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Exactly soluble Hamiltonian with a squared cotangent potential

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The exact ground and first-excited state eigenvalues and eigenfunctions are given for a one-dimensional Hamiltonian with the potential $\frac{1}{2}n(n-1)\cot^2(x)$ on the domain $x \in [0, \pi]$. Furthermore, an exact eigenvalue spectrum is proposed for all $n > 1$ and the exact eigenfunctions are proposed for $n = 3$. These are simply finite linear combinations of $\sin(mx)$ for integer m.

KEY WORDS: soluble, solvable, Hamiltonian, cotangent

1. Introduction

Any exactly soluble Hamiltonian is interesting because it serves as a model for comparison against Hamiltonians which are not exactly soluble. The most popular exactly soluble models in one-dimension are the particle-in-a-box and the harmonic oscillator model, both of which have a complete set of integrable eigenfunctions. The particle-in-a-finite-well model [1] is also exactly soluble but is more complicated because only some (if any) of the eigenfunctions are integrable, and those that are, are defined piece-wise. These three models can be found in most quantum mechanics and chemistry texts. Exact solutions for multiple finite wells have also been found [2]. The Morse potential also allows for exact solutions and modified Morse potentials have recently been investigated [3]. The *complex* square well also offers an exact solution [4].

Exactly soluble radial problems are also very interesting, the most significant being the hydrogenic atom. Many hydrogen-like potentials have exact solutions [5,6]. Of course there are also radial generalizations of the particle-in-a-box (infinite and finite) and harmonic oscillator. Multiparticle exactly soluble models [7] are even more difficult to come by and often have strange potentials [8]. Some, such as the Hooke-Law atom, are of particular interest in chemistry to study electron–electron interactions and test density functional theory [9–13].

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2. The general Hamiltonian

The eigenvalues and eigenfunctions of the following Hamiltonian on the domain $x \in [0, \pi]$ are exactly soluble for the special case $n = 3$:

$$H(n) = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{n(n-1)}{2}\cot^2(x). \tag{1}$$

The solution is presented below. This Hamiltonian conveniently reduces to the particle-in-a-box Hamiltonian for $n = 1$. It was determined by trial and error that the lowest two eigenfunctions and eigenvalues (measured in hartrees throughout) for this Hamiltonian are:

$$\psi_1(n) = \sin^n(x), \qquad \lambda_1(n) = n/2, \tag{2a}$$

$$\psi_2(n) = \sin^{n-1}(x)\sin(2x), \qquad \lambda_2(n) = (3n+1)/2. \tag{2b}$$

We started with the function $\sin^n(x)$ and determined its potential and eigenvalue by direct calculation using the kinetic energy operator, $-\frac{1}{2}\mathrm{d}^2/\mathrm{d}x^2$. The first excited-state eigenfunction $\psi^2(n)$ was then guessed. That these are correct can easily be verified using the Hamiltonian. While these solutions are valid for all $n > 0$, $n < 1$ causes the potential to approach $-\infty$ at both $x = 0$ and $x = \pi$ and makes physical interpretation problematic since these points are the boundaries. In this note we consider only $n \geqslant 1$. Further attempts at guessing more eigenfunctions failed. Numerical calculations gave evidence that the eigenvalue differences are related by

$$\lambda_{k+1}(n) - \lambda_k(n) = \lambda_k(n) - \lambda_{k-1}(n) + 1. \tag{3}$$

For example, for $n = 3$: $\lambda_2 - \lambda_1 = 3.5$, $\lambda_3 - \lambda_2 = 4.5$, $\lambda_4 - \lambda_3 = 5.5$, etc. as can be seen in table 1. This led us to suggest that the entire eigenvalue spectrum for all $n \geqslant 1$ can thus be deduced merely from the difference of the first two eigenvalues, which are exactly known:

$$\begin{aligned}\lambda_k(n) &= \lambda_1(n) + \sum_{i=1}^{k-1}\big(\lambda_2(n) - \lambda_1(n) + i - 1\big)\\ &= \frac{n}{2} + \sum_{i=1}^{k-1}(n + i - 1/2) = \frac{1}{2}\big(k^2 + 1 - n + 2k(n-1)\big).\end{aligned} \tag{4}$$

Table 1
Approximate eigenvalues for $H(n)$.

