ON EIGENFUNCTION APPROXIMATIONS FOR TYPICAL NON-SELF-ADJOINT SCHRÖDINGER OPERATORS

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Abstract. We construct efficient approximations for the eigenfunctions of non-self-adjoint Schrödinger operators in one dimension. The same ideas also apply to the study of resonances of self-adjoint Schrödinger operators which have dilation analytic potentials. In spite of the fact that such eigenfunctions can have surprisingly complicated structures with multiple local maxima, we show that a suitable adaptation of the JWKB method is able to provide accurate global approximations to them.

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1. Introduction

The motivation for this study was, to a great extent, our recent paper [1], where we discovered that extreme spectral instability was typical for many non-self-adjoint Schrödinger operators, and also for complex resonances of self-adjoint Schrödinger operators with dilation analytic potentials. The full analysis of such operators involves the determination not only of their spectra, but also of their eigenfunctions, which may be highly non-orthogonal. It is especially important to have a powerful tool for approximating eigenfunctions in situations in which numerical computations turn out to be intrinsically unstable and, therefore, standard routines are insufficiently reliable. This is the case for the spectral problems we have been dealing with in the mentioned paper. We start by testing the JWKB analysis of section 2 on a typical Schrödinger operator whose spectrum has been studied in [1]. Then the same technique is applied to another operator with a dilation analytic potential. Although the two operators have different dilation analytic potentials, they exhibit surprisingly similar spectral properties. However, in the course of this work

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we were primarily interested in constructing their eigenfunctions rather than comparing the corresponding eigenvalues. In section 3 we bring together the results of computations and report the conclusions drawn from their comparative analysis. This allows us to suggest that the technique we have developed can be used as a general method for a wide range of similar problems.

JWKB analysis is known to be an extremely useful technique when applied to a range of spectral problems. To be more precise, this notion includes a vast variety of methods, each associated with certain asymptotic formulae. The general asymptotic theory has been developed in a number of books among which monographs [5, 7, 13] can be mentioned. There exists an extensive literature on numerical analysis of ODEs where purely numerical procedures are combined with and strengthened by proper JWKB methods. Examples of different asymptotic formulae can, for instance, be found in papers [8, 9, 11]. Apart from this, one can take advantage of similar techniques for strictly analytical purposes, including spectral analysis of Schrödinger operators. Recent papers on the subject include [3, 4, 6, 10]. In the papers [3, 4] relevant JWKB-type formulae have been used to construct the semi-classical modes for non-self-adjoint Schrödinger operators in order to study their spectral properties. A major aspect of [3, 4] is that the JWKB functions are defined globally, not just asymptotically at infinity, and do not involve analytic continuation to complex phase space. We develop the basic approach of [4] in the next section, working out efficient eigenfunction approximations.

Another feature of our method which makes it different from the standard approach was suggested by our numerical results. Having studied the spectra of several operators, we became interested in their eigenfunctions. The latter, although more difficult to compute than the spectra, were also calculated by the transfer method followed by a conventional routine. The modes we have found are quite unexpected: some of them look like linear combinations of several complex Gaussian functions whose centres are quite distinct. It is this circumstance that prompted our decision to try to approximate the eigenfunctions globally by linear combinations of several JWKB approximate eigenfunctions. This permitted us to approximate rather accurately all the eigenfunctions except those associated with eigenvalues which are close to the origin, whereas using just one JWKB function usually only works for substantially larger eigenvalues. The results of section 3 show that in our examples each eigenvalue (starting from a certain number) is associated with two JWKB functions, one of them playing the leading role for lower and the other for higher eigenvalues. Linear combinations of these functions are proved to provide fairly good approximations for the eigenfunctions involved in our examples, in spite of the fact that we only retain the lowest order terms in the JWKB expansion in this paper. Having observed this phenomenon numerically for different examples, we propose a method suitable for approximating eigenfunctions by several easily obtained JWKB functions. Their number can be arbitrary and depends on the potential of the operator under consideration.

2. JWKB Formulae

We are interested in computing the eigenvalues and eigenfunctions of the Schrödinger operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \tag{1}$$

where $V(x)$ is a complex-valued continuous potential. Since we will adapt the JWKB method we study instead the Schrödinger operator acting in $\mathcal{L}_2(\mathbf{R})$ given by

$$H_h := -h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x),$$

where $h > 0$. Throughout the paper the potential is taken to be even; this simplification is not necessary, but enables us to restrict our computations to the half-line $\mathbf{R}_+$ instead of $\mathbf{R}$.

