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

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Abstract We generalize a small-energy expansion for one-dimensional quantum-mechanical models proposed recently by other authors. 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 Schrödinger 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.

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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 monotonically 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 $\psi(0, E_0) = 0$ in the case of symmetric potentials $V(-x) = V(x)$. By means of a suitable modification of this approach the authors were also able to treat parity-time invariant Hamiltonians with one-dimensional complex potentials that satisfy $V(-x)^* = V(x)$. 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. To this end, in Sect. 2 we derive the method in a more general way focussing on the logarithmic derivative of the eigenfunction. In Sect. 3 we briefly consider an exactly-solvable symmetric potential bounded from below and above. The reason for including such an example in the present paper is that Bender and Jones only considered problems with an infinite number of bound states. In Sect. 4 we discuss an exactly-solvable finite non-symmetric well and illustrate the application of the generalized perturbation method. In Sect. 5 we consider three non-symmetric infinite wells, one of which is not exactly solvable. Two of them are non-symmetric versions of the problems discussed by Bender and Jones. Finally, in Sect. 6 we summarize the main results of the paper and draw conclusions.

2 The method

Consider the dimensionless one-dimensional Schrödinger equation

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

where $V(x)$ is bounded from below. The solution satisfies the boundary conditions

$$\lim_{|x| \to \infty} \psi(x, E) = 0, \tag{2}$$

when E is one of the bound-state eigenvalues $E_0 < E_1 < \ldots$. If E is not exactly one of those eigenvalues then $\psi(x, E)$ can satisfy at most one of the boundary conditions.

Suppose, for example, that $\psi(x, E)$ satisfies the right boundary condition

$$\lim_{x \to \infty} \psi(x, E) = 0, \tag{3}$$

for an arbitrary value of E. Let $\psi_0(x) = \psi(x, 0)$ be a solution to Eq. (1) that satisfies the same boundary condition (3) for $E = 0$. The function $\phi(x, E)$ defined by

$$\psi(x, E) = \psi_0(x)\phi(x, E), \tag{4}$$

satisfies $\phi(x, 0) \equiv 1$ and enables us to reduce the Schrödinger Eq. (1) to the simpler form

$$\left(\psi_0^2 \phi'\right)' = -E\psi_0^2\phi. \tag{5}$$

If we expand $\phi(x, E)$ in a Taylor series about $E = 0$

$$\phi(x, E) = \sum_{j=0}^{\infty} \phi_j(x) E^j, \tag{6}$$

where $\phi_0(x) = \phi(x, 0) \equiv 1$, then we can easily obtain the coefficients $\phi_j(x)$ of this perturbation expansion iteratively from Eq. (5) as:

$$\left(\psi_0^2 \phi_j'\right)' = -\psi_0^2 \phi_{j-1}, \ j = 1, 2, \ldots. \tag{7}$$

The method of Bender and Jones [1] applies to symmetric potentials $V(-x) = V(x)$ for which $\psi(-x, E_n) = (-1)^n \psi(x, E_n)$. In this case the logarithmic derivative of the solution

$$L(x, E) = \frac{\psi'(x, E)}{\psi(x, E)} = L(x, 0) + \frac{\phi'(x, E)}{\phi(x, E)}, \tag{8}$$

satisfies $L(0, E_0) = 0$ so that the function

$$f(E) = 1 - \frac{L(0, E)}{L(0, 0)} = -\frac{\phi'(0, E)}{L(0, 0)\phi(0, E)} \tag{9}$$

increases monotonically from $f(0) = 0$ to $f(E_0) = 1$ [1]. It follows from Eq. (6) that this function can be expanded in the small-energy series

$$f(E) = \sum_{j=1}^{\infty} c_j E^j. \tag{10}$$

Since $\psi(0, E_1) = 0$ both $L(0, E)$ and $f(E)$ are singular at $E = E_1$ and the radius of convergence of the small-energy series cannot be greater than E_1 (the case in which $V(x)$ supports just one bound state will be discussed later on in Sect. 3).

The calculation of the perturbation coefficients c_j can be greatly simplified by choosing a convenient normalization condition. For example, if we choose $\psi(0, E) = \psi_0(0) = 1$ then $\phi(0, E) = 1$ and

$$f(E) = -\frac{\phi'(0, E)}{\psi_0'(0)}, \tag{11}$$

so that

$$c_j = -\frac{\phi_j'(0)}{\psi_0'(0)}. \tag{12}$$

Obviously we can obtain E_0 as a root of either $f(E_0) = 1$ or $L(0, E_0) = 0$, where

