Exercise 02

1 Spectral decomposition of an operator (10 points)

Let $\hat{A}$ be a self-adjoint, linear operator with eigenvalues a_i and eigenvectors ϕ_i. Prove that it can be represented by its spectral decomposition:

$$\hat{A} = \sum_i a_i \, |\phi_i\rangle\langle\phi_i| \tag{1}$$

2 Basis of commuting operators (5 points)

Using the spectral decomposition, prove that if two operators $\hat{A}$ and $\hat{B}$ have the same basis, then they commute.

3 Development of a function of a Hermitian operator (25 points)

Let's consider an Hamiltonian operator:

$$H = T + V = -\frac{\hbar}{2m}\partial_x^2 + V(x) \tag{2}$$

with kinetic energy T and potential:

$$V(x) = \frac{m\omega^2}{2}x^2 = \frac{k}{2}x^2 \tag{3}$$

This operator is present on a grid from x_{min} to x_{max} with N points. The lattice step is denoted by Δx and the grid points are are $x_i = x_{min} + (i-1)\Delta x$ with $i \in [1, N]$. To numerically find the eigenvectors of the Hamiltonian, it is necessary to use its matrix representation. First of all, the term ∂_x^2 can be approximated using the Taylor expansion:

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2 + \frac{1}{6}f'''(x)\Delta x^3 + \mathcal{O}(x^4) \tag{4}$$

$$f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{1}{2}f''(x)\Delta x^2 - \frac{1}{6}f'''(x)\Delta x^3 + \mathcal{O}(x^4) \tag{5}$$

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + f''(x)\Delta x^2 + \mathcal{O}(x^4) \tag{6}$$

$$f''(x) = \frac{f(x+\Delta x) + f(x-\Delta x) - 2f(x)}{\Delta x^2} + \mathcal{O}(x^4) \tag{7}$$

In the case of the discrete lattice, the second derivative of $f(x)$ in the point x_i, is obtained as an approximation:

$$f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{\Delta x^2} \tag{8}$$

Finally the matrix representation of the kinetic energy is:

$$T \simeq \frac{\hbar}{2m\Delta x^2}\begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix} \tag{9}$$

while the potential $V_i = V(x_i)$ is:

$$V = \begin{pmatrix} V_1 & 0 & 0 & \cdots & 0 \\ 0 & V_2 & 0 & \cdots & 0 \\ 0 & 0 & V_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & 0 & V_N \end{pmatrix} \tag{10}$$

Exercise

1. Using the atomic units (i.e.: $\hbar = m_e = e = 1$), find the eigenvectors ψ_n of the Hamiltonian with a force constant $k = \frac{\mathrm{E_h}}{\mathrm{a_0}^2}$ and the following parameters: $x_{min} = -10\mathrm{a}_0$, $x_{max} = 10\mathrm{a}_0$ and $N = 100$. Normalize the first four eigenvectors and plot them.

2. Compute the projection operator
$$P_n = |\psi_n\rangle\langle\psi_n| \tag{11}$$
Plot the vector of the diagonal elements of the matrices:
$$M_{N_{max}} = \sum_{n=1}^{N_{max}} P_n \tag{12}$$
with $N_{max} = 10, 50, 90, 100$. What can you observe?

3. Compute and normalize the Gaussian function:
$$\phi(x) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \exp\left(-(x-2)^2\right) \tag{13}$$
Calculate the expansion coefficients:
$$c_n = \langle\psi_n|\phi\rangle \tag{14}$$
Calculate the sum:
$$\sum_{n=1}^{M} |c_n|^2 \tag{15}$$
For which values M is it greater than 0.999?
Compute and plot the vector:
$$V_K = \sum_{n=1}^{K} c_n|\psi_n\rangle \tag{16}$$
for $K = 1, 3, 6, 9$. What can you observe?

MATLAB functions To solve these exercises the following functions can be useful:

- conj(X) $\rightarrow$ complex conjugate of X
- diag(V,K) $\rightarrow$ when V is a vector with N components, diag(V,K) is a square matrix, of order $N + |K|$, with the elements of V on the K^{th} diagonal.
- norm(X) $\rightarrow$ euclidean norm of X

For the first two exercises you can write a report by hand and deliver it at the office 35.17. For the third exercise you should write a report and send the scripts by email to luca.donati@fu-berlin.de before next Wednesday at noon.