Time-independent Schroedinger equation with Python: 1D potentials

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I. INTRODUCTION

We obtain the exact numerical solutions for the eigen-energies and wavefunctions for arbitrary 1D potentials which allow bound states. We achieve this by computing the Hamiltonian matrix in a basis and then obtaining its eigenvalues and eigenvectors.

A. Theory

Consider a general potential $V(x)$ supporting at least one bound state in the region $-a < x < b$.

$$H\psi = E\psi,$$

where $H = T + V(x)$. In order to solve the system, we expand the solution in an orthonormal eigen basis,

$$\psi(x) = \sum_k c_k \phi_k(x)$$

where the functions $\phi_k(x)$ satisfy the orthonormal condition. In our calculations, we select the solutions of 1D harmonic potential : $V_h(x) = \omega^2 x^2/2$ as our basis [1]. Therefore,

$$H = H_h + V(x) - V_h(x)$$

where $H_h = T + V_h(x)$. Hence,

$$H_{mn} =< \phi_m|H|\phi_n >= \delta_{mn}(m + 1/2)\omega + \int \phi_m(x)[V(x) - V_h(x)]\phi_n(x)dx$$

Now, let $U[i]$ and $W[j,i]$ be the sorted eigenvlaue-array and eigenvector-matrix of H_{mn}, respectively (computed using *numpy.linlag.eig()*). Then the wavefunction to a specific eigenvalue E_n can be obtained using,

$$\psi_n(x) = \sum_k W[k,n]\phi_k(x)$$

B. Results

In the following Figures, from 1 to 4, we show the solutions to various 1D potentials. The user can play with the code: sch1dpots.py to obtain the solutions to an arbitrary 1D potential which has bound states.

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[1]

$$\phi_k(x) = (\omega/\pi)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\sqrt{\omega}x)e^{-\omega x^2/2}$$

Note that $mass = 1, \hbar = 1$. H_n is the n^{th} order Hermite polynomial. Using the recurrence relation for H_n, we have

$$\phi_k = (\sqrt{2\omega}x\phi_{k-1} - \sqrt{k-1}\phi_{k-2})/\sqrt{k}$$

with $\phi_{-1} = 0$ and $\phi_0 = e^{-\omega x^2/2}(\omega/\pi)^{1/4}$

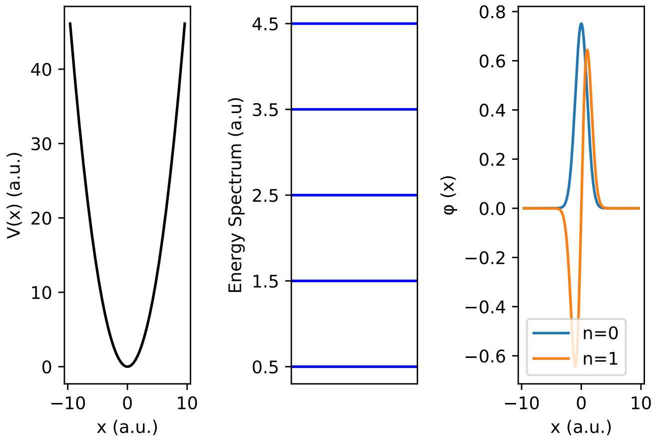

FIG. 1: Solutions to the Harmonic potential $kx^2/2$. Energy spectrum and the first two wavefunctions are shown in the rightmost panels (for the case $k = 1$).

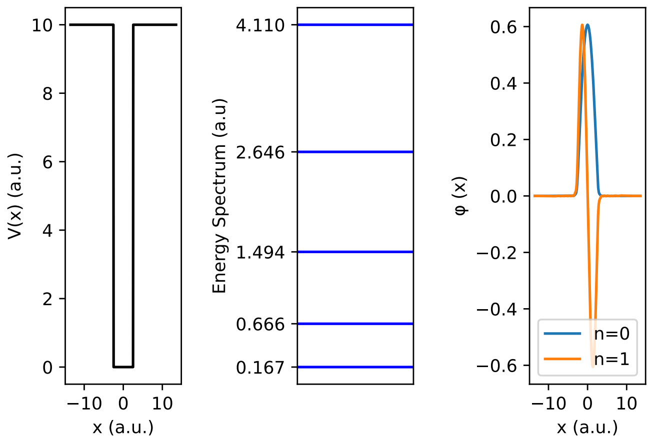

FIG. 2: Solutions to the 1D finite square well potential. Note the approximate n^2 scaling between the ratio $E_1/E_0, E_2/E_0$ etc.

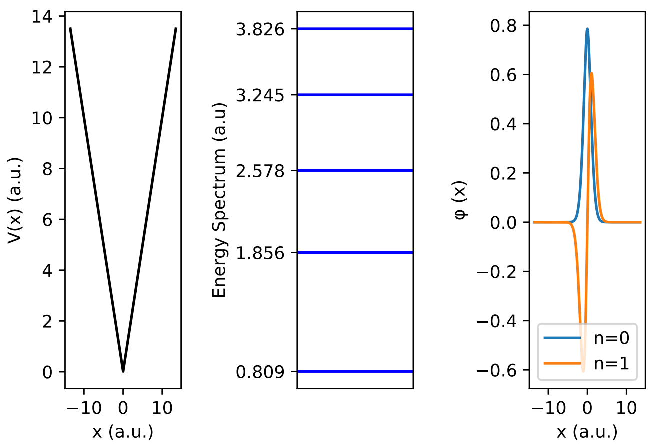

FIG. 3: Solutions to the $|x|$ potential

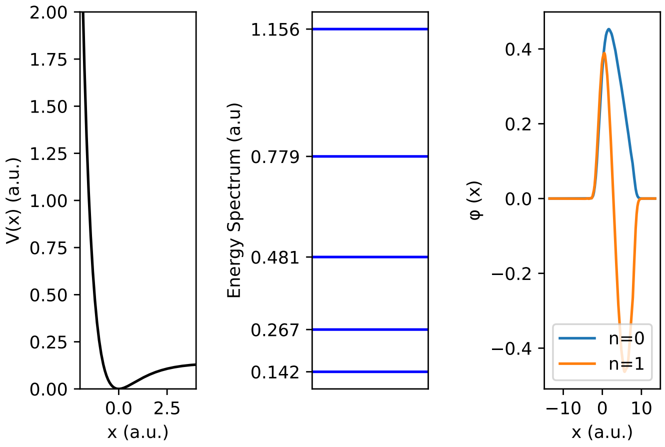

FIG. 4: Solutions to the 1D Morse potential.