Quantum Energy Eigenvalue Spectra for Very Flat Potentials

Rodney O. Weber
School of Mathematics and Applied Statistics
University of Wollongong
Northfields Avenue, Wollongong, NSW 2522
Australia
rweber@uow.edu.au

Abstract

An infinite sequence of potential well functions is considered. A numerical method is used for the Schrödinger equation to obtain the energy eigenvalue spectra for a number of these potential well functions. The results for the ground state energy are compared to a trial function method. The energy eigenvalue spectra are as one would expect although most of them have not been previously reported.

1. Introduction

The quantum theory of a particle in a potential has been much studied over the last hundred years. The infinite square well and harmonic potentials are two of the best known examples where a complete analytic solution is possible and all of the energy levels (eigenvalues) and wave functions (eigenfunctions) can be completely determined; e.g. Davies (1990). Most potential functions do not admit exact analytic solution, but fortunately there are useful analytic methods that can be used to approximately solve for the eigenvalues and eigenfunctions. In the current work we will calculate numerical results for the energy eigenvalue spectra for a select number of examples of a sequence of potentials, beginning with the harmonic potential, each one getting progressively flatter (and for comparison purposes we will also list the results for the infinite square well). The numerical solution is a method from Trefethan (2000) and implemented using Octave™. We will also compare the results for the ground state energies with a trial wavefunction method used by us previously (Weber, 2018). Our results are as one would expect (although most of them have not been previously reported) and are given in tabular form. An additional useful observation from our work is that the energies are partitioned between two contributions, similar to a kinetic energy part and a potential energy part and that the energies have a predictable, useful, functional dependence.

2. Non-dimensionalisation

We consider the Schrödinger equation with the same square well sequence of potentials as in Weber (2018); namely

\[- \frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + \mu \left( \frac{x}{a} \right)^N \psi = E \psi,\]

(1)

where \(\mu\) and \(a\) are constants and \(N\) is a positive natural number, usually assumed to be even; however, one can use the absolute value of \(\frac{x}{a}\) and raise it to any power greater than or equal to 2 and then the Schrödinger equation (with such a potential that employs the absolute value of \(\frac{x}{a}\)) admits the usual family of eigen-wave-function and eigen-energy-value solutions similar to those that are well known to anyone who has studied elementary quantum mechanics and the familiar harmonic oscillator potential. Our first task is to use non-dimensional variables to re-cast the Schrödinger in as simple
a form as possible. To this end one first observes that the non-dimensional length $\xi = \frac{x}{a}$ will simplify it to
\begin{equation}
-\frac{\hbar^2}{2ma^2} \frac{d^2\psi}{d\xi^2} + \mu \xi^N \psi = E\psi, \tag{2}
\end{equation}
Note that this form of the Schrödinger equation makes it obvious that the physical dimensions of the combination $\frac{\hbar^2}{2ma^2}$ is energy, the same as the physical dimensions of $\mu$ and $E$; i.e., the physical constants in our equation appear to be such that there are two energies that will be involved in any expression that we may finally obtain for the energy eigenvalue $E$.

