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Eigenvalue bounds for a class of singular potentials in N dimensions

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Abstract. The eigenvalue bounds obtained earlier (Hall R L and Saad N 1998 *J. Phys. A: Math. Gen.* **31** 963) for smooth transformations of the form $V(x) = g(x^2) + f(\frac{1}{x^2})$ are extended to N dimensions. In particular a simple formula is derived which bounds the eigenvalues for the spiked harmonic oscillator potential $V(x) = x^2 + \frac{\lambda}{x^\alpha}$, $\alpha > 0$, $\lambda > 0$, and is valid for all discrete eigenvalues, arbitrary angular momentum l and spatial dimension N.

1. Introduction

Recently [1], we obtained a simple formula that bounds the eigenvalues E_n of Schrödinger's equation

$$-\psi'' + \left(g(x^2) + f\left(\frac{1}{x^2}\right)\right)\psi = E_n\psi \qquad \psi(0) = 0 \tag{1}$$

where g and f are two smooth transformations of x^2 and $\frac{1}{x^2}$ respectively. We showed that E_n can be approximated by the expression

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

This formula provides a lower bound ($\approx\, = \,\geqslant$) or an upper bound ($\approx\, = \,\leqslant$) to the exact eigenvalues E_n of equation (1) according to the transformation functions g and f, which are both convex ($g'' > 0$, $f'' > 0$) or both concave ($g'' < 0$, $f'' < 0$). This allowed us, for example, to obtain simple expressions which bound the spectrum of the spiked harmonic oscillator potential $V(x) = \lambda x^2 + \frac{\mu}{x^\alpha}$, $\alpha \geqslant 1$, $n = 0, 1, 2, \ldots$, namely

$$E_n \approx \epsilon_n(\hat{t}) = \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{\hat{t}^\alpha} + 2\lambda\hat{t}^2 + 2\sqrt{\lambda}(2n + 1) \tag{3}$$

where $\hat{t}$ is the real positive 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 $\alpha < 2$. The purpose of this paper is to extend these results to the N-dimensional case with arbitrary angular momentum number l.

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2. Extension to N dimensions

We notice first that the exact eigenvalues [2, 3]

$$E_{nl} = \sqrt{\lambda}\left(4n + 2 + \sqrt{4\mu + (2l+1)^2}\right) \qquad n = 0, 1, 2, \ldots$$

of Schrödinger's equation with the Gol'dman and Krivchenkov potential $V(x) = \lambda x^2 + \frac{\mu}{x^2}$ in three dimensions can be extended [4] to the N-dimensional case by replacing l with $l + \frac{N}{2} - \frac{3}{2}$. Indeed, these exact solutions could be generated from the well known solutions of harmonic oscillator potential by two simple transformations: first replace the angular momentum l in the harmonic oscillator energy expression $\sqrt{\lambda}(4n+2l+3), n = 0, 1, 2, \ldots$ by $-\frac{1}{2}+\sqrt{\mu + (l+\frac{1}{2})^2}$; then replace l with $l + \frac{N}{2} - \frac{3}{2}$. Thus, the exact eigenvalues of the N-dimensional Schrödinger equation with the Gol'dman and Krivchenkov potential are

$$E_{nl}^{(N)} = 2\sqrt{\lambda}\left(2n + 1 + \sqrt{\mu + (l + N/2 - 1)^2}\right) \qquad n, l = 0, 1, 2, \ldots. \tag{4}$$

The method used to develop the results, equations (5) and (6) of [1], can now be followed, but instead of formula (2) of [1] we use equation (4) above and obtain

$$E_{nl}^{(N)} \approx \min_{s,t>0} \epsilon_{nl}^{(N)}(s, t)$$

where

$$\epsilon_{nl}^{(N)}(s,t) = \Bigg\{ g(s^2) - s^2 g'(s^2) + f\left(\frac{1}{t^2}\right) - \frac{1}{t^2} f'\left(\frac{1}{t^2}\right) + 2\sqrt{g'(s^2)}\left(2n + 1 + \sqrt{f'\left(\frac{1}{t^2}\right) + (l + N/2 - 1)^2}\right)\Bigg\}. \tag{5}$$

