Small-energy series for one-dimensional quantum-mechanical models with non-symmetric potentials

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Abstract. We generalize a recently proposed small-energy expansion for one-dimensional quantum-mechanical models. The original approach was devised to treat symmetric potentials and here we show how to extend it to non-symmetric ones. Present approach is based on matching the logarithmic derivatives for the left and right solutions to the Schrdinger equation at the origin (or any other point chosen conveniently) . As in the original method, each logarithmic derivative can be expanded in a small-energy series by straightforward perturbation theory. We test the new approach on four simple models, one of which is not exactly solvable. The perturbation expansion converges in all the illustrative examples so that one obtains the ground-state energy with an accuracy determined by the number of available perturbation corrections.

1. Introduction

In a recent paper Bender and Jones [1] proposed a convergent perturbation series for the calculation of the eigenvalues of the Schrödinger equation in one dimension. The approach consists of the expansion of the eigenfunction as a power series of the energy E itself and the construction of a function $f(E)$ that vanishes when $E = 0$ and increases monotonously till $f(E_0) = 1$, where E_0 is the lowest eigenvalue. This strategy is based on the fact that the eigenfunction $\psi(x, E)$ satisfies $\psi_0(0, E_0) = 0$ in the case of symmetric potentials $V(-x) = V(x)$. The authors also showed how to extend the approach for the treatment of parity-time invariant complex potentials $V(-x)^* = V(x)$. The method is not restricted to the ground state; the zeros of the Padé approximants for the small-energy expansion of $f(E) - 1$ are estimates of the energies of the excited states [1].

The purpose of this paper is to extend the approach proposed by Bender and Jones to non-symmetric potentials. In section 2 we outline the method of Bender and Jones but focus on the logarithmic derivative of the eigenfunction instead of on the eigenfunction itself. In section 3 we briefly consider an exactly solvable symmetric potential. However, instead of choosing an example that supports an infinite number of eigenvalues like those of Bender and Jones we concentrate on a finite well. In section 4 we discuss a finite non-symmetric well and develop the extension of the method of Bender and Jones in terms of the logarithmic derivative of the wavefunction. In section 5 we illustrate the application of the the generalized approach on three non-symmetric infinite wells, one of which is not exactly solvable. Finally, in section 6 we summarize the main results and draw conclusions.

2. The method of Bender and Jones

Consider the Schrödinger equation

$$\psi''(x) = [V(x) - E]\psi(x) \tag{1}$$

where $\psi(x)$ vanishes at $\pm\infty$. The method applies to symmetric potentials $V(-x) = V(x)$ that are bounded from below and, without loss of generality, we assume that $V(x) \geq V(0) = 0$.

The method of Bender and Jones [1] is based on the small-energy expansion for $\psi(x)$

$$\psi(x, E) = \sum_{j=0}^{\infty} \psi_j(x) E^j \tag{2}$$

For convenience, in what follows we consider the alternative expansion of the logarithmic derivative

$$L(x, E) = \frac{\psi'(x, E)}{\psi(x, E)} \tag{3}$$

in the form

$$L(x, E) = \sum_{j=0}^{\infty} L_j(x) E^j \tag{4}$$

Because of the symmetry of the potential the solutions to the equation (1) are either even or odd. In particular, the ground state $\psi(x, E_0)$ is even so that $\psi'(0, E_0) = 0$ and $L(0, E)$ vanishes when E is the ground-state energy E_0. Therefore, the function

$$f(E) = 1 - \frac{L(0, E)}{L_0(0)} \tag{5}$$

satisfies $f(0) = 0$ and $f(E_0) = 1$. Besides, $f(E)$ can be expanded as [1]

$$f(E) = \sum_{j=1}^{\infty} c_j E^j \tag{6}$$

Since $\psi(x,E)$ is odd when E is the energy of the first-excited state E_1, then $\psi(0,E_1)=0$ and $E=E_1$ is a pole of $f(E)$. Consequently, the radius of convergence of (6) cannot be greater than E_1.

Note that we can also obtain E_0 as a root of $L(0,E)=0$ that can be obtained approximately from the small-energy series

$$L(0,E)=\sum_{j=0}^{\infty}L_j(0)E^j \tag{7}$$

3. Finite symmetric well

Bender and Jones studied several symmetric wells that are unbounded from above and therefore support an infinite number of bound states. Although the aim of this paper is the application of the small-energy expansion to non-symmetric potentials we first consider symmetric wells that are bounded from below and above. Without loss of generality we assume that $0\leq V(x)\leq V_R$. It is well-known that such a potential supports a bound state no matter how small the well depth V_R. If there is only one bound state, then one expects the pole of $f(E)$ closest to the origin in the complex E plane to be a resonance. This is the main reason for discussing such symmetric well here.

