Finite Square Wells in Quantum Mechanics

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Statement of the Problem

My goal was to investigate wavefunctions and energies corresponding to finite square wells in quantum mechanics using an eigenvalue approach.

TI Schroedinger Equation

Starting from the time independant Schroedinger equation

$$E\psi(x) = \left[\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\right]\psi(x).$$

Nondimensionalizing by setting $x = aq$ for dimensionless q we get

$$\left[\frac{d^2}{dq^2} + \tilde{V}(q)\right]\psi(q) = \tilde{E}\psi(q)$$

with dimensionless $\tilde{E} = \frac{2ma^2}{\hbar^2}E$ and $\tilde{V}(q) = \frac{2ma^2}{\hbar^2}V(q)$. Given some potential $V(q)$, we are looking for the wave function $\psi(q)$. We project onto a grid $q_j = j\,\Delta q$ so that the functions $\psi(q_j)$ and $\tilde{V}(q_j)$ become a lists of values, ψ_j and $\tilde{V}_j$.

The Eigenvalue Problem

We can turn this problem into an eigenvalue problem using the methods we learned in class[1]! The equation we're trying to solve becomes:

$$\mathbb{D}\vec{\psi}_j = \tilde{E}\vec{\psi}_j$$

with a matrix $\mathbb{D}$ that takes care of the second derivative and the potential. The eigenvectors of $\mathbb{D}$ give us $\vec{\psi}_j$, and the eigenvalues give us $\tilde{E}$.

Getting the $\mathbb{D}$

Discretizing a double derivative with

$$\left.\frac{d^2\psi(q)}{dq^2}\right|_{q_j} \approx \frac{\psi_{j+1} - 2\psi_j + \psi_{j-1}}{\Delta q^2}$$

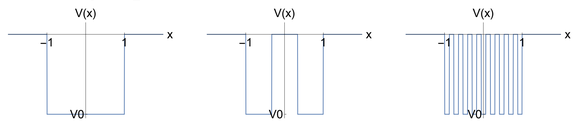
gives us an N by N matrix of the form:

$$\mathbb{D} = \begin{pmatrix} \frac{2}{\Delta q^2} + V_1 & -\frac{1}{\Delta q^2} & 0 & 0 \\ -\frac{1}{\Delta q^2} & \frac{2}{\Delta q^2} + V_2 & -\frac{1}{\Delta q^2} & 0 \\ 0 & -\frac{1}{\Delta q^2} & \frac{2}{\Delta q^2} + V_3 & -\frac{1}{\Delta q^2} \\ 0 & 0 & -\frac{1}{\Delta q^2} & \frac{2}{\Delta q^2} + V_4 \end{pmatrix}$$

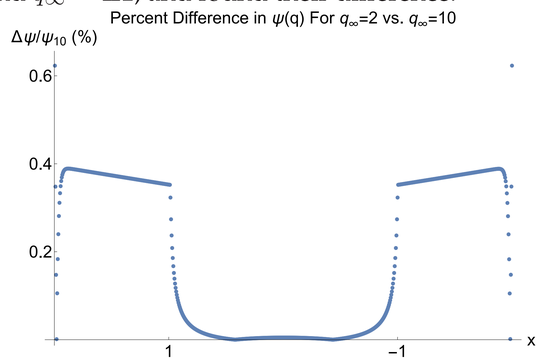
Here, for example, $N = 4$.

Comparing Boundary Conditions

By definition, ψ goes to zero at infinity. I've defined my square wells to from $q = -1$ to $q = 1$,

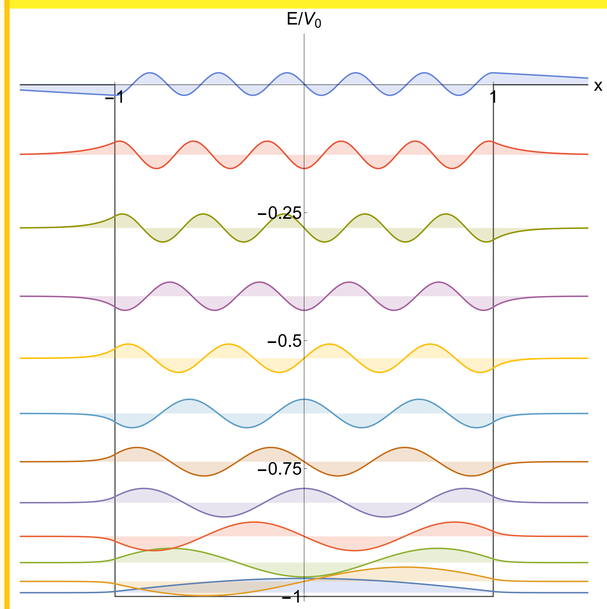


I figured I could saftely set $q_\infty = \pm 10$. Computation took longer than desired so in the interest of savings, I examined the ψ's generated by $q_\infty = \pm 10$ and $q_\infty = \pm 2$, and found their difference:



The cost of setting "infinity" at 2 instead of 10 is around 0.4% or less. Because we must invert a matrix, this shortcut shaves off 96% of the computation time.

