The Sine Transform

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Abstract

For certain potentials it is difficult to find bound states using the piecewise constant method. In these cases the sine transform is a simple method for computing the bound states. The procedure for this transform is outlined and then the bound states for a deep gaussian potential are computed. Finally the answers are checked using the more arduous piecewise constant method.

1 Introduction

The Sine, or Prufer transform is a method for finding bound states of a potential well [1] . It is based on the fact that the eigenfunctions corresponding to bound states are qualitatively similar to sine functions. Consequently, the wavefunctions will have the form

$$\psi(x) = A(x)\sin(\phi(x)) \tag{1}$$

where $\phi(x)$ is the phase.

But it is a requirement that the zeros of the wavefunction occur due to the natural increase in phase and not because of a zero in the amplitude. This can be facilitated by putting the wavefunction in the following form which ensures the amplitude is always greater than zero.

$$\psi(x) = e^{S(x)}\sin(\phi(x)) \tag{2}$$

The transformation is made complete by imposing the extra condition

$$\frac{d\psi(x)}{dx} = e^{S(x)}\cos(\phi(x)) \tag{3}$$

Now (2) is differentiated to give

$$\frac{d\psi(x)}{dx} = e^{S(x)}\cos(\phi(x))\phi'(x) + e^{S(x)}\sin(\phi(x))S'(x) \tag{4}$$

and by equating to (3) gives

$$e^{S(x)}\cos(\phi(x))\phi'(x) + e^{S(x)}\sin(\phi(x))S'(x) = e^{S(x)}\cos(\phi(x)) \tag{5}$$

Then, $\frac{d^2\psi(x)}{dx^2}$ is found by taking the derivative of (3).

$$\frac{d^2\psi(x)}{dx^2} = -e^{S(x)}\sin(\phi(x))\phi'(x) + e^{S(x)}\cos(\phi(x))S'(x) \tag{6}$$

This is now equated to the Schrödinger equation[1] to give

$$-e^{S(x)}\sin(\phi(x))\phi'(x) + e^{S(x)}\cos(\phi(x))S'(x) = -\frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)e^{S(x)}\sin(\phi(x)) \tag{7}$$

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

1

By canceling out the $e^{S(x)}$ term and putting in matrix form the equations become

$$\begin{bmatrix} \cos(\phi(x)) & \sin(\phi(x)) \\ -\sin(\phi(x)) & \cos(\phi(x)) \end{bmatrix} \begin{bmatrix} \phi'(x) \\ S'(x) \end{bmatrix} = \begin{bmatrix} \cos(\phi(x)) \\ -\frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)\psi(x) \end{bmatrix} \tag{8}$$

Solve for the derivatives to find

$$\begin{aligned} \begin{bmatrix} \phi'(x) \\ S'(x) \end{bmatrix} &= \begin{bmatrix} \cos(\phi(x)) & -\sin(\phi(x)) \\ \sin(\phi(x)) & \cos(\phi(x)) \end{bmatrix} \begin{bmatrix} \cos(\phi(x)) \\ -\frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)\psi(x) \end{bmatrix} \\[2mm] &= \begin{bmatrix} \cos^2(\phi(x)) + \frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)\sin^2(\phi(x)) \\[2mm] \left(1 - \frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)\right)\sin(\phi(x))\cos(\phi(x)) \end{bmatrix} \end{aligned} \tag{9}$$

Now it is seen that $\phi'(x)$ is independent of S. The wavefunction must vanish in the asymptotic regions but it can only vanish through the sine term so $\phi(-\infty)$ and $\phi(\infty)$ will always be integer multiples of π. Therefore

$$\int_{-\infty}^{\infty} \phi'(x)dx = \phi(x \to \infty) - \phi(x \to -\infty) = n\pi \tag{10}$$

This gives an easy way to locate the bound state energies for the well. The equation

$$\phi'(x) = \cos^2(\phi(x)) + \frac{2m}{\hbar^2}\left(\mathcal{E} - \mathcal{V}(x)\right)\sin^2(\phi(x)) \tag{11}$$

is integrated, choosing values of $\mathcal{E}$ in small steps[2] from the bottom to the top of the potential. By choosing an initial value of $\phi(-\infty) = 0$, equation (10) gives

$$\phi(\infty) = n\pi \tag{12}$$

Therefore as the energy increases, the phase will only change in integer multiples of π. This can be seen in Figure 1.

