of the effects due to the random eigenvalue errors expected in practice. To investigate the effectiveness of the regularized method in more realistic circumstances, the standard and regularized solutions were computed using the first sixteen eigenvalues of the Mathieu potential with random perturbations uniformly distributed in the interval $[-.1, .1]$. The values of the maximum error in each of the two solutions over fifty trials are displayed as a scatter plot in Figure 3. Of particular note here is the large variation of the error in the standard solution compared with its regularized counterpart. As a point of reference the maximum error for the two solutions using the exact eigenvalues is also marked on the figure. It can be seen that the error in the regularized solution is almost independent of the eigenvalue perturbation, thus indicating that the potential advantages of regularization outweigh any possible loss of accuracy in the recovered solution unless it is known that the eigenvalues are very accurate.

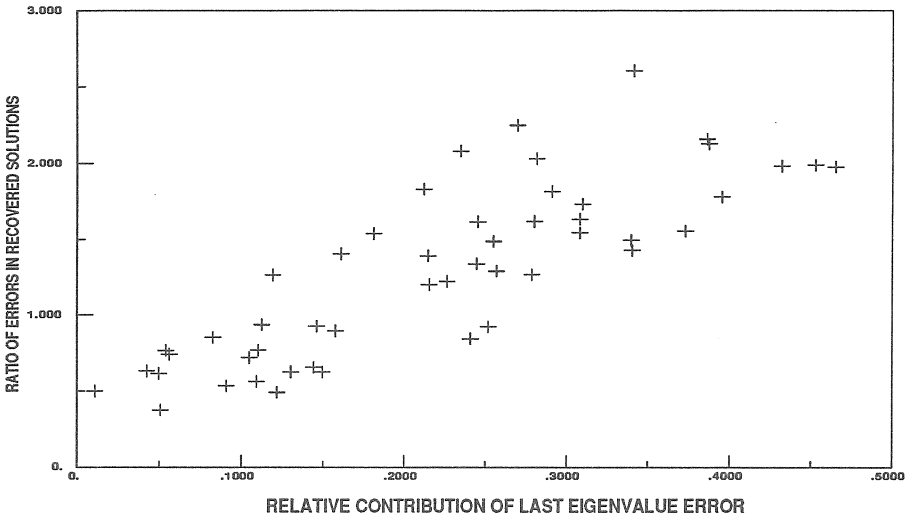

Figure 4. Dependance of the ratio of the maximum error in the standard solution to that of the regularized solution on the relative size of the perturbation in the largest eigenvalue used.

To further investigate the effectiveness of regularization, the ratio of the maximum error for the two recovered solutions is displayed in Figure 4. Here the horizontal axis is taken to be the relative contribution of the last component in the error vector so that the dependence of the error on this component can also be illustrated.

These results show that there is a strong correlation between the error in the largest eigenvalue and the size of the error in the standard solution. The regularization process therefore appears to be fairly effective in removing such errors without also diminishing the accuracy of the solution too greatly. However when the error in the last eigenvalue is relatively small, the regularization process can adversely affect the accuracy of the recovered solution. Figures 5 and 6 display the error in the standard and regularized solutions for the perturbed problems which gave the smallest (0.37 in Figure 5) and largest (2.61 in Figure 6) ratios of the maximum errors. The errors in the regularized solutions are very similar in both cases, whereas the errors for the standard solutions are quite different, thus confirming the lack of sensitivity of the regularized solution to the errors in the specified eigenvalues.

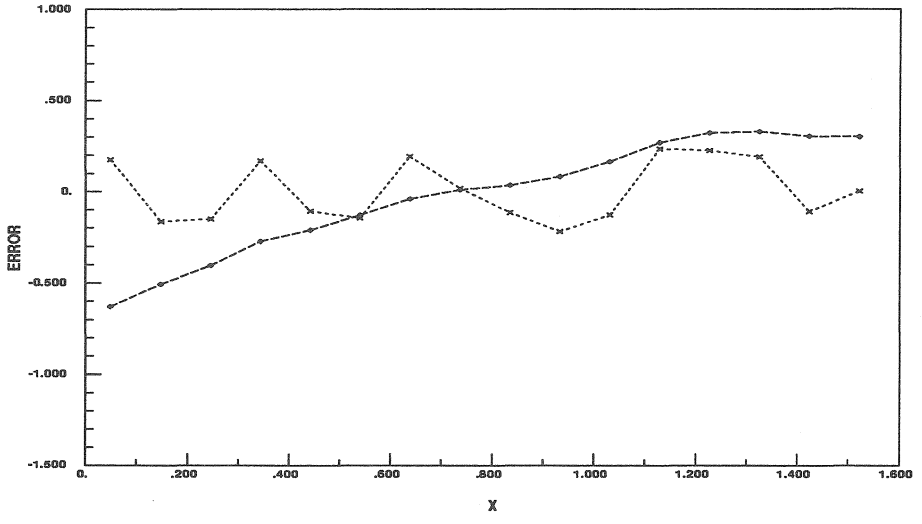

Figure 5. Errors in the standard : ·····,and regularized : ----- solutions for the random perturbation which gave the smallest ratio of maximum errors.

