Introduction to Computational Physics SS2019

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Exercise 5 from May 22, 2019
Return by noon of May 31, 2019

1 Numerical linear algebra methods: unperturbed quantum mechanical oscillator

Use your own scripts or the numerical recipes routines to study the unperturbed quantum mechanical oscillator. You can obtain these routines from the lecture webpage for `Fortran` and `C`. There are also equivalent scripts for `python`. The idea is to use Householder transformations to bring the matrix into tri-diagonal form, followed by a QR decomposition to obtain the eigenvalues and eigenvectors.

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

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

(c) Test you approach by applying it to the unperturbed harmonic oscillator. In dimensionless form, the corresponding Hamiltonian reads

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

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

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

The best approach is to consider this problem in second quantisation and use the properties of the creation and annihilation operators, a^* and a, as discussed in the lecture. (8 points)

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

(c) Calculate the eigenvalues analytically using the linearized form of the equation, i.e. consider only the terms on the diagonal. (4 points)

(d) BONUS QUESTION: Determine the eigenvalues by employing the Wentzel, Kramers, and Brillouin (WKB) approximation applied to this system. Compare to the results in (b) and (c) and discuss possible differences. (10 bonus points)