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Eigenvalue bounds for a class of singular potentials

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Abstract. We study smooth transformations $V(x) = g(x^2) + f(\frac{1}{x^2})$ of the solvable potentials $\lambda x^2 + \frac{\mu}{x^2}$. Eigenvalue approximation formulae are obtained which provide lower or upper energy bounds for all the discrete energy eigenvalues E_n, $n = 0, 1, 2, \ldots$, accordingly as the transformation functions g and f are both convex or both concave. Detailed results are presented for the special case of two-term singular potentials of the form $V(x) = \lambda x^\beta + \frac{\mu}{x^\alpha}, \alpha, \beta > 0$, and also for the potentials $V(x) = \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$ and $V(x) = \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$, $\lambda > 0$, $\mu > 0$, for $0 \leqslant n \leqslant 10$.

1. Introduction and main result

In many cases the exactly solvable problems in non-relativistic quantum mechanics provide simple and effective models illustrating the most relevant features of actual physical phenomena. Further, they may provide a starting point for more accurate approximations based on a variational or perturbation method, or on geometric properties of the Hamiltonian involved [1, 2]. In envelope theory [3], for example, the exactly solvable models play a basic role in the development of the energy approximation expressions. There are many excellent sources available in the literature for exactly solvable models in quantum mechanics [4–10]. Gol'dman and Krivchenkov [5], for example, have provided a clear description of the exact solution for the following one-dimensional Schrödinger equation (in units $\hbar = 2m = 1$):

$$-\psi'' + (\lambda x^2 + \frac{\mu}{x^2})\psi = \mathcal{E}_n \psi \qquad \psi(0) = 0 \qquad \lambda > 0,\ \mu > 0. \tag{1}$$

They showed that the energy spectrum of (1) is given by

$$\mathcal{E}_n = \sqrt{\lambda}\left(4n + 2 + \sqrt{4\mu + 1}\right) \qquad n = 0, 1, 2, \ldots. \tag{2}$$

The purpose of the paper is to use such solutions to investigate the spectrum of the Schrödinger equation:

$$-\psi'' + V(x)\psi = E_n \psi \qquad \psi(0) = 0 \tag{3}$$

where

$$V(x) = g(x^2) + f\left(\frac{1}{x^2}\right) \tag{4}$$

is a sum of two smooth transformations respectively of x^2 and $\frac{1}{x^2}$, and E_n is the eigenvalue. We shall show that E_n can be approximated by the expression

$$E_n \approx \epsilon_n = \min_{s,t>0}\left\{g(s^2) - s^2 g'(s^2) + f\left(\frac{1}{t^2}\right) - \frac{1}{t^2} f'\left(\frac{1}{t^2}\right)\right.$$

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$$+\sqrt{g'(s^2)}\left(4n+2+\sqrt{4f'\left(\frac{1}{t^2}\right)+1}\right)\Bigg\} \qquad n=0,1,2,\ldots. \tag{5}$$

This formula provides a lower bound ($\approx=\geqslant$) or an upper bound ($\approx=\leqslant$) to the exact eigenvalues according to whether the transformation functions g and f are both convex or both concave. This allows us, for example, to obtain simple expressions which bound the spectrum of the spiked harmonic oscillator potential $V(x) = \lambda x^2 + \frac{\mu}{x^\alpha}$, $\alpha \geqslant 1$, $n = 0, 1, 2, \ldots$, a problem which is of considerable interest [11–18]. Indeed, formula (5) implies that the energy of spiked harmonic oscillator can be approximated by

$$E_n \approx \epsilon_n(\hat{t}) = \left(1-\frac{\alpha}{2}\right)\frac{\mu}{\hat{t}^\alpha} + 2\lambda\hat{t}^2 + 2\sqrt{\lambda}(2n+1) \tag{6}$$

where $\hat{t}$ is the real root of

$$2\mu\alpha t^{2-\alpha} - 4\lambda t^4 + 1 = 0.$$

Here $\epsilon_n(\hat{t})$ is lower bound to E_n when $\alpha > 2$ and an upper bound when $\alpha < 2$.