Clearly one can divide by $\frac{\hbar^2}{2ma^2}$ in equation (2) and then the coefficient in front of $\xi^N$ will be $\mu$ divided by $\frac{\hbar^2}{2ma^2}$. Noticing that there is the second power of $\xi$ involved in the second derivative, as well the $N^{th}$ power of $\xi$ in the potential suggests that we introduce a new constant; let’s call it $\sigma$, such that
\begin{equation}
\sigma^{N+2} = \frac{\mu}{\frac{\hbar^2}{2ma^2}}. \tag{3}
\end{equation}
We can then divide equation by $\sigma^2$ to give
\begin{equation}
-\frac{1}{\sigma^2} \frac{d^2\psi}{d\xi^2} + \sigma^N \xi^N \psi = \frac{1}{\sigma^2} \frac{E}{\frac{\hbar^2}{2ma^2}} \psi. \tag{4}
\end{equation}
Then we rescale with $\xi^* = \sigma \xi$ and arrive at a very tidy expression for the Schrödinger equation; namely
\begin{equation}
-\psi'' + \xi^{*N} \psi = \lambda \psi, \tag{5}
\end{equation}
with
\begin{equation}
\lambda = \frac{1}{\sigma^2} \frac{E}{\frac{\hbar^2}{2ma^2}}. \tag{6}
\end{equation}
Equation (5) is to be solved for the eigenvalues $\lambda$ and corresponding eigenfunctions $\psi$ for each value of $N$ that is of interest to us. Then the energy eigenvalues for the original Schrödinger equation are obtained by re-arranging equation (6) to give
\begin{equation}
E = \lambda \sigma^2 \frac{\hbar^2}{2ma^2}. \tag{7}
\end{equation}
And using the definition of $\sigma$ from equation (3) we are able to write the result for the energy in our final form
\begin{equation}
E = \lambda \left( \frac{\hbar^2}{2ma^2} \right)^{1-\frac{1}{\beta}} \mu^{\frac{1}{\beta}}. \tag{8}
\end{equation}
Here we have introduced $\beta = \frac{1}{2}(N + 2)$ as it allows us to write the result for the energy in a reasonably compact and neat form. It also facilitates a direct comparison with the result given in our previous paper (Weber, 2018) where we used a trial wavefunction to estimate ground state energies for the Schrödinger equation (1) for several values of $N$ and commented on being able to interpret the result as a partitioning of energy into two parts.

In the present work we numerically solve equation (5) to obtain eigenvalues $\lambda$ for several values of $N$. In the case of the lowest eigenvalues (and consequently the ground state
energies) we will compare the numerical results with the results from the trial function approach. Furthermore, we will tabulate the energy levels for several values of $N$ in order to clearly see and better understand how the square well sequence influences these energy levels. In some respects the results will not be at all surprising; however, it is still of interest to see them clearly displayed. Also, we will speculate on how this may be relevant to zero point energy calculations, as we intend to follow this up in future work.

3. Numerical Results

The numerical results are obtained using Octave™. We have actually used Matlab™ programs from Trefethen (2000) and with minimal adaptation have been able to obtain numerical results for the various $N$ values of interest to us in the current work. The accuracy can be checked by changing the number of nodes and we have been content with reporting the results to four significant figures as we are here interested in demonstrating the process and at the same time displaying a table of results that illuminate the physical behaviour described by the Schrödinger equation that is of direct interest to us.

Specific details of the numerical method employed by us in the current work are not our original ideas. Rather we have used the programs available in the book by Trefethen (2000) (and there are also many more available on his work website as referred to in the book). The essence of the numerical method is to approximate the second derivative using spectral methods and turn the ordinary differential equation eigenvalue problem (5) into a matrix eigenvalue problem. Background and details for this method for eigenvalue problems for ordinary differential equations is discussed and can also be found in the references given in Trefethen (2000).

In table 1 we show the ground state energy eigenvalues obtained by the trial wavefunction method as described in Weber (2018) compared to the numerical results. For the harmonic oscillator potential ($N = 2$) the trial wavefunction happens to be exactly correct and the numerical method agrees with the result for the minimum eigenvalue to a high degree of accuracy. As $N$ increases (and we have chosen $N = 3, 4, 5, 6, 7, 8$) it is quite obvious that the trial wavefunction method consistently returns a result for the ground state eigenvalue that is higher than the numerical result and in fact the percentage by which it is higher increases as $N$ increases. This is because the trial wavefunctions (generalised Gaussians) are poorer approximations to the actual ground state wavefunction as $N$ gets larger. From the variational analysis methods for trial wavefunctions, as described in many quantum mechanics texts, including Davies (1990), it is possible to prove that the ground state energy estimate obtained from using any trial wavefunction will always be greater than (or equal to) the actual ground state energy. The results in table 1 are perfectly in accordance with this theorem and indeed we are confident that the numerical results for the ground state energies are very close to exact.

| $N$ | 2   | 3  | 4  | 5  | 6  | 7  | 8   |
|-----|-----|----|----|----|----|----|-----|
| Trial Wavefunction Method | 1.000 | 1.053 | 1.157 | 1.288 | 1.434 | 1.592 | 1.758 |
| Numerical Method          | 1.003 | 1.023 | 1.060 | 1.102 | 1.145 | 1.186 | 1.226 |