The case where $g(x^2) = \lambda x^\beta$ and $f(\frac{1}{x^2}) = \frac{\mu}{x^\alpha}$ implies, from (5), that

$$\epsilon_{nl}^{(N)}(s,t) = \lambda\left(1 - \frac{\beta}{2}\right)s^\beta + \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{t^\alpha} + \sqrt{2\lambda\beta s^{\beta-2}}\left(2n + 1 + \sqrt{\frac{\mu\alpha}{2t^{\alpha-2}} + (l + N/2 - 1)^2}\right). \tag{6}$$

In particular, for the spiked harmonic oscillator potential with $\beta = 2$ it follows from (5) that the eigenvalue approximation is given by

$$\epsilon_{nl}^{(N)}(t) = \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{t^\alpha} + 2\lambda t^2 + 2\sqrt{\lambda}(2n+1) \tag{7}$$

where t is the real positive root of

$$2\lambda t^4 - \mu\alpha t^{2-\alpha} - 2(l + N/2 - 1)^2 = 0. \tag{8}$$

We now prove that for optimal t there is only one positive real root given by (8). If we let $h(t) = 2\lambda t^4 - \mu\alpha t^{2-\alpha} - 2(l+N/2-1)^2$, then for $\alpha < 2$: $h(t) \to -2(l+N/2-1)^2$ as $t \to 0$ and $h(t) \to \infty$ as $t \to \infty$. On the interval $(0, \infty)$ the function $h(t)$ has only one minimum occurring at

$$t_{\min} = \left(\frac{\lambda\alpha(2-\alpha)}{8\mu}\right)^{\frac{1}{2+\alpha}}.$$

Consequently for $\alpha < 2$, equation (8) has only one real positive root. For $\alpha > 2$, $h(t) \to -\infty$ as $t \to 0^+$ and to $+\infty$ as $t \to \infty$. On the interval $(0, \infty)$, $h(t)$ is monotone increasing on the open interval $(0, \infty)$ and we conclude that (8) has only one real positive solution for all α. The

Table 1. Upper bounds E_{00}^U using (7) for $H = -\Delta + x^2 + \frac{10}{x^{1.9}}$ for dimension $N = 2$–10. The 'exact' values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}	E_{00}^U
2	8.485 38	8.511 90
3	8.564 36	8.590 21
4	8.795 44	8.819 47
5	9.163 09	9.184 61
6	9.646 70	9.665 48
7	10.225 05	10.241 20
8	10.879 08	10.892 89
9	11.592 98	11.604 78
10	12.354 18	12.364 29

Table 2. Lower bounds E_{21}^L using (7) for $H = -\Delta + x^2 + \frac{10}{x^{2.1}}$ for dimension $N = 2$–10. The 'exact' values E_{21} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{21}^L	E_{21}
2	16.457 73	16.543 63
3	16.826 41	16.904 44
4	17.312 54	17.381 71
5	17.895 07	17.955 44
6	18.554 81	18.607 07
7	19.275 58	19.320 69
8	20.044 44	20.083 41
9	20.851 25	20.885 02
10	21.688 22	21.717 61

above discussion leads to the following simple expression for the energy bound approximations for the spiked harmonic oscillator potential valid for all dimensions $N \geqslant 2$, arbitrary angular momentum $l \geqslant 0$, and $n \geqslant 0$:

$$\begin{aligned}&\epsilon_{nl}^{(N)}(\hat{t}) = \left(1 - \frac{\alpha}{2}\right)\frac{\mu}{\hat{t}^{\alpha}} + 2\lambda\hat{t}^2 + 2\sqrt{\lambda}(2n+1)\\ &\hat{t} \quad \text{is the root of} \quad 2\lambda t^4 - \mu\alpha t^{2-\alpha} - 2(l + N/2 - 1)^2 = 0.\end{aligned} \tag{9}$$

3. Two examples

In table 1 we exhibit the upper bounds E_{00}^U obtained by use of formula (7) for dimensions $N = 2$–10 with $\alpha = 1.9$, $\lambda = 1$, and $\mu = 10$, along with some accurate values obtained by direct numerical integration of Schrödinger's equation. Similar accurate numerical results could also be obtained by the use of perturbation methods such as the renormalized hypervirial perturbation method of Killingbeck [5]. In table 2 we exhibit the corresponding lower bounds E_{21}^L obtained by use of formula (7) for dimensions $N = 2$–10 with $\alpha = 2.1$, $\lambda = 1$, and $\mu = 10$.