Given an eigenvalue z of H_h, let us solve the equation

$$(H_h - z)f(x) \;=\; 0. \tag{2}$$

We impose one of the conditions

$$f(0) = 0 \qquad \text{or} \qquad f'(0) = 0$$

bearing in mind that the eigenfunctions of H_h are either even or odd. Our aim is to approximate the true eigenfunctions $f(x)$ by means of relevant JWKB asymptotic formulae. Following [4], we assume for now that h is sufficiently small and represent the approximate solution $y(x)$ of (2) as

$$y(x) = y(a+s) = \xi(s;h)\exp\left(-h^{-1}\psi(s)\right) \tag{3}$$

about some $a > 0$ to be determined. One expects $\xi(s;h)$ to be asymptotically expanded in powers of h:

$$\xi(s;h) \sim \sum_{k=0}^{\infty} h^k \xi_k(s), \qquad h \to +0. \tag{4}$$

As in [4], $\psi(s)$ is taken to be the solution of the eikonal equation

$$\psi'(s)^2 = V(a+s) - V(a) - \eta^2, \qquad \psi(0) = 0,$$

where real η and a satisfy $z = \eta^2 + V(a)$. Thus, we have

$$\psi(s) \;=\; i\eta \int_0^s \left(1 - \frac{V(a+t) - V(a)}{\eta^2}\right)^{1/2} \mathrm{d}t. \tag{5}$$

Here the sign of η and the branch of the square root in the integrand are chosen so that $\mathrm{Re}\,\psi(s) > 0$ for small s. An important consequence of the fact that V is complex-valued is that generically the integrand never vanishes, and thus a unique continuous branch of the square root is defined globally on the real line by the above formula. Substituting the expansion (3) into (2) and equating the coefficients by equal powers of h, we get a series of equations for ξ_k, $k = 0, 1, \ldots$. To normalise the function $y(x)$ we impose the initial conditions $\xi_0(0) = 1$, $\xi_k(0) = 0$, $k > 0$, so that $y(a) = 1$. A direct calculation gives us

$$2\xi_0'\psi' + \xi_0\psi'' = 0$$

and, therefore,

$$\xi_0(s) = \left(1 - \frac{V(a+s) - V(a)}{\eta^2}\right)^{-1/4}.$$

The function $\xi_0(s)$ is globally well-defined and continuous.

The other functions ξ_k, $k = 1, 2, \ldots$, can be successively determined as well. In this initial study, we omit the higher order terms in (4) and finally obtain the approximate solution

$$y(x) \;=\; \xi_0(s) \exp\left(-\frac{i\eta}{h} \int_0^s \xi_0(t)^{-2} \mathrm{d}t\right). \tag{6}$$

We substitute y directly into (2) to confirm that

$$\frac{(H_h - z)y}{y} = O(h^2), \qquad h \to +0.$$

Although the above analysis is only justified asymptotically as $h \to +0$, we apply the formulae obtained to the case $h = 1$, that is to the operator defined by (1). We refer to [4] for a justification of this for large eigenvalues and for a wide class of smooth potentials. Thus we actually consider the eigenvalue problem

$$(H - \lambda)\, f = 0 \tag{7}$$

in the rest of the paper. We expect the basic JWKB modes $y(x)$ defined by (6) to provide good first approximations for the eigenfunctions related to the eigenvalues λ of H as

$|\lambda| \to \infty$. The above relation (6) becomes the approximate formula for the eigenfunction of H related to λ:

$$y(a+s) = \left(1 - \frac{V(a+s) - V(a)}{\eta^2}\right)^{-1/4} \exp\left(-i\eta \int_0^s \left(1 - \frac{V(a+t) - V(a)}{\eta^2}\right)^{1/2} \mathrm{d}t\right) \tag{8}$$

where the pair of real numbers (a, η) solves

$$\lambda = \eta^2 + V(a). \tag{9}$$

Here $a > 0$ since we consider $x \in \mathbf{R}_+$; the sign of η is chosen so that for small s in (5) we have $\mathrm{Re}\, \psi(s) > 0$ for the selected branch of the square root in the integrand. In what follows we shall use the key formulae (8), (9) systematically. The actual efficiency of these formulae can be judged by the numerical results discussed in the next section.

Note that apart from (8) there are other ways of approximating $f(x)$. The expression (8) can, for instance, be further approximated by

$$\tilde{y}(x) = \left(1 - \frac{V'(a)s}{2\eta^2}\right)^{-1/2} \exp\left(-i\eta s + \frac{iV'(a)s^2}{4\eta}\right).$$

This formula is easier to deal with than (8) because of its explicit expression. Naturally, $\tilde{y}(x)$ is expected and proved to be less accurate for our aims than the original JWKB function $y(x)$. One can also continue the process and work out more terms ξ_k, $k = 1, 2, \ldots$. However, the formula (8) provides quite satisfactory eigenfunction approximations, which is justified by the results of computations related to two typical examples (see, in particular, table 6 of subsection 3.4).