n	$\lambda_1^{(n)}$	$\lambda_2^{(n)}$	$\lambda_3^{(n)}$	$\lambda_4^{(n)}$	$\lambda_5^{(n)}$	$\lambda_6^{(n)}$
2	1.000	3.500	7.000	11.500	17.000	23.500
3	1.500	5.000	9.500	15.000	21.500	29.000
4	2.000	6.500	12.000	18.500	26.000	34.500
4.25	2.125	6.875	12.625	19.375	27.125	35.875

Table 2
Coefficients $c_m^{(k)}$ of $\sin(mx)$ in the expansions of the first seven odd-indexed eigenfunctions $\psi_k(3)$.

k	Coefficient $c_m^{(k)}$ of ... for $\psi_k(3)$							
	$\sin(x)$	$\sin(3x)$	$\sin(5x)$	$\sin(7x)$	$\sin(9x)$	$\sin(11x)$	$\sin(13x)$	$\sin(15x)$
1	3	−1	0	0	0	0	0	0
3	1/2	3/2	−1	0	0	0	0	0
5	1/5	3/5	5/5	−1	0	0	0	0
7	3/28	9/28	15/28	21/28	−1	0	0	0
9	1/15	3/15	5/15	7/15	9/15	−1	0	0
11	1/22	3/22	5/22	7/22	9/22	11/22	−1	0
13	3/91	9/91	15/91	21/91	27/91	33/91	39/91	−1

The simplicity of eigenvalue difference is similar to that of the harmonic oscillator Hamiltonian. In the latter case the eigenvalue difference is constant. In our case the eigenvalue difference increases by one.

The approximate eigenvalues determined in table 1 were calculated variationally using a basis set consisting of the orthonormal functions $(2/\pi)^{1/2}\sin(mx)$ for $m = 1$ to 100. The accuracy of the results for the Hamiltonian with $n = 3$ indicated that the results were probably exact. Smaller caluculations were then done with infinite precision in *Mathematica* [14] and the eigenfunctions calculated as well. When the resulting eigenfunctions were tested using the Hamiltonian operator (not the Hamiltonian matrix) all but two were found to be exact for a variety of sized matrices. These two solutions were not exact because of the finite nature of the matrix; the final eigenfunction of each symmetry (odd and even about $x = \pi/2$) is determined, not by minimization, but merely by orthogonality to the others of its symmetry, and thus are poor approximate eigenfunctions.

3. Odd-indexed eigenfunctions for $H(3)$

The first seven unnormalized odd-indexed eigenfunctions for $H(3)$ are listed in table 2. Although the ground-state eigenfunction ($k = 1$) is listed as $3\sin(x) - \sin(3x)$, standard trigonometric relations show that this is proportional to $\sin^3(x)$, the ground-state eigenfunction given in ($2a$). A pattern is immediately obvious. The kth eigenfunction of the Hamiltonian has $\sin[(k+2)x]$ as the highest sine term in its expansion. When its coefficent, $c_{k+2}^{(k)}$, is taken as -1 the coefficient, $c_m^{(k)}$, of another $\sin(mx)$ for odd $m < k+2$ is m times the coefficient, $c_1^{(k)}$, of $\sin(x)$. Coefficients of $\sin(mx)$ for even m are zero. Determination of the coefficient of $\sin(x)$ for the kth eigenfunction is then necessary. Analysis of the coefficient of $\sin(x)$ for different k reveals another pattern shown in table 3.

The difference in the denominators of $c_1^{(k)}$ (when 3 is chosen as the numerator) is easily seen to start at $5 = (1 + 4)$ and then increase as $9 = (1 + 4 + 4)$, $13 =$

Table 3
Coefficients $c_1^{(k)}$ of $\sin(x)$.

k	1	3	5	7	9	11	13
$c_1^{(k)}$	3/1	3/6	3/15	3/28	3/45	3/66	3/91

$(1+4+4+4), \ldots$. From this one can deduce that the coefficients of $\sin(x)$ are:

$$c_1^{(2j-1)} = \frac{3}{\sum_{i=1}^{j} 1 + 4(i-1)} = \frac{3}{2j^2 - j} \tag{5}$$

for positive integer j. Thus in summary, the odd-indexed eigenfunctions of $H(3)$ are given by

$$\psi_{2j-1}(3) = \sum_{i=1}^{j+1} c_{2i-1}^{(2j-1)} \sin[(2i-1)x] \quad \text{for } j = 1, 2, 3, \ldots,$$
$$c_1^{(2j-1)} = \frac{3}{2j^2 - j}, \qquad c_{2i-1}^{(2j-1)} = (2i-1)c_1^{(2j-1)} \quad \text{for } 1 < i \le j, \qquad c_{2j+1}^{(2j-1)} = -1 \tag{6}$$