For the particular test problem discussed here, other approximation methods might also be considered. For example, if we let $E(\alpha)$ represent an eigenvalue of the operator $H(\alpha) = -\Delta + x^2 + \mu x^{-\alpha}$ with μ *fixed*, then an immediate first-order approximation 'formula' is provided by

$$E(\alpha) \approx E(2) + (\alpha - 2)E'(2). \tag{10}$$

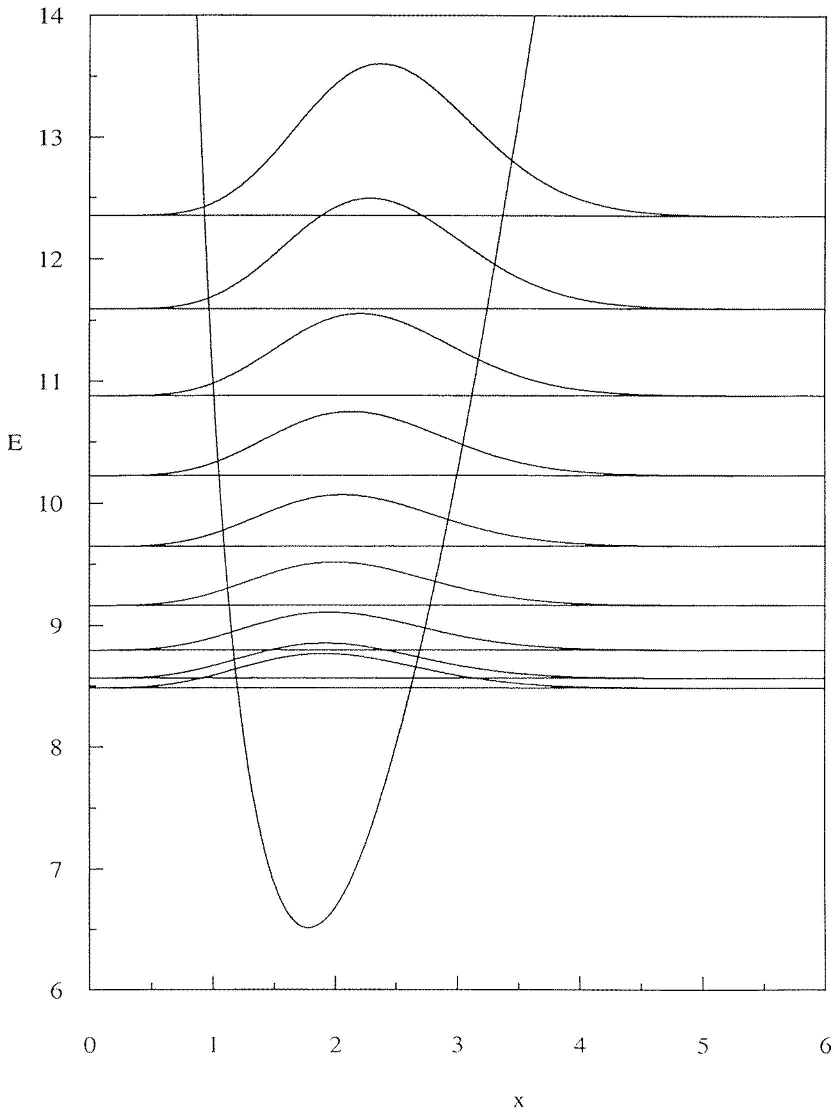

Figure 1. Graph of the eigenvalues $E = E_{00}$ for the Schrödinger equation with the potential $V(x) = x^2 + \frac{10}{x^{1.9}}$ and corresponding unnormalized wavefunctions in dimensions $N = 2$ (bottom) to 10 (top).