Several final remarks are in order. The functions defined by (8) do not generally lie in $\mathcal{L}_2(\mathbf{R})$, even when they are good approximations to the eigenfunctions in some interval. In subsection 3.2 we discuss a further truncation procedure needed to obtain $\mathcal{L}_2(\mathbf{R})$ functions without sacrificing the fact that they satisfy the eigenvalue equation approximately. Secondly the number of solutions of (9) for a given eigenvalue λ depends on the potential V, and each of the corresponding JWKB functions may make a contribution to the eigenfunction, as we show in subsection 3.3. In our examples the number of solutions is always 0, 1 or 2. Finally the absence of turning points typical for the complex equation (2) should be once again mentioned. It allows us to define the functions ψ and ξ globally on $\mathbf{R}$ without applying any special complex analysis technique. This reflects the different nature of the approach presented here and the standard JWKB analysis.

3. Numerical Experiments

3.1. **JWKB Parameters.** To find the approximate eigenfunction $y(x)$ we have to solve equation (9) first. In this section we consider several operators of type (1) starting by the harmonic oscillator operator H_o with the complex potential $V_o(x) = (cx)^2$, $c \in \mathbf{C}$. In particular, for the m-th eigenvalue of H_o we have the equation

$$c(2m+1) = \eta^2 + (ca)^2, \qquad m = 0, 1, \dots ,$$

which is solved exactly. The solution $(a,\, \eta)$ such that $\eta > 0$, $a > 0$ defines the JWKB mode $y(x)$ decaying at infinity.

As mentioned in [1], the eigenvalues of this and similar operators are extremely unstable under small perturbations, which makes numerical analysis quite difficult. To be able to compute higher eigenvalues and relevant eigenfunctions numerically one needs some additional information. For instance, when solving eigenvalue problem (7) by the transfer method it is helpful to have at least rough estimates for the location of $\operatorname{argmax}|f(x)|$. Here we take advantage of the JWKB analysis to find the centres of the eigenfunctions.

For comparison purposes along with equation (9) let us introduce its more sophisticated version:

$$\lambda + \frac{iV'(a)}{2\eta}(a, \eta) - \eta^2 - V(a) = 0. \tag{10}$$

It is obtained if we replace the eigenfunction associated with an eigenvalue λ by the approximation

$$f(x) = \exp\left(-i\eta s + \frac{iV'(a)s^2}{4\eta}\right).$$

For the harmonic oscillator problem we denote the roots of (9) by (a', η'), those of (10) by (a'', η''). Below we tabulate the values of $\tau' := \operatorname{argmax}|f(x)| - a'$ and $\tau'' := \operatorname{argmax}|f(x)| - a''$. The eigenfunctions are computed with the use of the same basic method as in [1]. In our numerical exercises we take a typical value of $c = \mathrm{e}^{i\pi/8}$ throughout the paper.

Table 1. Parameters a, τ for H_o

m	a'	a''	argmax$\lvert f_m(x)\rvert$	τ'	τ''
10	3.371	3.535	3.678	0.307	0.143
20	4.711	4.822	4.831	0.120	0.009
30	5.746	5.835	5.839	0.093	0.004
40	6.621	6.698	6.700	0.079	0.002
50	7.393	7.462	7.464	0.071	0.002
60	8.092	8.155	8.156	0.064	0.001
70	8.736	8.793	8.794	0.058	0.001
80	9.335	9.389	9.389	0.054	0.0
90	9.897	9.948	9.949	0.052	0.001
100	10.430	10.478	10.479	0.049	0.001

Equation (10) easily solved by a standard iterative method provides somewhat more accurate information about the centres of the eigenfunctions of H_o (and other considered operators) than (9) does. However, for our primary aim of eigenfunction approximation this is not vital, and the parameters obtained from (9) turn out to be more suitable. For the examples considered below we use a standard NAG routine to find the real roots of the equations of type (9) and (10).

An interesting example where we apply the JWKB method is an operator with a dilation analytic potential studied in [1]. This operator is given by

$$H_c = -c^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(\sqrt{c}x), \qquad V(x) = x^2\exp(-x^2/b^2),$$

where $c \in \mathbf{C}$, $b \in \mathbf{R}$ as in [1]. Equation (9) then becomes

$$\lambda_m c = \eta^2 + cV(\sqrt{c}a) \tag{11}$$

where λ_m denotes the m-th eigenvalue. Another typical quantum mechanical operator $\tilde{H}_c$ to be considered here has a similar form to H_c:

$$\tilde{H}_c = -c^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tilde{V}(\sqrt{c}x),$$

$$\tilde{V}(x) = \alpha\left(\exp(-\gamma(x-\beta)^2) + \exp(-\gamma(x+\beta)^2)\right), \qquad \alpha, \beta, \gamma \in \mathbf{R}.$$

Both H_c and $\tilde{H}_c$ are the operator families parametrised by a complex c; their eigenvalues are known to be independent of c in a sense explained in [1]. If one puts $c = 1$ then the corresponding operators H_1 and $\tilde{H}_1$ are self-adjoint and known to have complex resonances which are the eigenvalues of the original non-self-adjoint operators (see, for example, [2] where the theory of dilation analytic resonances is exposed).

