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Computational Quantum Physics Exercise 1

FS 10
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Problem 1.1 Anharmonic oscillator

In this exercise we will calculate properties of the anharmonic oscillator. The quantum mechanical description is based on an eigenvalue problem (the stationary 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 Hamilton operator which acts on vectors in $\mathcal{H}$,
- E are the energy eigenvalues.

To solve this problem, we will choose a basis set and truncate to a finite dimension, set up the eigenvalue problem and find the eigenvalues numerically.
The Hamiltonian of the anharmonic oscillator is given by

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

where x and p are operators that generally do not commute, $xp - px \neq 0$.
The harmonic part of this Hamiltonian can be written as

$$H_{\text{harmonic}} = \hbar\omega(a^\dagger a + \frac{1}{2}) \tag{4}$$

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

$$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{ip}{\sqrt{2m\hbar\omega}} \tag{5}$$

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - \frac{ip}{\sqrt{2m\hbar\omega}}, \tag{6}$$

where $[a, a^\dagger] = 1$.
The eigenstates $|n\rangle$ of the count operator $N = a^\dagger a$ build a natural set of basis states for the harmonic oscillator. Their energy eigenvalues are 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 truncate at a finite n.

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 $\mathcal{H}$ in the basis $|n\rangle$.
3. Set up the matrix and diagonalize it numerically for finite n and small K.

Problem 1.2 1-D quantum scattering problem

We consider a particle in one dimension, which is scattered at a potential barrier. This problem can be numerically solved using the Numerov algorithm.
Proceed as described in the lecture notes in section 3.1.2. You can use a constant potential ($V = 1$) in the interval $[0, a]$.

1. Observe the tunneling effect for energies $E \in [0, V]$, where the transmission probability $T = 1/|A|^2$ is non-vanishing.
2. Plot T versus the barrier width a and observe the exponential decay.

This dependency $T(a)$ plays a crucial role for the realization of the scanning tunneling microscope (STM). (Review of Modern Physics 59, 615 (1987). Nobel prize 1986).