$$L(0, E) = \psi_0'(0) + \phi'(0, E). \tag{13}$$

This function can also be expanded in a small-energy series

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

$$L_0 = \psi_0'(0), \ L_j = \phi_j'(0), \ j > 0 \tag{14}$$

In the more general case of a non-symmetric potential $V(-x) \neq V(x)$ we need the left $\psi^{(L)}(x, E)$ and right $\psi^{(R)}(x, E)$ solutions to the Schrödinger Eq. (1) that satisfy

$$\lim_{x \to -\infty} \psi^{(L)}(x, E) = 0$$

$$\lim_{x \to \infty} \psi^{(R)}(x, E) = 0. \tag{15}$$

We also need the corresponding reference solutions, or solutions of order zero, $\psi_0^{(L)}(x) = \psi^{(L)}(x, 0)$ and $\psi_0^{(R)}(x) = \psi^{(R)}(x, 0)$ that satisfy similar left and right boundary conditions, respectively. In this case it is also useful to choose the normalization conditions $\psi^{(L,R)}(x_0, E) = \psi_0^{(L,R)}(x_0) = 1$ at a convenient coordinate point x_0.

The left and right logarithmic derivatives

$$L_L(x, E) = \frac{\psi'^{(L)}(x, E)}{\psi^{(L)}(x, E)}$$

$$L_R(x, E) = \frac{\psi'^{(R)}(x, E)}{\psi^{(R)}(x, E)}, \tag{16}$$

match at $x = x_0$ if and only if E is one of the bound-state eigenvalues:

$$L_R(x_0, E_n) - L_L(x_0, E_n) = 0. \tag{17}$$

If we define $\phi^{(L)}(x, E)$ and $\phi^{(R)}(x, E)$ by

$$\psi^{(L,R)}(x, E) = \psi_0^{(L,R)}(x)\phi^{(L,R)}(x, E), \tag{18}$$

then the left and right logarithmic derivatives become

$$L_{L,R}(x_0, E) = \psi_0'^{(L,R)}(x_0) + \phi'^{(L,R)}(x_0, E). \tag{19}$$

The perturbation approach is similar to the one outlined above; we simply expand

$$\phi^{(L,R)}(x, E) = \sum_{j=0}^{\infty} \phi_j^{(L,R)}(x) E^j, \tag{20}$$

where $\phi_0^{(L,R)}(x) \equiv 1$, and obtain the perturbation corrections $\phi_j^{(L,R)}(x)$ from two equations similar to (7). Straightforward integration leads to

$$\phi_n^{(L)}(x) = \int_x^{x_0} \frac{ds}{\psi_0^{(L)}(s)^2} \int_{-\infty}^s dt \, \psi_0^{(L)}(t)^2 \phi_{n-1}^{(L)}(t)$$

$$\phi_n^{(R)}(x) = \int_{x_0}^x \frac{ds}{\psi_0^{(R)}(s)^2} \int_s^\infty dt \, \psi_0^{(R)}(t)^2 \phi_{n-1}^{(R)}(t), \tag{21}$$

that provide the perturbation corrections iteratively for $n = 1, 2, \ldots$ starting from $\phi_0^{(L,R)}(x) \equiv 1$. The second expression is identical to the one derived by Bender and Jones for the symmetric case.

Since $\psi_0^{(L)}(x)$ and $\psi_0^{(R)}(x)$ decay to the left and right, respectively, then $\psi_0'^{(L)}(x_0) > 0$ and $\psi_0'^{(R)}(x_0) < 0$. On the other hand, since $\phi_n'^{(L)}(x_0) < 0$ and $\phi_n'^{(R)}(x_0) > 0$ we conclude that $L_L(x_0, E)$ and $L_R(x_0, E)$ are monotonically decreasing an increasing, respectively, matching at $E = E_0$.

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 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 the singularity of $f(E)$ closest to the origin in the complex E plane cannot be an excited state. This is the main reason for discussing such symmetric wells here.

The simplest exactly-solvable model is given by

$$V(x) = \begin{cases} 0, & |x| < 1 \\ V_R > 0, & |x| > 1 \end{cases}. \tag{22}$$

A straightforward calculation yields the logarithmic derivative at the origin

$$L(0, E) = \frac{\sqrt{E}\left(\sqrt{E}\sin\left(\sqrt{E}\right) - \sqrt{V_R - E}\cos\left(\sqrt{E}\right)\right)}{\sqrt{E}\cos\left(\sqrt{E}\right) + \sqrt{V_R - E}\sin\left(\sqrt{E}\right)}, \tag{23}$$

that can be expanded in the E-series

Table 1 Bound-state eigenvalue of the symmetric well (22) of depth $V_R = 1$ estimated by means of the expansion (24) 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