2. Transformed potentials

In order to lay down a framework to the approximation method we are about to construct, we consider a Schrödinger Hamiltonian of the form

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g(x^2) + f\left(\frac{1}{x^2}\right) \tag{7}$$

where g and f are smooth transformations of x^2 and $\frac{1}{x^2}$, respectively. For example, when g and f are identity transformations, the problem has the exact solution (2) for all n and arbitrary positive values of λ and μ. Standard envelope theory [3] suggests the following approach to treat a Hamiltonian of the form (7). We may approximate the shape of $V(x) = g(x^2) + f(\frac{1}{x^2})$ by some suitable potential, called base potential, with known spectrum. Using the well known comparison theorem (or refinements thereto [19]) for $V(x)$ with this base potential, we can obtain eigenvalue bounds for H. This method has been applied to obtain a simple lower bound formula for eigenvalues of the spiked harmonic oscillator $V(x) = x^2 + 1/x^\alpha$, $\alpha \geqslant 1$ using a harmonic oscillator as a base potential [18].

Here we add a new idea which leads to energy bounds which are both more general and sharper. Instead of approximating $V(x)$ by a single potential, as in [18], we use the tangent approximation for $g(x^2)$ and $f(\frac{1}{x^2})$, separately. That is to say, we replace g and f by their corresponding tangent approximations

$$\begin{aligned} g^{(s)}(x^2) &= a(s) + b(s)x^2 \\ f^{(t)}\left(\frac{1}{x^2}\right) &= c(t) + \frac{d(t)}{x^2} \end{aligned} \tag{8}$$

respectively, where s is a contact point between $g(x^2)$ and its tangent approximation $g^{(s)}(x^2)$, and t plays a similar role for f. Elementary analysis implies that $V(x)$ in (4) can thus be approximated by

$$V^{(s,t)}(x) = g(s^2) - s^2 g'(s^2) + g'(s^2)x^2 + f\left(\frac{1}{t^2}\right) - \frac{f'(\frac{1}{t^2})}{t^2} + \frac{f'(\frac{1}{t^2})}{x^2}. \tag{9}$$

With this approximation for $V(x)$, we may use the result of Gol'dman and Krivchenkov (2) for the eigenvalues of Schrödinger equation

$$-\psi'' + V^{(s,t)}(x)\psi = \epsilon_n(s,t)\psi. \tag{10}$$

Table 1. Some lower bounds E_0^L and upper bounds E_0^U using (6) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{1000}{x^\alpha}$. The 'exact' values E_0^N were obtained by direct numerical integration of Schrödinger's equation.

	$\mu = 1000$		
α	E_0^L	E_0^N	E_0^U
0.5	—	415.889 79	416.309 77
1	—	190.723 31	190.992 13
1.5	—	104.410 22	104.539 93
1.9	—	71.061 58	71.086 86
2	65.253 46	65.253 46	65.253 46
2.1	60.127 04	60.152 01	—
2.5	44.833 49	44.955 49	—
3	33.079 40	33.316 76	—
3.5	25.762 04	26.108 85	—
4	20.918 65	21.369 64	—
4.5	17.552 18	18.101 83	—
5	15.117 58	15.761 13	—
5.5	13.298 42	14.031 07	—
6	11.901 53	12.718 62	—

Table 2. lower bounds E_0^L using (6) for $H = -\frac{d^2}{dx^2} + x^2 + \frac{\mu}{x^{5/2}}$ with different values of μ. The 'exact' values E_0^N were obtained by direct numerical integration of Schrödinger's equation.

	$\alpha = \frac{5}{2}$	
μ	E_0^L	E_0^N
1000	44.833 49	44.955 49
100	17.419 00	17.541 89
10	7.611 69	7.735 11
5	6.173 94	6.296 47
1	4.204 53	4.317 31
0.5	3.746 16	3.848 55
0.1	3.204 95	3.266 87
0.05	3.109 54	3.152 43
0.01	3.023 36	3.036 70
0.005	3.011 78	3.019 05
0.001	3.002 37	3.003 97

Thus we have

$$\epsilon_n(s,t) = g(s^2) - s^2 g'(s^2) + f\left(\frac{1}{t^2}\right) - \frac{1}{t^2} f'\left(\frac{1}{t^2}\right) + \sqrt{g'(s^2)}\left(4n + 2 + \sqrt{4f'\left(\frac{1}{t^2}\right) + 1}\right). \tag{11}$$

For the eigenvalues of Schrödinger equation (3), we have

(a) $E_n \leqslant \epsilon_n(s,t)$ if g and f are both convex.