The procedure for finding the bound states is to integrate (11) for increasing energy and keep list of values for $\phi(\infty)$[3] If a plot is made of $\phi(x)/\pi$ versus $\mathcal{E}$ there will be discontinuous jumps that correspond to the energy eigenvalues.

2 Finding Bound States: Gaussian Potential

The following is this procedure illustrated for the gaussian potential shown in Figure 2.

$$\mathcal{V}(x) = 20\left(1 - e^{-\left(\frac{x}{15/4}\right)^2}\right) \tag{13}$$

Equation (11) is integrated for different energies in some small stepsize[4] from the bottom of the potential to the top. Theoretically the numerical integration is carried from $-\infty$ to ∞ but in practical application I integrate from -100 to 100. The resulting phase is evaluated at the far right and divided by π ($\phi(100)/\pi$).

Looping through for increasing values of energy, each value of ($\phi(100)/\pi$) is saved and then a plot of all values is constructed. Figure 3 shows these values. Each time the energy increases above a bound state, there will an integer jump in phase. In the plot, tick marks are drawn at each jump.

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[2]Choose the steps as small as you wish for the desired accuracy

[3]In a numerical scheme like this it is obviously impossible to evaluate $\phi(\infty)$ so choose a value sufficiently far away from the potential.

[4]Whatever accuracy you desire. I found that below about 0.01, there is no increased resolution
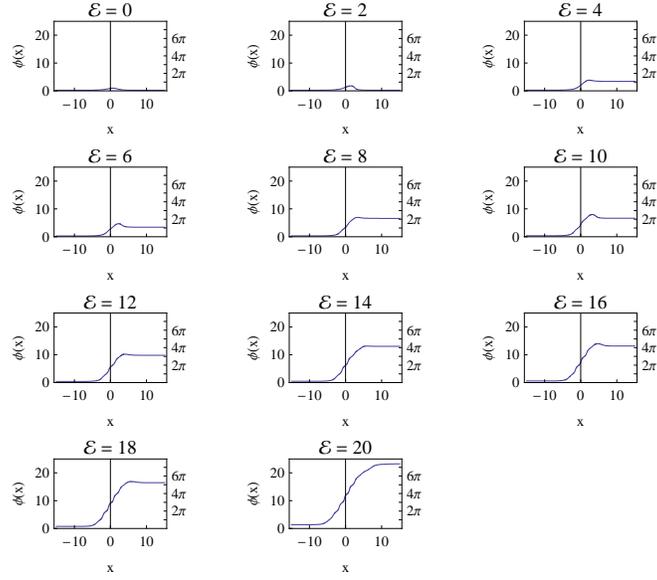
Figure 1: *Multiple plots with increasing energy of the phase across the potential. Notice that there is a jump across the potential but at the far right, the phase always ends at some integer multiple of π.*
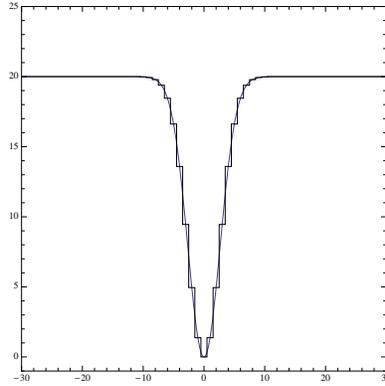
Figure 2: *The potential $\mathcal{V}(x) = 20\left(1 - e^{-\left(\frac{x}{15/4}\right)^2}\right)$ shown as the smooth curve and a piecewise approximation (for calculation using the methods described earlier in [1]).*

3 Validation of Answer

It is useful whenever using a new numerical method, to check the validity of the answer by using another method. This can either be by finding an analytical solution, or using another *well tested* numerical method. I this case I use the method of piecewise approximation as outlined in [1].

The twenty-one piece approximation is shown in Figure 2. First the height of every piece of the potential including the values in the asymptotic regions is saved. Then, looping through different values of energy, the 2×2 matrix, $M(\mathcal{E})$ is constructed according to

$$M(\mathcal{E}) = \prod_j^N M(\mathcal{V}_j; L_j) \tag{14}$$

where L is the width of the piecewise constant potential. The condition needed for a bound state to exist is then

$$t_{11}((E)) = \frac{1}{2}\left((m_{11} + m_{22}) - \left(\kappa m_{12} + \frac{1}{\kappa} m_{21} \right) \right) \tag{15}$$

This function is plotted, and its zero crossings correspond to bound state energies. In this case the function oscillates wildly with very large maxima. Figure 4 is a log plot of $t11(\mathcal{E})$. Due to resolution issues, the plot was unable to show the entire line as it crosses the zero point. The zero crossings were computed numerically once $t11(\mathcal{E})$ was found and they are labeled in the plot. Compare Figure 4 with Figure 3.