$$L(0, E) = -\frac{\sqrt{V_R}}{\sqrt{V_R} + 1} + \frac{\left(2V_R^{3/2} + 6V_R + 6\sqrt{V_R} + 3\right) E}{6\sqrt{V_R}\left(\sqrt{V_R} + 1\right)^2}$$
$$+ \frac{\left(8V_R^3 + 48V_R^{5/2} + 120V_R^2 + 180V_R^{3/2} + 180V_R + 135\sqrt{V_R} + 45\right) E^2}{360 V_R^{3/2}\left(\sqrt{V_R} + 1\right)^3}$$
$$+ \dots, \tag{24}$$

which clearly shows that it is monotonically increasing. Its radius of convergence is determined by $E = V_R > E_0$ so that the perturbation expansion will enable us to obtain the lowest eigenvalue E_0 with arbitrary accuracy. For example, Table 1 shows the rate of convergence of the approximate eigenvalue estimated from the expansion (24) for $V_R = 1$.

4 Finite non-symmetric well

As a first illustrative example of non-symmetric potential we choose the exactly-solvable finite well

$$V(x) = \begin{cases} V_L > 0, & x < -1 \\ 0, & |x| < 1 \\ V_R > 0, & x > 1 \end{cases}. \tag{25}$$

The exact logarithmic derivatives at the origin

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

$$L_R(0, E) = \frac{\sqrt{E}\left(\sqrt{E}\sin\left(\sqrt{E}\right) - \sqrt{V_R - E}\cos\left(\sqrt{E}\right)\right)}{\sqrt{E}\cos\left(\sqrt{E}\right) + \sqrt{V_R - E}\sin\left(\sqrt{E}\right)}, \tag{26}$$

can be expanded as

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

$$L_R(0, E) = -\frac{\sqrt{V_R}}{\sqrt{V_R} + 1} + \frac{\left(2V_R^{3/2} + 6V_R + 6\sqrt{V_R} + 3\right)E}{6\sqrt{V_R}\left(\sqrt{V_R} + 1\right)^2}$$
$$+ \frac{\left(8V_R^3 + 48V_R^{5/2} + 120V_R^2 + 180V_R^{3/2} + 180V_R + 135\sqrt{V_R} + 45\right)E^2}{360V_R^{3/2}\left(\sqrt{V_R} + 1\right)^3}$$
$$+ \ldots . \tag{27}$$

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 (27) for increasing truncation order.

5 Infinite wells

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

$$V(x) = \begin{cases} -a_L x, & x < 0 \\ a_R x, & x > 0 \end{cases}, \tag{28}$$
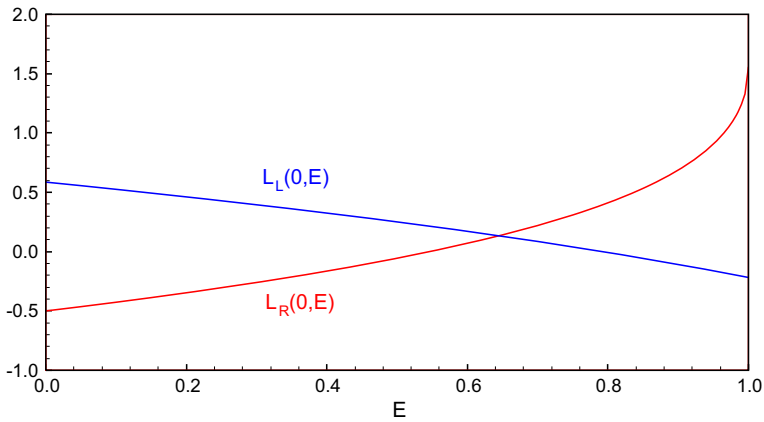
Fig. 1 $L_R(0, E)$ and $L_L(0, E)$ for the non-symmetric well (25) with $V_L = 2$ and $V_R = 1$

Table 2 Bound-state eigenvalue of the non-symmetric well (25) 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

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

$$L_L(0, E) = -\frac{a_L^{1/3} A_i'\left(-E/a_L^{2/3}\right)}{A_i\left(-E/a_L^{2/3}\right)}$$

$$L_R(0, E) = \frac{a_R^{1/3} A_i'\left(E/a_R^{2/3}\right)}{A_i\left(E/a_R^{2/3}\right)}, \qquad (29)$$

where $A_i(z)$ is an Airy function [2].