with eigenvalues

$$\lambda_{2j-1}(3) = \frac{4j^2 + 4j - 5}{2}. \tag{7}$$

4. Even-indexed eigenfunctions for $H(3)$

Although the first excited-state eigenfunction ($k = 2$) is listed in table 4 as $2\sin(2x) - \sin(4x)$, standard trigonometric relations show that this is proportional to $\sin^2(x)\sin(2x)$ – the first excited-state eigenfunction given in (2b). As in section 3, the coefficient of $\sin(mx)$ reveal a pattern. The kth eigenfunction of the Hamiltonian has $\sin[(k+2)x]$ as the highest sine term in its expansion. When its coefficent, $c_{k+2}^{(k)}$, is taken as -1 the coefficients, $c_m^{(k)}$, of another $\sin(mx)$ for even $m < k+2$ is $m/2$ times the coefficient, $c_2^{(k)}$, of $\sin(2x)$. Coefficients of $\sin(mx)$ for odd m are zero. Determination of the coefficient of $\sin(2x)$ for the kth eigenfunction is necessary. Analysis of the coefficient of $\sin(2x)$ for different k reveals another pattern shown in table 5.

The difference in the denominators of $c_2^{(k)}$ (when 6 is chosen as the numerator) is easily seen to start at $7 = (4+4-1)$ and then increase as $11 = (4+4+4-1)$, $15 = (4+4+4+4-1), \ldots$. From this one can deduce that the coefficients of $\sin(2x)$ are:

$$c_2^{(2j)} = \frac{6}{\sum_{i=1}^{j} 4i - 1} = \frac{6}{2j^2 + j} \tag{8}$$

Table 4
Coefficients $c_m^{(k)}$ of $\sin(mx)$ in the expansions of the first even-indexed eigenfunctions $\psi_k(3)$.

	Coefficient $c_m^{(k)}$ of ... for $\psi_k(3)$							
k	$\sin(2x)$	$\sin(4x)$	$\sin(6x)$	$\sin(8x)$	$\sin(10x)$	$\sin(12x)$	$\sin(14x)$	$\sin(16x)$
2	2	−1	0	0	0	0	0	0
4	3/5	6/5	−1	0	0	0	0	0
6	2/7	4/7	6/7	−1	0	0	0	0
8	1/6	2/6	3/6	4/6	−1	0	0	0
10	6/55	12/55	18/55	24/55	30/55	−1	0	0
12	1/13	2/13	3/13	4/13	5/13	6/13	−1	0
14	2/35	4/35	6/35	8/35	10/35	12/35	14/35	−1

Table 5
Coefficients $c_2^{(k)}$ of $\sin(2x)$.

k	2	4	6	8	10	12	14
$c_2^{(k)}$	6/3	6/10	6/21	6/36	6/55	6/78	6/105

for positive integer j. Thus in summary, the even-indexed eigenfunctions of $H(3)$ are given by

$$\psi_{2j}(3) = \sum_{i=1}^{j+1} c_{2i}^{(2j)} \sin[2ix] \quad \text{for } j = 1, 2, 3, \ldots,$$
$$c_2^{(2j)} = \frac{6}{2j^2 + j}, \qquad c_{2i}^{(2j)} = i c_2^{(2j)} \quad \text{for } 1 < i \le j, \qquad c_{2j+2}^{(2j)} = -1 \tag{9}$$

with eigenvalues

$$\lambda_{2j}(3) = 2j^2 + 4j - 1. \tag{10}$$

5. Summary

For the Hamiltonian (1) with potential $\frac{1}{2}n(n-1)\cot^2(x)$ the ground and first excited-state eigenvalues and eigenfunctions are known exactly for $n \geqslant 1$. An eigenvalue spectrum for all $n \geqslant 1$ is suggested and backed by numerical evidence. This spectrum is certain, however, only in the case for $n = 1$ which reduces (1) to the particle-in-a-box Hamiltonian. In the case $n = 3$, a complete set of exact eigenfunctions are proposed to complement the eigenvalue spectrum. The solutions (6)–(7) and (9)–(10) were symbolically tested and confirmed for $j = 1$ to 100. We are confident that these eigenfunctions are correct for all integer j, but this has not been proven. Completeness is guaranteed since the set of functions $\sin(mx)$ for integer m (which is complete) can be constructed from the proposed eigenspace.

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