# Introduction to Computational Physics SS2017

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**Exercise 6** from May 24, 2017
Return by noon of June 2, 2017

## 1 Numerical linear algebra methods: unperturbed quantum mechanical oscillator

Use the numerical recipes routines to study the unperturbed quantum mechanical oscillator. You can obtain these routines from the lecture webpage for `Fortran` and `C` or find them in the web for other languages.

(a) Reduce symmetric matrices to tri-diagonal form using `tred2`.

(b) Calculate the eigenvalues and eigenvectors of a tri-diagonal matrix using `tqli`.

(c) Consider the unperturbed harmonic oscillator. In dimensionless form, it follows the Hamiltonian

$$h_0 = \frac{H}{\hbar\omega} = \left(\frac{1}{2}\Pi^2 + \frac{1}{2}Q^2\right)$$

with eigenvalues $n + 1/2$. The matrix form of the diagonalized operator $h_0$ is

$$(h_0)_{nm} = \left(n + \frac{1}{2}\right)\delta_{nm}$$

## 2 Homework: perturbed quantum mechanical oscillator

Calculate the eigenvalues of the perturbed quantum mechanical harmonic oscillator for $n = 0 \dots 9$ by approximating the operators in Hilbert space by matrices with finite dimension in the range $N = 15 \dots 30$.
The dimensionless Hamiltonian reads

$$h = \frac{H}{\hbar\omega} = \left(\frac{1}{2}\Pi^2 + \frac{1}{2}Q^2 + \lambda Q^4\right)$$

$$(h)_{nm} = (h_0)_{nm} + \lambda(Q^4)_{nm}$$

where $(h_0)_{nm} = \left(n + \frac{1}{2}\right)\delta_{nm}$ is the unperturbed Hamiltonian.

(a) Determine the matrix form of $Q^4$ using (see lecture script)

$$Q_{nm} = \frac{1}{\sqrt{2}}\left(\sqrt{n+1}\delta_{n,m-1} + \sqrt{n}\delta_{n,m+1}\right) .$$ (6 points)

(b) Compute the eigenvalues of $(h)_{nm}$ for the parameter $\lambda = 0.1$ as function of the matrix size ($N = 15 \dots 30$) using `tred2`. Demonstrate that your program works properly, just listing the eigenvalues is not sufficient. (8 points)

(c) Calculate the eigenvalues analytically. (6 points)