The spectra of H_o and H_c for sufficiently large b are proved to be very close to each other; the same can be said about the eigenfunctions of the two operators. For $b = 100$ let us tabulate the JWKB parameters a'' found from (10) (where obvious changes are made to suit H_c) to make sure they also approximate the actual values of $\mathrm{argmax}|f_m(x)|$.

Table 2. Parameters a'', τ'' for H_c; $b = 100$

m	a''	$\mathrm{argmax}\lvert f_m(x)\rvert$	τ''
10	3.537	3.682	0.145
20	4.826	4.836	0.010
30	5.842	5.850	0.008
40	6.708	6.713	0.005
50	7.475	7.479	0.004
60	8.172	8.175	0.003
70	8.815	8.817	0.002
80	9.414	9.415	0.001
90	9.982	9.983	0.001
100	10.519	10.520	0.001

Comparing tables 1 and 2 one can see that the results obtained for H_o and H_c ($b = 100$) are quite similar. The plots of the computed eigenfunctions indicate the same fact. The comparison of the actual eigenfunctions of these two operators contributes to our study of their spectra. From the numerical point of view it may turn out to be useful to have the values of the parameter a'' found from (10) which approximate the centres of the eigenfunctions reasonably accurately.

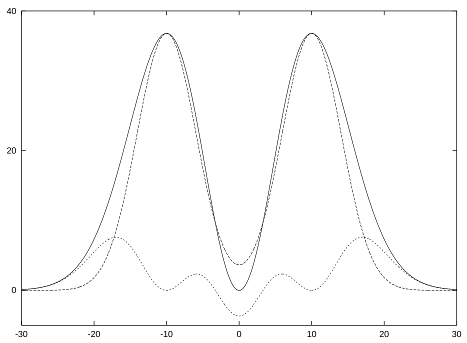

Figure 1. Potentials $V(x)$ (solid line) and $\tilde{V}(x)$ (dotted line); values of $V - \tilde{V}$

From now on we shall concentrate on the two operators H_c at $b = 10$ and $\tilde{H}_c$ where $\gamma = 0.03$, $\alpha = 100/\mathrm{e}$, $\beta = 10$. The choice of the parameters α, β, γ involved into $\tilde{H}_c$ is systematic rather than random. Our idea is to take two close self-adjoint operators H_1 and $\tilde{H}_1$ and transform them into non-self-adjoint operators by the dilation analyticity technique (as has been done for H_1 in [1]). In fact, the potentials $V(x)$ and $\tilde{V}(x)$ at the chosen values of b and α, β, γ are relatively close to one another: $\|V(x)-\tilde{V}(x)\|/\|V(x)\| \approx 0.18$; see also figure 1 where V, $\tilde{V}$ and $V - \tilde{V}$ are plotted. (Here and below by $\|\cdot\|$ we understand the $\mathcal{L}_2$-norm.) Of course, the complex potentials $V(\sqrt{c}x)$ and $\tilde{V}(\sqrt{c}x)$ thus obtained are no longer similar to each other. Remarkably, the operators H_c and $\tilde{H}_c$, although different, prove to have similar spectral properties. Namely, their lower eigenvalues are real (up to a chosen accuracy); starting from a certain number they turn sharply into the lower half-plane. This behaviour of the complex resonances observed in [1, 12] seems to be typical for a range of operators, and the results quoted here provide yet another numerical evidence of the fact.

Below we quote the even eigenvalues of $\tilde{H}_c$ calculated by means of the same procedure as proposed and implemented in our earlier paper. The eigenvalues of H_c are tabulated in [1] (see table 10 there and also figure 2 below for comparisons).

Table 3. Eigenvalues $\tilde{\lambda}_m$ of $\tilde{H}_c$

m	$\tilde{\lambda}_m$		m	$\tilde{\lambda}_m$		m	$\tilde{\lambda}_m$
0	4.4063		18	30.2243		36	$46.9295 - 7.3270i$
2	7.3902		20	32.6595		38	$48.7860 - 9.0639i$
4	10.3846		22	$34.8766 - 0.0005i$		40	$50.6604 - 10.9142i$
6	13.3718		24	$36.6986 - 0.0736i$		42	$52.5485 - 12.8733i$
8	16.3358		26	$38.1852 - 0.6680i$		44	$54.4504 - 14.9375i$
10	19.2609		28	$39.8085 - 1.6721i$		46	$56.3613 - 17.1037i$
12	22.1312		30	$41.5232 - 2.8670i$		48	$58.2803 - 19.3695i$
14	24.9295		32	$43.2907 - 4.2188i$		50	$60.2058 - 21.7326i$
16	27.6357		34	$45.0959 - 5.7093i$		52	$62.1367 - 24.1910i$

Given the eigenvalues, we find the values of a and η from (11). In a generic situation this equation may have several real solutions $(a_k,\, \eta_k)$ such that $a_k > 0$ and η has the appropriate sign as discussed in section 2. This is the case for both of the operators H_c and $\tilde{H}_c$, unlike the former two operators. Namely, for higher eigenvalues there exist two solutions providing $|y(a_k+s)| < |y(a_k)|$ for sufficiently small s. The values of a_k, η_k, $k = 1, 2$, $a_2 > a_1$, are tabulated below (see table 4). The results for H_c and $\tilde{H}_c$ are qualitatively similar; the second solution of (11) appears for the 28-th and 30-th eigenvalue respectively.

Table 4. Solutions of (11): a, η relate to H_c, $\tilde{a}$, $\tilde{\eta}$ to $\tilde{H}_c$

m	a	η	$\tilde{a}$	$\tilde{\eta}$		m	a	η	$\tilde{a}$	$\tilde{\eta}$
20	5.0880	3.9262	5.4144	3.8701		40	3.5726	6.3897	4.4905	6.2876
26	5.4023	4.3319	5.8455	4.2843			12.3112	-3.5569	11.4371	-3.3463
28	5.2223	4.5915	5.7562	4.5455		42	3.2224	6.6574	4.1567	6.5730
	10.7554	-0.3678					12.6198	-3.9050	11.6097	-3.7166
30	5.0489	4.8785	5.6270	4.8273		44	2.7926	6.9310	3.7719	6.8549
	10.9252	-1.3639	10.7532	-0.1320			12.9812	-4.2601	11.7924	-4.0723
32	4.7845	5.1944	5.4631	5.1183		46	2.2971	7.1949	3.3172	7.1332
	11.1804	-1.9060	10.8609	-1.4247			13.3664	-4.6127	11.9855	-4.4182
34	4.5351	5.5016	5.2676	5.4124		48	1.6747	7.4508	2.7555	7.4085
	11.4189	-2.3884	10.9854	-2.0364			13.7846	-4.9684	12.1898	-4.7583
36	4.2522	5.8023	5.0413	5.7065		50	0.6079	7.7002	1.9911	7.6815
	11.6864	-2.8042	11.1241	-2.5247			14.2496	-5.3334	12.4065	-5.0958
38	3.9280	6.0983	4.7833	5.9985		52			0.2650	7.9532
	11.9881	-3.1856	11.2750	-2.9532					12.6375	-5.4334

Figure 2 explains why the second solution (a, η) appears. Here the complex potentials $cV(\sqrt{c}x)$ and $c\tilde{V}(\sqrt{c}x)$ are plotted for $0 \le x \le X$, X being sufficiently large. We treat x as a parameter and represent the data in the form (Re (cV), Im (cV)) for each x. The dots in the figure denote the values of $\lambda_m c$, i.e., the eigenvalues of the operators H_c and $\tilde{H}_c$ multiplied by c (only even eigenvalues are pictured for both operators). These pictures refer to equation (11) and show how it is solved graphically. Clearly, if a dot $\lambda_m c$ is 'inside' the graph then the two possible values of $\eta^2 = \text{Re}\,(\lambda_m c) - \text{Re}\,(cV)$ have opposite signs, while dots lying 'outside' determine two positive values of η^2. Hence in the former case there is only one real pair (a, η) solving (11) (provided the proper sign of η is chosen), whereas in the latter (11) has two solutions of this kind. As is seen, the critical points are $m = 28$ for the first operator and $m = 30$ for the second. It is from these numbers onwards that the behaviour of eigenfunctions changes (see figure 3 where eigenfunctions of H_c are plotted).

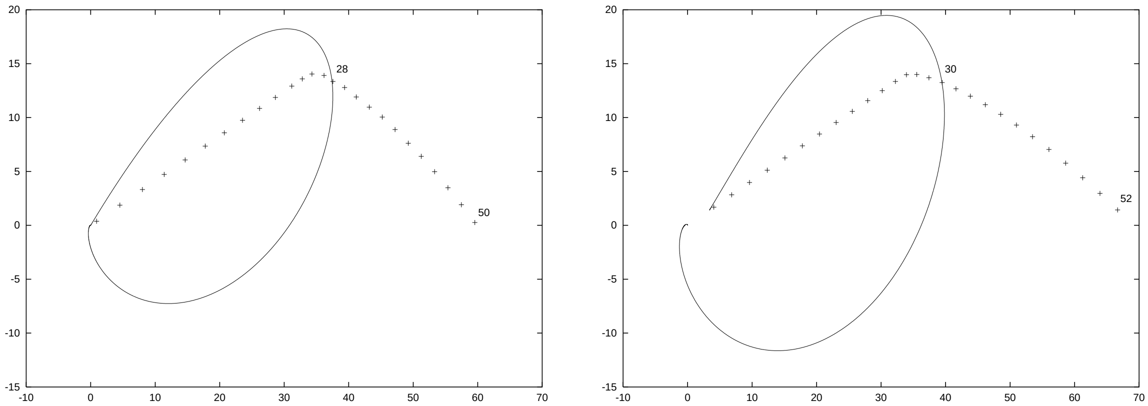

Figure 2. Potential and eigenvalues of H_c (left) and $\tilde{H}_c$ (right)

The graphs of the true eigenfunctions also suggest that for a certain range of m ($28 \leq m \leq 40$ and $30 \leq m \leq 44$ for H_c and $\tilde{H}_c$ respectively) the solution of (7) has to be sought as a linear combination of two JWKB modes rather than a single function of type (8). These modes are determined by the corresponding values of $(a,\, \eta)$. Of course the problem (7) itself can have only one $\mathcal{L}_2$ eigenfunction for each eigenvalue, but the peculiarities of the solutions indicate that the existence of more than one JWKB approximation has great significance for our problem.

3.2. **Cut-Off Technique.** There is a possibility that Re $(-i\eta\xi_0(s)^{-2}) > 0$ for some range of s for particular JWKB modes. Therefore, we cannot use the formula (8) to approximate $\mathcal{L}_2$-functions f on the whole $\mathbf{R}_+$. In fact, most of the modes defined by (8) in our examples, although good around their centres where s is small enough, either increase as $s \to \infty$ or change rapidly near $s = -a$.

When this problem occurs, we modify the original functions y defined by (8) putting

$$\frac{y_1'(x)}{y_1(x)} = \frac{y_1'(s_1)}{y_1(s_1)},\ s \geq s_1, \qquad \frac{y_2'(x)}{y_2(x)} = \frac{y_2'(s_2)}{y_2(s_2)},\ s \leq s_2, \tag{12}$$

where the points s_1, s_2 are chosen properly for each JWKB function. Otherwise the functions are not changed anywhere. Our aim is to replace the formerly defined modes by decaying exponentials beyond $[s_2, s_1]$ if necessary; we shall keep the same notation $y(x)$ for the modified functions in what follows.

It is clear that our results depend on the choice of these s_k. Generally, in practical computations we have to vary two parameters to minimise the approximation error for each particular eigenfunction (see the next subsection for corresponding formulae). To get optimal results one can take the initial values of s_1 and s_2 reasonably close to the corresponding local minima of $|y_1|$ and $|y_2|$ respectively, replacing y_k by exponentially decaying functions according to (12). Then the values of s_k providing the best possible approximations among those given by the above formulae are found by a standard minimisation procedure.

However, this general routine can be substituted by a simple although not quite universal method. We observe that in the examples considered here a possible way of choosing s_k is as follows. For the original functions y_k we evaluate

$$\frac{y_k'(x)}{y_k(x)} = -i\eta_k\xi_k(x) - \frac{\xi_k'(x)}{2\xi_k(x)},$$

then take

$$s_k = \operatorname{argmax}\left|\mathrm{Re}\,\frac{y_k'(x)}{y_k(x)}\right|.$$

The reasoning leading to this choice, although not rigorous, may prove to work in a generic situation. Replacing y_k'/y_k by constants beyond the points s_k as in (12), we obtain our final modes which are almost orthogonal to one another. Their suitable linear combinations approximate the actual eigenfunctions of our operators fairly well. This is the subject of the remaining subsections.

3.3. **Constructing Eigenfunctions.** In a generic situation when equation (9) has several real roots of proper signs, we have to approximate the relevant eigenfunction by the linear combination of the corresponding JWKB functions:

$$\phi(x) = \sum_{k=1}^{n} c_k y_k(x). \tag{13}$$

Here $y_k(x)$ are basic JWKB modes related to (a_k, η_k). The number of modes entering (13) can be arbitrary; in our examples $n = 1$ or 2. The coefficients c_k are to be determined.

One approach to computing these constants is as follows. Let c_k minimise the value of

$$\Delta := \frac{\|f(x) - \phi(x)\|}{\|f\|}. \tag{14}$$

Denote $d(x) := f(x) - \phi(x)$; a direct calculation gives us

$$\|d\|^2 = \|f(x) - \sum_{k=1}^{n} c_k y_k(x)\|^2 = \|f\|^2 - 2\mathrm{Re}\left(\sum_{k=1}^{n} c_k\bar{u}_k + \sum_{j,k=1}^{n} a_{jk}c_k\bar{c}_j\right) \tag{15}$$

where

$$u_k = \int_0^\infty f\bar{y}_k \mathrm{d}x, \qquad a_{jk} = \int_0^\infty y_k\bar{y}_j \mathrm{d}x.$$

Differentiating (15) with respect to c_k and putting the variation equal to zero, we obtain the desired constants:

$$C = A^{-1}U, \quad C = (c_1, \dots, c_n)^T, \quad U = (u_1, \dots, u_n)^T, \quad A = (a_{jk}), \; j,k = 1, \dots, n. \tag{16}$$

The integrals involved into (16) are easily computed by means of the routine described in [1] in terms of f'/f, y_k'/y_k. This procedure does not require computing the eigenfunctions themselves: it is only the values of u_k, a_{jk}, $j,k = 1, \dots, n$, that we have to calculate. Then the constants c_k, $k = 1, \dots, n$, are found from (16). Obviously, for a given eigenfunction our c_1, c_2 must depend on the normalisation of the functions f and y_k while the value of $|c_2/c_1|$ must not. We take $\|f\| = \|e_1\| = \|e_2\| = 1$ to make the matrix A well-conditioned and then repeat computations for several different values of $\|e_k\|$ to double-check our results (we leave $\|f\| = 1$ throughout the paper). The procedure developed in [1] turns out to be suitable for our purposes and provides reliable answers.

Let us tabulate $c := |c_2/c_1|$ for the examined eigenvalues of the operators H_c and $\tilde{H}_c$ (as above, m denotes the number of an eigenvalue).

Table 5. Values of c for the operators H_c and $\tilde{H}_c$

m	H_c	$\tilde{H}_c$		m	H_c	$\tilde{H}_c$
28	0.0447			42	277.2584	13.5057
30	0.0928	0.0328		44	1434.62	48.2824
32	0.2083	0.0621		46	7615.34	177.1347
34	0.7876	0.1420		48	41623.37	660.8588
36	2.9866	0.3890		50	354757.06	2486.87
38	13.4820	1.1897		52		10590.02
40	65.6680	3.9086				

The contents of the above table is illustrated qualitatively by the plots of the eigenfunctions (see figure 3). Indeed, for a certain range of eigenvalues the relevant eigenfunctions have two distinct components clearly seen in the plots. For lower eigenvalues the first mode y_1 is dominating, while the contribution of y_2 is more significant for the high energy spectrum. All our numerical results including the plots of the eigenfunctions indicate the transition from the first leading JWKB function y_1 to y_2 in formula (13). This phenomenon is observed for both examples studied here.

In the previous subsection we mentioned the parameters s_k entering the modified functions y_k. The formulae of this subsection contain these parameters fixed at some starting values. After minimising Δ with respect to c_k as described we minimise the obtained function with respect to s_k, and thus get the final results to be tabulated in the next subsection.

3.4. **The Efficiency of Approximations.** Having found c_k, $k = 1, 2$, we then compute Δ defined by (14) in terms of the calculated coefficients u_k, a_{jk}. The values of Δ tabulated below characterise the accuracy of the JWKB approximations we use.

As is seen from table 6, not only do the JWKB modes approximate eigenfunctions corresponding to higher eigenvalues but they also turn out to be surprisingly efficient even for the lower part of the spectrum. The plots of $|d_m|$ in comparison with $|f_m|$ (see figure 4) also indicate the effectiveness of the approximations obtained by our approach. The corrections d_m for other values of m either look similar to those shown in figure 4 or are invisible compared to the corresponding eigenfunctions.

These numerical results complete our study of eigenfunction approximations.

Table 6. Minimal values of Δ

m	H_c	$\tilde{H}_c$		m	H_c	$\tilde{H}_c$
10	0.132627	0.153114		32	0.015264	0.015016
12	0.042214	0.048187		34	0.017776	0.015332
14	0.029275	0.032804		36	0.014177	0.020596
16	0.021119	0.024966		38	0.009434	0.025885
18	0.015969	0.019302		40	0.006557	0.025631
20	0.012366	0.011576		42	0.004796	0.012372
22	0.011045	0.009765		44	0.003873	0.007280
24	0.010724	0.009110		46	0.002828	0.005568
26	0.014866	0.008487		48	0.002236	0.004359
28	0.015133	0.009798		50	0.001732	0.003464
30	0.015232	0.012214		52		0.003133

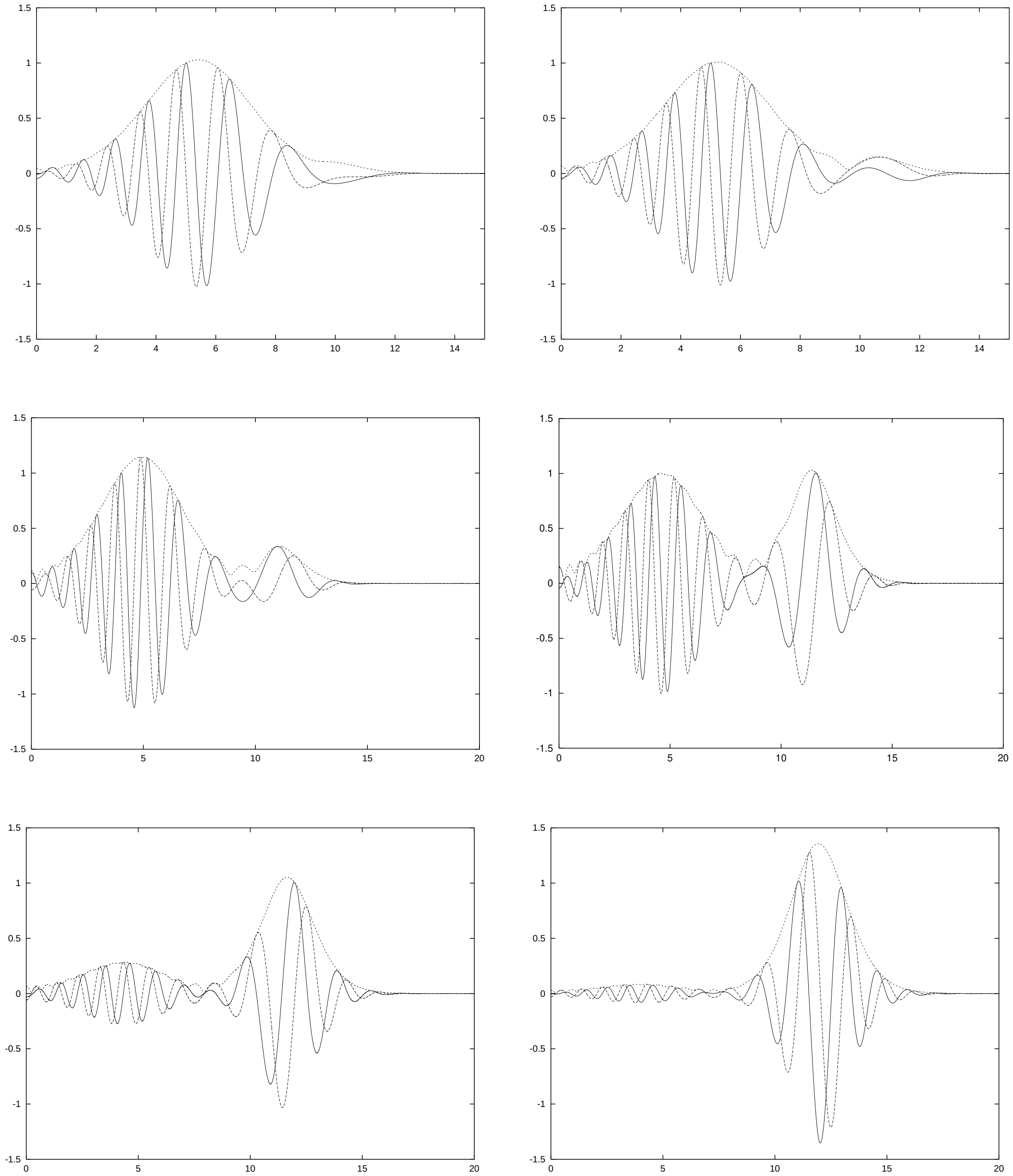

Figure 3. Eigenfunctions of H_c: Re f_m, Im f_m, $|f_m|$. From left to right, top to bottom: $m = 28,\ 30,\ 32,\ 34,\ 36,\ 38$

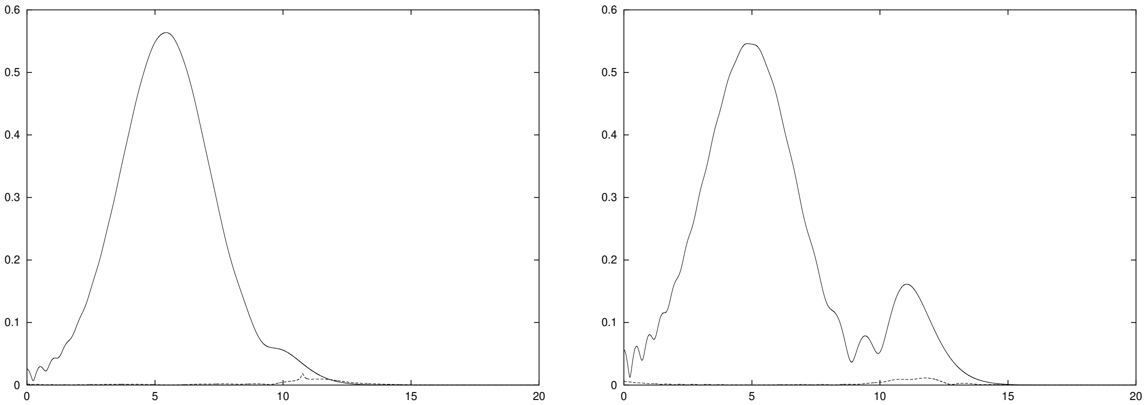

Figure 4. Plots of $|f_m|$ and $|d_m|$ for H_c. From left to right: $m = 28,\ 32$

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