In table 2 we show the ground state energies and the first five energies for the excited states for $N = 2, 3, 4, 5, 6, 7, 8, \infty$. For larger $N$ and higher excited states the numerical
calculations using our simple method are at first not as accurate, so we have had to increase the number of nodes for the spectral methods from 36 to 60 and then through to 80 in order to examine the accuracy of the simple numerical method for these higher excited states. Other than for $N = 2$, the eigenvalues are all reported to four significant figures, including the results for the infinite square well (infinite $N$) which are obtained from the well known exact solution. Importantly, we can clearly see the pattern for the eigenvalue spectra for the Schrödinger equation using our square well sequence of potentials as $N$ increases. Namely, larger $N$ means that the spacing between energy eigenvalues gets progressively greater (and for comparison we have also tabulated the exact results for the energy eigenvalues for the infinite square well which can be obtained by direct solution as explained in texts such as Davies, 1990). These results are all exactly as one would expect and some of the numbers have been reported before; but to the author’s knowledge, most of these eigenvalues have not been previously reported.

| $n$:N | 2     | 3     | 4     | 5     | 6     | 7     | 8     | $\infty$ |
|-------|-------|-------|-------|-------|-------|-------|-------|----------|
| 1     | 1.023 | 1.060 | 1.102 | 1.145 | 1.186 | 1.226 | 2.467 |
| 2     | 3.451 | 3.800 | 4.089 | 4.339 | 4.559 | 4.756 | 9.870 |
| 3     | 6.370 | 7.456 | 8.337 | 9.073 | 9.700 | 10.25 | 22.21 |
| 4     | 9.522 | 11.64 | 13.43 | 14.94 | 16.23 | 17.34 | 39.48 |
| 5     | 12.87 | 16.26 | 19.19 | 21.71 | 23.90 | 25.81 | 61.69 |
| 6     | 16.37 | 21.24 | 25.54 | 29.30 | 32.60 | 35.50 | 88.83 |

4. Conclusion and Further Work

We have used a numerical method to obtain the energy eigenvalue spectra for a family of potentials. The results are as one would expect, although most of them have not been previously reported in the literature. An additional useful observation from equation (7) is that there is a particular combination of the constants in the problems that always appears in the equation for the eigenvalues and hence the energies; namely powers of $\frac{\hbar^2}{2ma^2}$ and powers of $\mu$. Checking the dimensions of the result is easy as $\frac{\hbar^2}{2ma^2}$ has the dimensions of energy, as does $\mu$. And the two powers always add to one. Hence, it is as though the ground state energy is partitioned between the two contributions; one kinetic energy and the other potential energy. The comparison with a previous trial function method for the ground state energy level is also given. Further work on different trial wavefunctions is being considered as is the extension of the numerical method to a broader class of potential functions.

Zero point energy calculations, such as in the Casimir effect, begin with the ground state energy eigenvalues for the harmonic potential. The results that are then obtained for the force between parallel plates have been compared with recent experimental measurements. What we wish to stress in this current work, is that the ground state energies for any potentials (for example the square well sequence of potential wells considered by us) depends on a fundamental length scale in the problem ($a$ in our formulation of the Schrödinger equation) and the potential strength ($\mu$ in our case). It is our intention to next repeat some of the zero point energy calculations to see how these parameters ($\mu$ and $a$) influence the results.
References
P.C.W. Davies (1984) Quantum Mechanics. Chapman & Hall (reprinted 1990)
N.Trefethen (2000) Spectral Methods in Matlab. SIAM, Philadelphia.
R.O.Weber (2018) arXiv:1803.02207

Acknowledgments
The author would like to thank Dr.J.S.Chapman for assistance with LaTeX and R.

Authors’ Contributions
This paper is solely the work of the single author.

Competing Interests
The author declares no competing interests.

Data Accessibility
This paper has no data.

Ethics Statement
There were no ethical considerations required for this work.

Funding Statement
This work was done without funding.