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

$$\begin{aligned}
L_L(0) = {}& 0.9184964715 - 0.4218178838\, E - 0.05628088100\, E^2 \\
& - 0.01242379097\, E^3 - 0.003082268481\, E^4 + \ldots \\
L_R(0) = {}& -0.7290111325 + 0.5314572310\, E + 0.1125617620\, E^2 \\
& + 0.03944307773\, E^3 + 0.01553365974\, E^4 + \ldots. \qquad (30)
\end{aligned}$$

The singularities of $L_L(0, E)$ and $L_R(0, E)$ for this particular choice of potential parameters are located at $E = 3.711514163$ and $E = 2.338107410$, respectively. Since both are larger than E_0 the perturbation expansions (30) are suitable for the calculation of this eigenvalue with arbitrary accuracy. 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

$$V(x) = \begin{cases} a_L x^2, & x < 0 \\ a_R x^2, & x > 0 \end{cases}, \qquad (31)$$

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

$$L_L(0) = \sqrt{2} a_L^{1/4} \frac{D_{(E+\sqrt{a_L})/(2\sqrt{a_L})}(0)}{D_{(E-\sqrt{a_L})/(2\sqrt{a_L})}(0)}$$

$$L_R(0) = -\sqrt{2} a_R^{1/4} \frac{D_{(E+\sqrt{a_R})/(2\sqrt{a_R})}(0)}{D_{(E-\sqrt{a_R})/(2\sqrt{a_R})}(0)}, \qquad (32)$$

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

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

$$\begin{aligned}
L_L(0) = {}& 0.8038781325 - 0.4464420544\, E - 0.06011306588\, E^2 - 0.01251356963\, E^3 \\
& - 0.002831976530\, E^4 + \ldots \\
L_R(0) = {}& -0.6759782395 + 0.5309120676\, E + 0.1010977236\, E^2 + 0.02976245185\, E^3 \\
& + 0.009525595408\, E^4 + \ldots, \qquad (33)
\end{aligned}$$

Table 3 Lowest eigenvalue of the non-symmetric linear well (28) 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 Lowest eigenvalue of the non-symmetric quadratic well (31) 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

for the left and right solutions, respectively. Table 4 shows the convergence of the series for the lowest eigenvalue of the non-symmetric quadratic well (31) estimated from the truncated small-energy series (33).

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

$$V(x) = x^4 + \lambda x^3, \tag{34}$$

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.
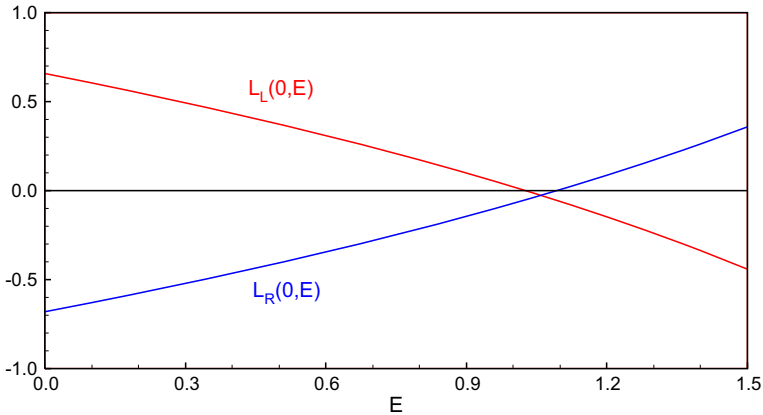
Fig. 2 $L_R(0, E)$ and $L_L(0, E)$ for the non-symmetric anharmonic oscillator (34) with $\lambda = 1$

In this case we do not attempt to calculate the small-energy series for the left and right logarithmic derivatives and instead 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 (8) can be expanded in a Taylor series about $x = 0$

$$L(x, E) = \sum_{j=0}^{\infty} g_j x^j, \tag{35}$$

where the coefficients g_j, $j > 0$, depend on both g_0 and E. The Hankel determinants $H_D^d(E, g_0) = \left| g_{i+j+d-1} \right|_{i,j=1}^D$, 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 $L_R(0, E)$. For each value of E the RPM yields both $L_L(0, E)$ and $L_R(0, E)$ simultaneously as limits of two sequences of roots of the same sequence of Hankel determinants.

For concreteness we restrict ourselves to $\lambda = 0.1$ that is sufficiently small to 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 (from above and below, respectively) 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 $H_D^{d,e}(E, g_0) = \left| g_{2i+2j+2d-2} \right|_{i,j=1}^D$ and $H_D^{d,o}(E, g_0) = \left| g_{2i+2j+2d-1} \right|_{i,j=1}^D$ [3]. In this case, sequences of roots of the set of nonlinear equations $\left\{ H_D^{d,e}(E, g_0) = 0, H_D^{d,o}(E, g_0) = 0 \right\}$ converge towards E_0 and $L(0, E_0)$. For $\lambda = 0.1$ we obtain

$$E_0 = 1.0590028460380260258$$
$$L_L(0, E_0) = L_R(0, E_0) = -0.02652946094577843397, \tag{36}$$

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

6 Conclusions

The aim of this paper is the generalization of 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 a chosen coordinate point. 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 and intersect at $L(0, E_0) = 0$.

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 that should have been carried out in an entirely numerical way 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 another version of the RPM.

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