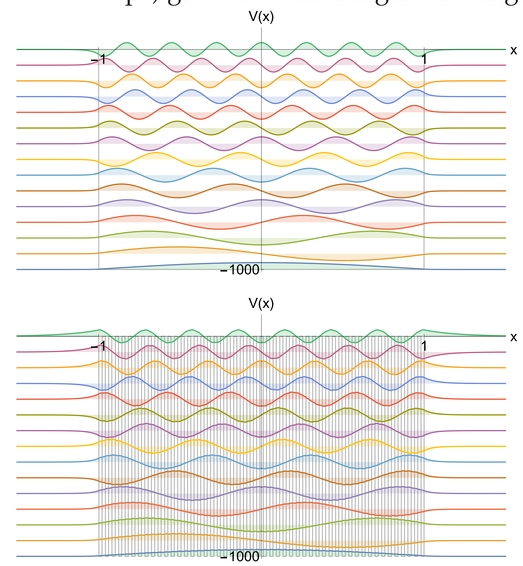
Finite Potential Well



The first 12 solutions to the Schroedinger equation for a finite well of $V_0 = 300$. (Energies scaled.)

One Well vs. Fifty Wells

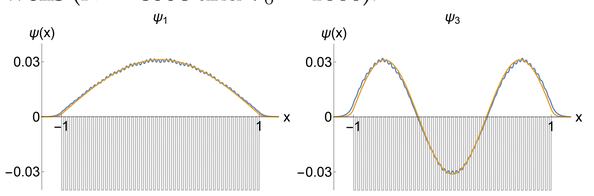
Computing the first 15 wavefunctions for 1 finite potential well and for 50 finite potential wells (with $N = 3998$ steps) gives us something interesting:



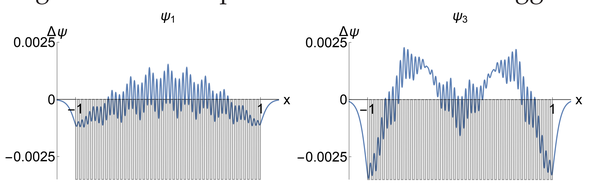
the wavefunctions appear to be almost identical! In the 50 well case, the width of each well and barrier is the same. (Energies not scaled.)

Similarity in $\psi_n(x)$

We can get a better sense of the behavior by focusing, like a laser, on the first and third wavefunctions. Comparing the wavefunctions between the potential of one well against the potential of 50 wells ($N = 3998$ and $V_0 = 1000$):



"Integrating" under the curves shows that normalization is preserved ($\int |\psi(x)|^2 dx = 1$) in all cases. Substracting the pairs of wavefunctions produces the residuals, which show us that ψ changes on a larger scale to compensate for small scale wiggles:



Periodicity of $\psi_n(x)$

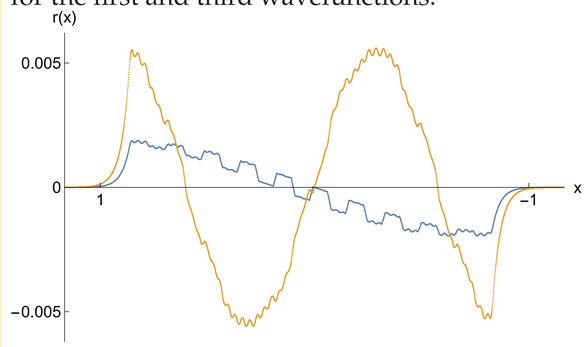
We can see how closely our wavefunctions fit the model of an infinite periodic potential using Bloch's Theorem:

$$\psi(x + a) = \psi(x)e^{ika}$$

which requires a potential $V(x) = V(x + a)$. Since our potential is semi periodic, we can find k near in the middle of the well (when it is most periodic) and calculate the residual:

$$r(x) = \psi(x + a) - \psi(x)e^{ika}$$

for the first and third wavefunctions.



Comparing E_n

Solving the finite square analytically never seems to work out. Everytime, we get stuck at an impossible equation [2]:

$$\tan(za) = \frac{2\sqrt{(\frac{z_0}{z})^2 - 1}}{2 - (\frac{z_0}{z})^2}$$

where ${z_0}^2 = V_0$ and $z^2 = {z_0}^2 - \tilde{E}$. We can find energies using a numerical root finding method (Newton's), and compare these to the energies from our eigenvalue method. Taking $N = 1998$ and $V_0 = 100$, we find that our eigenvalue approach has a max error of 0.01% for the first three energies.

The energies of 50 well system are very different from those in the single well system. For $V_0 = 100$:

	E_1/V_0	E_2/V_0	E_3/V_0
1 Well	$-.980$	$-.919$	$-.817$
50 Wells	$-.482$	$-.427$	$-.336$

References

[1] Franklin, J. *Computational Methods of Physics*. Cambridge University Press, 2013.

[2] Griffiths, D.J. *Introduction to Quantum Mechanics*. Pearson Prentice Hall, 2005.