The problem now is to find $E'(2)$. Since $E(\alpha) = (\psi(\alpha), H(\alpha)\psi(\alpha))$, differentiation with respect to α and the minimal property of the expectation $(\psi(\alpha), H(2)\psi(\alpha))$ with respect to α leads to the expression

$$E'(2) = -\mu(\psi(2), \log(x)x^{-2}\psi(2)). \tag{11}$$

As an illustration of this result we consider the first and last lines of table 1. We find for $N = 2$ that $E'(2) \approx -1.557$ and $E(1.9) = 8.4803$; meanwhile for $N = 10$, $E'(2) \approx -1.498$ and $E(1.9) \approx 12.3479$. The same reasoning and method can be applied to table 2. However, these results are particular to the example chosen for illustration, and they do not in general provide energy *bounds*. Given the correct convexity of the transformation functions, the geometrical

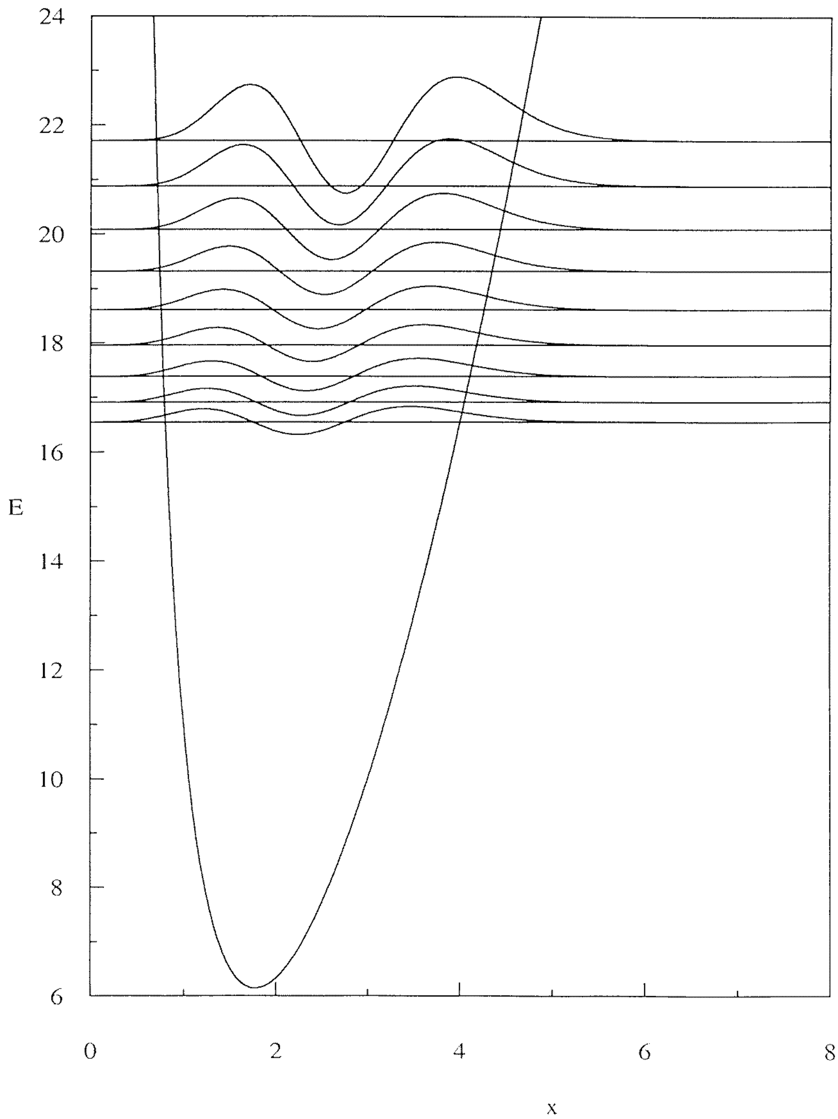

Figure 2. Graph of the eigenvalues $E = E^L_{21}$ for the Schrödinger equation with the potential $V(x) = x^2 + \frac{10}{x^{2.1}}$ and corresponding unnormalized wavefunctions in dimensions $N = 2$ (bottom) to 10 (top).

methods described in this paper provide energy bounds on all the discrete eigenvalues in all dimensions $N \geqslant 2$.

4. Conclusion

By extending the scope to N dimensions we have generalized our simple general eigenvalue approximation formulae for the potential

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

where g and f are smooth monotone transformations of x^2 and $\frac{1}{x^2}$ respectively. These results may be used for exploratory purposes and also for seeding direct numerical methods. In figures 1 and 2 we show the potential, the eigenvalues, and the unnormalized radial wavefunctions corresponding to the data in tables 1 and 2. The computation of such results is greatly helped by *a priori* knowledge of the approximate location of the eigenvalues.

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