The simplest exactly-solvable model is given by

$$V(x)=\begin{cases} 0, & |x|<1 \\ V_R>0, & |x|>1 \end{cases} \tag{8}$$

A straightforward calculation yields the logarithmic derivative at the origin

$$L(0,E)=\frac{\sqrt{E}\left(\sqrt{E}\sin\left(\sqrt{E}\right)-\sqrt{V_R-E}\cos\left(\sqrt{E}\right)\right)}{\sqrt{E}\cos\left(\sqrt{E}\right)+\sqrt{V_R-E}\sin\left(\sqrt{E}\right)} \tag{9}$$

that can be expanded in the E-series

$$\begin{aligned} L(0,E)= & -\frac{\sqrt{V_R}}{\sqrt{V_R}+1}+\frac{\left(2V_R^{3/2}+6V_R+6\sqrt{V_R}+3\right)E}{6\sqrt{V_R}\left(\sqrt{V_R}+1\right)^2} \\ & +\frac{\left(8{V_R}^3+48V_R^{5/2}+120{V_R}^2+180V_R^{3/2}+180V_R+135\sqrt{V_R}+45\right)E^2}{360V_R^{3/2}\left(\sqrt{V_R}+1\right)^3} \\ & +\ldots \end{aligned} \tag{10}$$

Its radius of convergence is determined by the root E_r of $\sqrt{E_r}\cos\left(\sqrt{E_r}\right) + \sqrt{V_R - E_r}\sin\left(\sqrt{E_r}\right) = 0$ with the smallest absolute value. As an illustrative example we choose $V_R = 1$ that supports only one bound state. In this case we have $E_r = 1.222635745 - 0.5925040566i$. Since $E_0 < 1 < |E_r|$ the perturbation expansion will enable us to obtain the lowest eigenvalue E_0 with increasing accuracy. For example, table 1 shows the rate of convergence of the approximate eigenvalue estimated from the expansion (10) for $V_R = 1$.

4. Finite non-symmetric well

As argued in the introduction, the aim of this paper is the extension of the method proposed by Bender and Jones to non-symmetric potentials that are bounded from below. As before, without loss of generality we assume that $V(x) \geq V(0) = 0$. For a given value of E we construct the logarithmic derivatives $L_L(x,E)$ and $L_R(x,E)$ from the left and right solutions $\psi^{(L)}(x,E)$ and $\psi^{(R)}(x,E)$ to the differential equation (1) that vanish when $x \to -\infty$ and x$\to \infty$, respectively. The continuity of the eigenfunction and its first derivative at $x = 0$ requires that the curves $L_L(0,E)$ and $L_R(0,E)$ intersect at each of the eigenvalues $E = E_n$. Obviously, we can obtain E-power series for both $L_L(0,E)$ and $L_R(0,E)$ in the way proposed by Bender and Jones; that is to say, we simply apply the method twice, one to the left of $x = 0$ and one to the right. The intersection of the two small-energy expansions thus derived provide an estimate of the lowest eigenvalue E_0.

In order to illustrate this approach we choose the exactly solvable non-symmetric finite well

$$V(x) = \begin{cases} V_L > 0, \ x < -1 \\ 0, \ |x| < 1 \\ V_R > 0, \ x > 1 \end{cases} \tag{11}$$

The exact logarithmic derivatives at the origin

$$L_L(0,E) = \frac{\sqrt{E}\left(\sqrt{V_L-E}\cos\left(\sqrt{E}\right)-\sqrt{E}\sin\left(\sqrt{E}\right)\right)}{\sqrt{E}\cos\left(\sqrt{E}\right)+\sqrt{V_L-E}\sin\left(\sqrt{E}\right)}$$

$$L_R(0,E) = \frac{\sqrt{E}\left(\sqrt{E}\sin\left(\sqrt{E}\right)-\sqrt{V_R-E}\cos\left(\sqrt{E}\right)\right)}{\sqrt{E}\cos\left(\sqrt{E}\right)+\sqrt{V_R-E}\sin\left(\sqrt{E}\right)} \tag{12}$$

can be expanded as

$$\begin{aligned} L_L(0,E) &= \frac{\sqrt{V_L}}{\sqrt{V_L}+1} - \frac{\left(2V_L^{3/2}+6V_L+6\sqrt{V_L}+3\right)E}{6\sqrt{V_L}\left(\sqrt{V_L}+1\right)^2} \\ &- \frac{\left(8{V_L}^3+48V_L^{5/2}+120{V_L}^2+180V_L^{3/2}+180V_L+135\sqrt{V_L}+45\right)E^2}{360V_L^{3/2}\left(\sqrt{V_L}+1\right)^3} + \ldots \\ L_R(0,E) &= -\frac{\sqrt{V_R}}{\sqrt{V_R}+1} + \frac{\left(2V_R^{3/2}+6V_R+6\sqrt{V_R}+3\right)E}{6\sqrt{V_R}\left(\sqrt{V_R}+1\right)^2} \\ &+ \frac{\left(8{V_R}^3+48V_R^{5/2}+120{V_R}^2+180V_R^{3/2}+180V_R+135\sqrt{V_R}+45\right)E^2}{360V_R^{3/2}\left(\sqrt{V_R}+1\right)^3} \\ &+ \ldots \end{aligned} \tag{13}$$

Figure 1 shows $L_L(0,E)$ and $L_R(0,E)$ when $V_L = 2$ and $V_R = 1$. These curves intersect at the ground-state energy as argued above. For such values of the potential parameters there is just one bound state. Table 2 shows the rate of convergence of the estimated lowest eigenvalue obtained from the intersection of the series (13) for increasing truncation order. In this case the radii of convergence of each expansion is determined by $E_{rL} = 2.125364032 - 0.3468294596i$ and $E_{rR} = 1.222635745 - 0.5925040566i$ and the approach is successful because both series converge at $E = E_0 < |E_{rR}| < |E_{rL}|$.

5. Infinite wells

As an extension of the model with the linear symmetric potential $V(x) = |x|$ discussed by Bender and Jones we consider the non-symmetric version

$$V(x) = \begin{cases} -a_L x, & x < 0 \\ a_R x, & x > 0 \end{cases} \tag{14}$$

where a_L, $a_R > 0$. In this case we have

$$\begin{aligned} L_L(0,E) &= -\frac{a_L^{1/3} A_i'\left(-E/a_L^{2/3}\right)}{A_i\left(-E/a_L^{2/3}\right)} \\ L_R(0,E) &= \frac{a_R^{1/3} A_i'\left(E/a_R^{2/3}\right)}{A_i\left(E/a_R^{2/3}\right)} \end{aligned} \tag{15}$$

where $A_i(z)$ is one of the Airy functions [2].

In order to carry out a sample calculation we choose $a_R = 1$ and $a_L = 2$ and obtain the series

$$\begin{aligned} L_L(0) &= 0.9184964715 - 0.4218178838\,E - 0.05628088100\,E^2 \\ &\quad - 0.01242379097\,E^3 - 0.003082268481\,E^4 + \ldots \\ L_R(0) &= -0.7290111325 + 0.5314572310\,E + 0.1125617620\,E^2 \\ &\quad + 0.03944307773\,E^3 + 0.01553365974\,E^4 + \ldots \end{aligned} \tag{16}$$

The singularities of $L_L(0,E)$ and $L_R(0,E)$ for this particular choice of potential parameters appear at $E = 3.711514163$ and $E = 2.338107410$, respectively. Since both are larger than E_0 the perturbation expansions (16) are suitable for the calculation of this eigenvalue. Table 3 shows the rate of convergence of the approach for the lowest eigenvalue E_0.

As a non-symmetric extension of the harmonic oscillator discussed by Bender and Jones we consider the potential

$$V(x) = \begin{cases} a_L x^2, & x < 0 \\ a_R x^2, & x > 0 \end{cases} \tag{17}$$

where a_L, $a_R > 0$. In this case we have

$$\begin{aligned} L_L(0) &= \sqrt{2} a_L^{1/4} \frac{D_{(E+\sqrt{a_L})/(2\sqrt{a_L})}(0)}{D_{(E-\sqrt{a_L})/(2\sqrt{a_L})}(0)} \\ L_R(0) &= -\sqrt{2} a_R^{1/4} \frac{D_{(E+\sqrt{a_R})/(2\sqrt{a_R})}(0)}{D_{(E-\sqrt{a_R})/(2\sqrt{a_R})}(0)} \end{aligned} \tag{18}$$

where $D_\nu(z)$ is the parabolic cylinder function [2].

For $a_L = 2$ and $a_R = 1$ we have the small-energy expansions

$$L_L(0) = 0.8038781325 - 0.4464420544\,E - 0.06011306588\,E^2 - 0.01251356963\,E^3$$

$$
\begin{aligned}
& - 0.002831976530\, E^4 + \ldots \\
L_R(0) = & - 0.6759782395 + 0.5309120676\, E + 0.1010977236\, E^2 + 0.02976245185\, E^3 \\
& + 0.009525595408\, E^4 + \ldots
\end{aligned} \tag{19}
$$

for the left and right solutions, respectively. Table 4 shows the convergence of the lowest eigenvalue of the non-symetric quadratic well (17) estimated from the truncated small-energy series (19).

Finally, we consider the Schrödinger equation (1) with the non-symmetric anharmonic potential

$$
V(x) = x^4 + \lambda x^3 \tag{20}
$$

that is not exactly solvable. Note that the minimum of the potential-energy function $V_{min} = V(x_{min})$ is not located at the origin but at $x_{min} = -3\lambda/4$ and that $V(0) = 0 > V_{min} = -27\lambda^4/256$ does not agree with the assumption made above. However, that arbitrary assumption was made for simplicity and is unnecessary for the application of the approach.

In this case we do not attempt to calculate the small-energy series for the left and right logarithmic derivatives but we can obtain $L_L(0, E)$ and $L_R(0, E)$ quite accurately by means of a variant of the Riccati-Padé method (RPM) [3].

The logarithmic derivative (3) can be expanded in a Taylor series about $x = 0$

$$
L(x, E) = \sum_{j=0}^{\infty} g_j x^j \tag{21}
$$

where the coefficients g_j, $j > 0$, depend on both g_0 and E. The Hankel determinants $H_D^d(E, g_0) = |g_{i+j+d-1}|_{i,j=1}^{D}$, where $D = 2, 3, \ldots$ is the determinant dimension and $d = 0, 1, \ldots$, are polynomial functions of g_0 and E. For a given value of E the RPM condition $H_D^d(E, g_0) = 0$ yields sequences of roots $g_0^{[D,d]}(E)$, $D = 2, 3, \ldots$ that converge towards $L_L(0, E)$ and $L_R(0, E)$. Since the RPM takes into account the left and right solutions simultaneously we cannot determine which sequence corresponds to either $L_L(0, E)$ or $L_R(0, E)$. However, this is not a serious drawback as we will see in what follows.

For concreteness we restrict ourselves to $\lambda = 0.1$ that is small and we therefore expect $L_L(0, E_0) = L_R(0, E_0) = L(0, E_0)$ to be close to zero. Figure 2 shows that the left and right logarithmic derivatives approach each other as E increases from $E = 0$ and intersect at E_0 as expected. In this straightforward application of the RPM we simply chose $d = 0$ and $2 \leq D \leq 15$.

We can also calculate the value of E_0 quite accurately by means of the standard RPM that is based on pairs of Hankel determinants $H_D^{d,e}(E, g_0) = |g_{2i+2j+2d-2}|_{i,j=1}^{D}$ and $H_D^{d,o}(E, g_0) = |g_{2i+2j+2d-1}|_{i,j=1}^{D}$ [3]. In this case, sequences of roots of the set of nonlinear equations $H_D^{d,e}(E, g_0) = 0$ and $H_D^{d,o}(E, g_0) = 0$ converge towards E_0 and $L(0, E_0)$. For $\lambda = 0.1$ we obtain

$$\begin{aligned} E_0 &= 1.0590028460380260258 \\ L_L(0, E_0) = L_R(0, E_0) &= -0.02652946094577843397 \end{aligned} \tag{22}$$

that agree with the intersection shown in Figure 2. Here we chose the same values of D and d indicated previously.

6. Conclusions

In this paper we generalized the method of Bender and Jones so that it can be applied to non-symmetric potentials. Present approach consists of matching the logarithmic derivatives of the left and right solutions at the origin. The matching procedure itself is well known but here it is combined with the original idea of the small-energy series proposed by those authors. The series are convergent as in the case of the symmetric potentials studied earlier. It is worth noting that the same procedure applies to symmetric potentials but in this case it is not necessary to carry out both calculations because the two curves $L_L(0, E)$ and $L_R(0, E)$ are symmetric with respect to the E axis.

As illustrative examples we explicitly considered three exactly solvable models and a nontrivial anharmonic oscillator. In the latter case we did not derive the small-energy series and restricted ourselves to the accurate calculation of the two logarithmic derivatives at origin by means of the RPM. In this way we showed that the two curves intersect at the ground-state energy that we also calculated accurately by means of the RPM. For the treatment of one-dimensional or separable problems the RPM is by far preferable to the perturbation approach but the latter may hopefully be applied to non-separable systems. For the time being we do not know how to apply this perturbation approach to multidimensional problems, but it is likely that one should have to resort to some kind of matching procedure like the one illustrated in this paper.

Acknowledgments

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Table 1. Eigenvalue of the symmetric well (8) of depth $V_R = 1$ estimated by means of the expansion (10) of order n. The exact result is $E_0 = 0.5462468341$.

n	E_0
4	0.5855444198
8	0.5516251660
12	0.5472622152
16	0.5464638914
20	0.5462964250
24	0.5462586560
28	0.5462497386
32	0.5462475642
36	0.5462470210
40	0.5462468826
44	0.5462468468
48	0.5462468375
52	0.5462468350
56	0.5462468344
60	0.5462468343
64	0.5462468341

Table 2. Eigenvalue of the non-symmetric well (11) with $V_L = 2$ and $V_R = 1$ estimated by means of the expansions of $L_R(0, E)$ and $L_L(0, E)$. The exact result is $E_0 = 0.6446113612$.

n	E_0
4	0.8367722372
8	0.6634864161
12	0.6487132635
16	0.6457463863
20	0.6449609259
24	0.6447254502
28	0.6446499927
32	0.6446247871
36	0.6446161202
40	0.6446130747
44	0.6446119860
48	0.6446115915
52	0.6446114469
56	0.6446113933
60	0.6446113734
64	0.6446113658
68	0.6446113630
72	0.6446113618
76	0.6446113615
80	0.6446113614
84	0.6446113614
88	0.6446113612

Table 3. Eigenvalue of the non-symmetric linear well (14) with $a_L = 2$ and $a_R = 1$ estimated by means of the expansions of $L_R(0, E)$ and $L_L(0, E)$. The exact result is $E_0 = 1.250207832$.

n	E_0
2	1.387352237
4	1.275507151
6	1.256485215
8	1.251913598
10	1.250686548
12	1.250343776
14	1.250246604
16	1.250218907
18	1.250210997
20	1.250208737
22	1.250208091
24	1.250207905
26	1.250207854
28	1.250207837
30	1.250207833
32	1.250207832

Table 4. Eigenvalue of the non-symmetric quadratic well (17) with $a_L = 2$ and $a_R = 1$ estimated by means of the expansions of $L_R(0, E)$ and $L_L(0, E)$. The exact result is $E_0 = 1.176933152$.

n	E_0
2	1.254541164
4	1.185370810
6	1.178091246
8	1.177102981
10	1.176958699
12	1.176937027
14	1.176933737
16	1.176933265
18	1.176933166

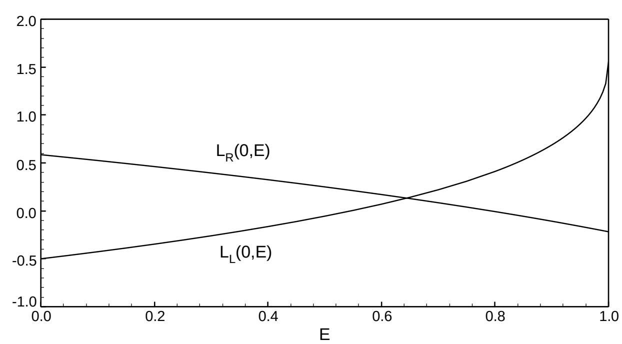

Figure 1. $L_R(E, 0)$ and $L_L(E, 0)$ for the non-symmetric well (11) with $V_L = 2$ and $V_R = 1$

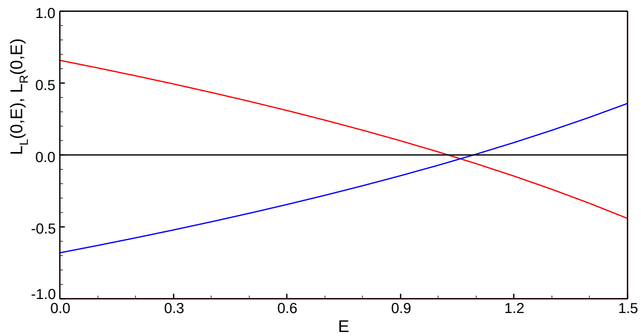

Figure 2. $L_R(E,0)$ and $L_L(E,0)$ for the non-symmetric anharmonic oscillator (20)