(b) $E_n \geqslant \epsilon_n(s,t)$ if g and f are both concave.

The proof is obtained by the following simple argument. For definiteness we consider case (a). Since g and f are convex, their graphs lie above their tangents. Consequently, we have from (9) that $V^{(s,t)}(x) \leqslant V(x)$. Case (a) then follows by an application of the

Table 3. Upper bounds E_n^U using (12) for $H = -\frac{d^2}{dx^2} + \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$ with different values of n. The 'exact' values E_n^N were obtained by direct numerical integration of Schrödinger's equation.

	$\lambda = \mu = 1$	
n	E_n^U	E_n^N
0	4.160 38	4.116 28
1	7.946 96	7.850 41
2	11.684 36	11.544 96
3	15.389 87	15.211 95
4	19.071 75	18.857 79
5	22.734 85	22.486 48
6	26.382 39	26.100 75
7	30.016 64	29.702 60
8	33.639 30	33.293 52
9	37.251 69	36.874 71
10	40.854 86	40.447 12

Table 4. Lower bounds E_n^L using (12) for $H = -\frac{d^2}{dx^2} + \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$ with different values of n. The 'exact' values E_n^N were obtained by direct numerical integration of Schrödinger's equation.

	$\lambda = \mu = 1$	
n	E_n^L	E_n^N
0	4.309 42	4.356 98
1	8.519 89	8.626 97
2	12.782 43	12.940 00
3	17.079 60	17.283 55
4	21.402 86	21.650 81
5	25.747 12	26.037 51
6	30.108 94	30.440 71
7	34.485 90	34.858 23
8	38.876 13	39.288 42
9	43.278 21	43.729 98
10	47.690 99	48.181 84

comparison theorem. Case (b) is proven in an analogous way if 'convex' is replaced by 'concave'. It is appropriate to mention here that the conclusions follow even if either f or g is the identity transformation. These bounds may, of course, be sharpened by optimization with respect to s and t, and moreover they are valid for the entire discrete spectrum $n \geqslant 0$.

3. Numerical results and conclusion

One of the interesting points concerning the bounds we have obtained, in section 2, is the large variety of approximations made possible by different choices of the transformations g and f. We consider, for example, the case where $g(x^2) = \lambda x^\beta$ and $f(\frac{1}{x^2}) = \frac{\mu}{x^\alpha}$. From (11) it follows that

$$\epsilon_n(s,t) = \lambda\left(1 - \frac{\beta}{2}\right)s^\beta + \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{t^\alpha} + \sqrt{\frac{\lambda\beta s^{\beta-2}}{2}}\left(4n + 2 + \sqrt{\frac{2\mu\alpha}{t^{\alpha-2}} + 1}\right). \tag{12}$$

For the spiked harmonic oscillator $\beta = 2$ and therefore it follows from (12) that the eigenvalue approximation is given by (6). In tables 1 and 2 we exhibit the results of the lower bounds obtained by using formula (6) for different values of α and for $\lambda = 1$ and different values of the coupling parameter μ, along with some accurate values obtained by direct numerical integration of Schrödinger equation.

For the potential $V(x) = \lambda x^{1.9} + \frac{\mu}{x^{1.9}}$, we take $\beta = 1.9$ and $\alpha = 1.9$ in formula (12), which provides upper bounds in this case. A comparison of some results obtained by this formula and the corresponding results obtained by direct numerical integration, for 11 energy levels, are reported in table 3. In table 4, we report the corresponding results for the case $\beta = 2.1$ and $\alpha = 2.1$, that is to say, for the potential $V(x) = \lambda x^{2.1} + \frac{\mu}{x^{2.1}}$. Similar numerical results could also be obtained by using perturbation methods such as the renormalized hypervirial perturbation method of Killingbeck [20].

The main point of the approach described in this paper is to provide a way to generate simple general approximate formulae to be used for exploratory purposes. Once the appropriate ranges of the potential parameters are established, direct numerical methods could be used to find more accurate eigenvalues.

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