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Computational Quantum Physics Exercise 2

FS 16
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In the following exercises we will approach the general problem of finding bound states of a quantum model. For this the quantum mechanical description is based on an eigenvalue problem (the time-independent Schrödinger equation),

$$H|\Psi\rangle = E|\Psi\rangle \tag{1}$$

where

- $|\Psi\rangle \in \mathcal{H}$ is a vector in some Hilbert space $\mathcal{H}$,
- H is the Hamiltonian operator which acts on vectors in $\mathcal{H}$,
- E are the energy eigenvalues.

It will be our goal to obtain normalizable solutions for this eigenvalue problem, i.e. solutions $|\Psi\rangle$ which can be made to satisfy $\langle\Psi|\Psi\rangle = 1$.

Problem 2.1 1D Numerov for a Finite Harmonic Well

The goal of this exercise is to find bound-state solutions ($E < 0$) to the 1D time-independent Schrödinger equation for a finite harmonic well, i.e. for a potential $V(x)$ satisfying

$$V(x) = c(x^2 - x), 0 \leq x \leq 1, \tag{2}$$

and zero everywhere else, where $c > 0$ is a positive constant.

Use the Numerov algorithm and a root solver as described in section 3.1.3 of the lecture notes. In particular, note that bound-state solutions exist only for discrete energy eigenvalues.

1. Plot the number of bound states as a function of the parameter c for some values inside the interval $(0, 1000]$.
2. Plot the bound-state spectrum and the wavefunctions for the value $c = 400$.

Start with finding the ground state energy (which has zero nodes) and proceed further with 1, 2, 3... nodes.

Hint: Check the number of zeros (nodes) in the solution. For your guessed energy, if you find more nodes in your solution than the desired number of nodes, decrease the trial energy and vice versa.

Problem 2.2 Truncated Exact Diagonalization of an Anharmonic Oscillator

The goal of this exercise is to approximate the low lying eigenvalues and eigenvectors for an anharmonic oscillator using exact diagonalization with a truncated basis set. To solve this problem we will choose a convenient basis set, truncate it to a finite dimension, set up the eigenvalue problem and find the eigenvalues numerically.

The Hamiltonian of the anharmonic oscillator is given by

$$\begin{aligned} H &= H_{\text{harmonic}} + H_{\text{anharmonic}} && (3) \\ &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 + Kx^4, && (4) \end{aligned}$$

where x and p are operators that do not commute, i.e. $[x, p] = i\hbar$.

The harmonic part of this Hamiltonian can be written as

$$H_{\text{harmonic}} = \hbar\omega(a^\dagger a + \frac{1}{2}) \tag{5}$$

with the operators a and $a^\dagger$ defined by

$$\begin{aligned} a &= \sqrt{\frac{m\omega}{2\hbar}}x + \frac{ip}{\sqrt{2m\hbar\omega}} && (6) \\ a^\dagger &= \sqrt{\frac{m\omega}{2\hbar}}x - \frac{ip}{\sqrt{2m\hbar\omega}}, && (7) \end{aligned}$$

where $[a, a^\dagger] = 1$.
The eigenstates $|n\rangle$ of the so-called *number* operator $N = a^\dagger a$ build a natural set of basis states for the harmonic oscillator with their energy eigenvalues being given by $\langle n|H_{harm}|n\rangle = \hbar\omega(n + \frac{1}{2})$. We will use this as a basis set for the anharmonic oscillator, but truncating it at some finite n. For convenience you may choose $\hbar = m = \omega = 1$.

1. Using the definitions of a and $a^\dagger$, express the anharmonic part of the oscillator in second-quantized form.

2. Calculate the non-vanishing matrix elements of H in the basis $|n\rangle$.[1]

3. Set up the hamiltonian matrix for some finite number of basis elements M.[2]

4. Diagonalize the matrix and plot the 5 lowest eigenvalues as a function of K for $K \in (0, 5]$. Monitor the behaviour of the eigenvalues as a function of your cut-off parameter M for the basis set.

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[1] Recall the way the operators a,$a^\dagger$ act on the states $|n\rangle$, i.e. $a|n\rangle = \sqrt{n}|n-1\rangle$ and $a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$, see script 2.4.1.

[2] Can you think of a way of doing this using only O(M) operations?