4 Summary

It has been shown that the sine transform is an accurate method for computing the bound states of a potential. As an alternative to the piecewise constant potential method, it is useful for potentials that are not easily approximated by constant pieces. These include smooth potentials that are either very long-range or very deep.

The sine transform is explicitly designed to exploit the fact that the phase is constant in the asymptotic regions of a bound state potential. This is in contrast to scattering states, where the phase constantly increases. A short study of the sine transform with scattering states confirmed this. Future research will attempt to find the analog of the sine transform for scattering states.

References

[1] R Gilmore. *Elementary Quantum Mechanics in One Dimension.* Johns Hopkins University Press, Jan 2004.
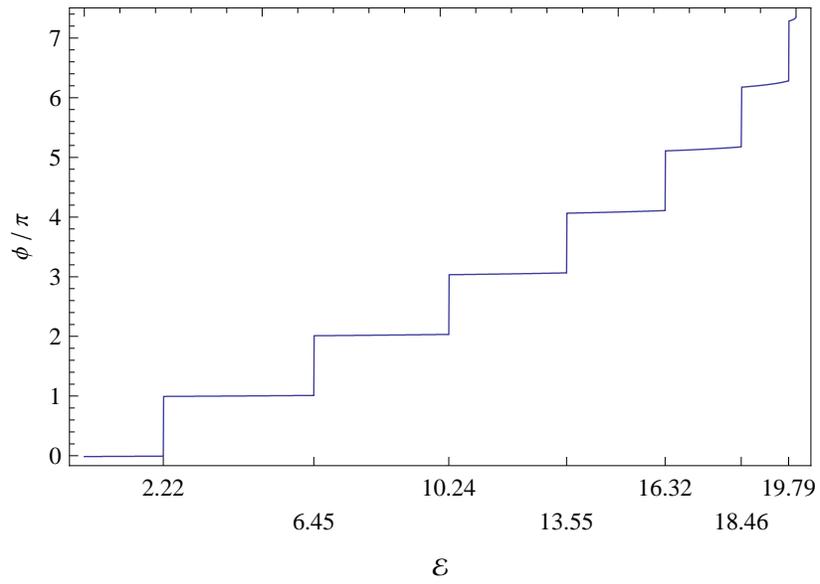
Figure 3: *A jump in phase is seen whenever the energy passes an energy eigenvalue.*
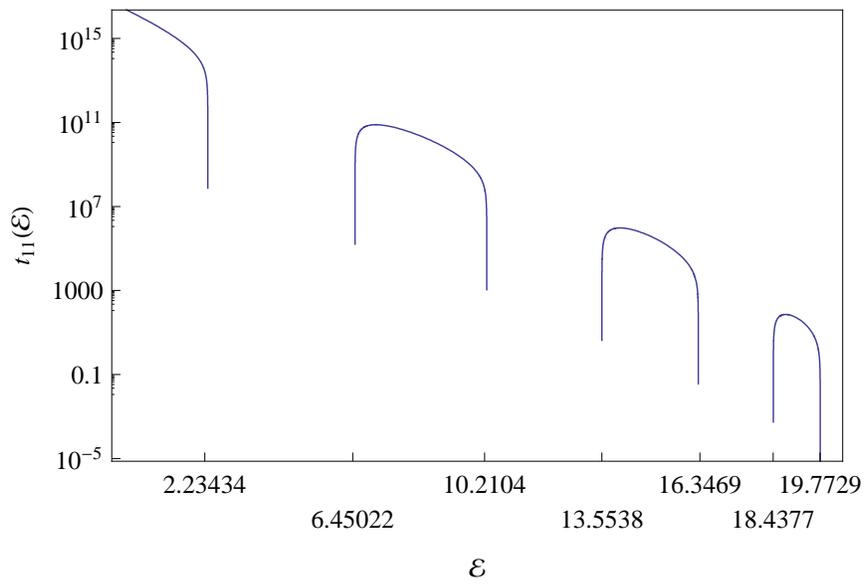
Figure 4: *Energy eigenvalues shown as zero crossings of $t_{11}(\mathcal{E})$*

5