4.5: A Symmetric Double Well Potential Illustrating Tunneling

Schrödinger's equation is solved numerically for a symmetric double well potential: $V = bx^4 - cx^2$, which resembles the double-well potential used to model the ammonia inversion in the previous tutorial. The integration algorithm is taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.

Set parameters:

$$\text{Increments:} \quad n = 100 \quad \text{Integration limits:} \quad xmin = 4 \quad \Delta = \frac{xmax - xmin}{n-1}$$
$$\text{Effective mass:} \quad \mu = 1 \quad \text{Constants:} \quad b = 1 \quad c = 6$$

Calculate position vector, the potential energy matrix, and the kinetic energy matrix. Then combine them into a total energy matrix.

$$i = 1..n \quad j = 1..n \quad x_i = xmin + (i-1)\Delta$$

$$V_{i,j} = \text{if}\left[i = j,\ b(x_i)^4 - c(x_j)^2,\ 0\right] \quad T_{i,j} = \text{if}\left[i = j,\ \frac{\pi^2}{6\mu\Delta^2},\ \frac{(-1)^{i-j}}{(i-j)^2\mu\Delta}\right]$$

Hamiltonian matrix:

$$H = T + V$$

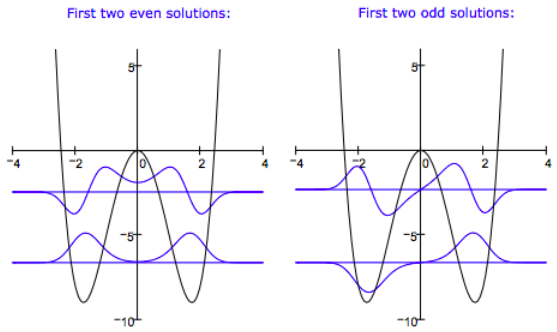
Calculate eigenvalues: E = sort(eigenvals(H))

Display selected eigenvalues: m = 1 .. 6

$$E_m = \begin{bmatrix} -6.6427 \\ -6.6406 \\ -2.4512 \\ -2.3156 \\ 0.4156 \\ 1.6785 \end{bmatrix}$$

Calculate selected eigenvectors: k = 1 .. 4 Ψ(k) = eigenvec(H, E_k)

Display the results graphically:



The numerical results show that the energy eigenvalues are paired due to the presence of the central barrier because the odd energy states have a node at the center of the internal potential barrier. The canonical solutions to Schrödinger's equation (stationary states) show that the wave functions are delocalized over the entire potential well and that tunneling is occurring because of the probability of being in a barrier of greater potential energy than that of the total eigenstate energy. But at this point tunneling does not imply motion, just a violation of a very important classical concept - kinetic energy cannot be negative!

We also see that the ground and first-excited states are very nearly degenerate. In the presence of a small perturbing electromagnetic field, the system would be forced into a superposition of these states which would exhibit oscillatory behavior. This effect is now demonstrated for the two lowest energy states. In the presence of this perturbation we see movement from one well to the other because the system is no longer in a stationary state.

This effect is demonstrated using Mathcad's animation capabilities.

Select quantum numbers of superposition states:

$$vi = 1 \quad vf = 2 \quad t = \frac{\text{FRAME}}{0.005}$$

Timed-dependent superposition of these states:

$$Phi_i = \frac{\Psi(vi)_i exp(-iE_{vi}t) + \Psi(vf)_i exp(-iE_{vf}t)}{\sqrt{2}}$$

To animate click on Tools, Animation, Record and follow the instructions in the dialog box. Recommended setting: From 0 To 40 in 5 Frames/Sec.