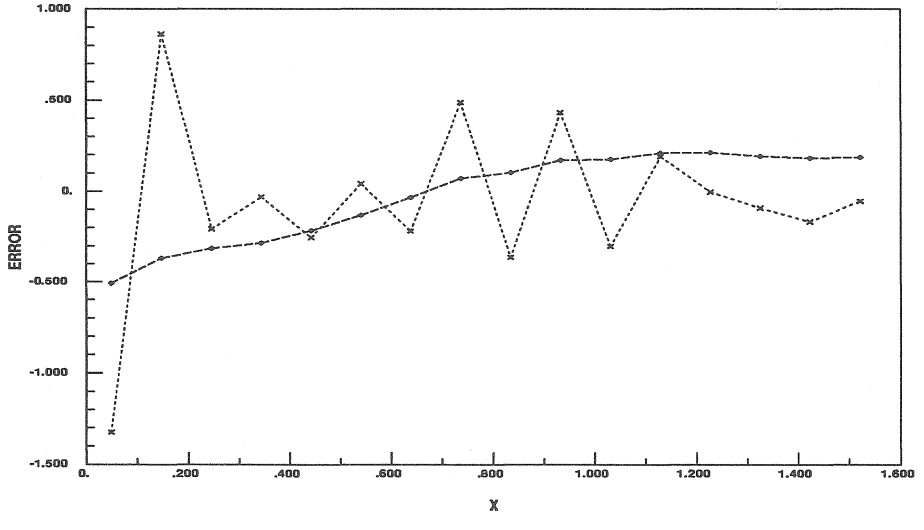

Figure 6. Errors in the standard : ·····,and regularized : ----- solutions for the random perturbation which gave the largest ratio of maximum errors.

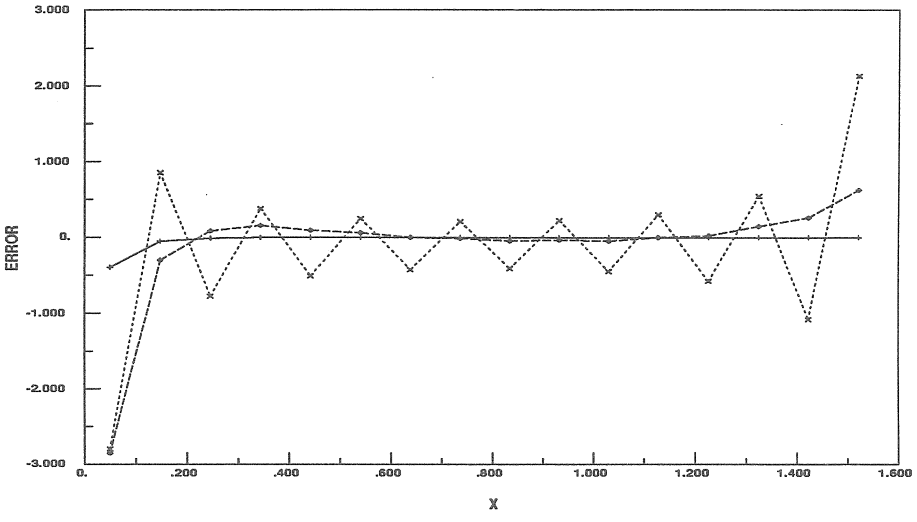

Figure 7. Errors in the piecewise constant approximation of the almost singular potential (3.1) using sixteen eigenvalues. Exact eigenvalues : ——— , perturbed eigenvalues : ····· , regularized solution : ------ .

As a final illustration of this method Figure 7 displays the errors in the potentials constructed using the first sixteen eigenvalues of the potential

$$((x+.1)(\pi+.1-x))^{-2} \tag{3.1}$$

using the standard method with exact and perturbed eigenvalues, and for the regularized method with $\alpha^2 = .001$ for the perturbed eigenvalues. The influence of the perturbations of the eigenvalues in this case is almost identical to that for the Mathieu potential. Once again the oscillations in the regularized solution have been substantially reduced, but the error near $x = 0$ has been increased marginally rather than reduced. This effect is to be expected as the origin is close to a singularity of the potential and so the solution is varying rapidly there.

References

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