Double Minimum Potential Well

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Schrodinger's equation is integrated numerically for a double minimum potential well: $V = bx^4 - cx^2$. The integration algorithm is taken from J. C. Hansen, *J. Chem. Educ. Software*, **8C2**, 1996.

Set parameters:

Increments: $n := 100$ Integration limits: $xmin := -4$ $xmax := 4$ $\Delta := \frac{xmax - xmin}{n - 1}$

Effective mass: $\mu := 1$ Constants: $b := 1$ $c := 6$

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

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

$$V_{i,j} := \mathrm{if}\left[i = j, b\cdot(x_i)^4 - c\cdot(x_i)^2, 0\right]$$

$$T_{i,j} := \mathrm{if}\left[i = j, \frac{\pi^2}{6\cdot\mu\cdot\Delta^2}, \frac{(-1)^{i-j}}{(i-j)^2\cdot\mu\cdot\Delta^2}\right]$$

Hamiltonian matrix: $H := T + V$

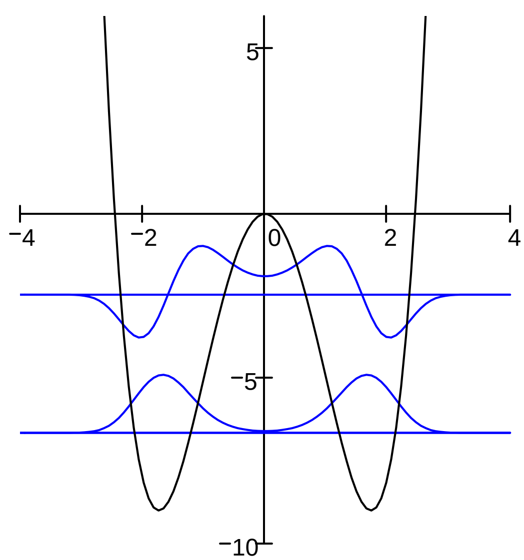
Calculate eigenvalues: $E := \mathrm{sort}(\mathrm{eigenvals}(H))$ Display selected eigenvalues: $m := 1 .. 5$ $E_m =$

-6.64272702
-6.64062824
-2.45118605
-2.3155705
0.41561275

Calculate selected eigenvectors: $k := 1 .. 4$ $\Psi(k) := \mathrm{eigenvec}(H, E_k)$

Display results:

First two even solutions:



First two odd solutions: