QTC, NWI-MOL112, exercises week 1

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Question 1: Quantum harmonic oscillator

The harmonic oscillator Hamiltonian for a particle with mass m and a harmonic potential with force constant k is

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2. \tag{1}$$

The corresponding Schrödinger equation,

$$\hat{H}_0\phi_n(x) = \epsilon_n\phi_n(x), \tag{2}$$

can be solved with the ladder operator method. The aim of this exercise, however, is to look up the answer in the (famous) "Handbook of Mathematical Functions" by Abramowitz and Stegun (A&S). A pdf version of the book can be easily found online, or, from within the `www.ru.nl` domain:

`www.theochem.ru.nl/cgi-bin/dbase/search.cgi?abramowitz:64`

and its content is also available on `dlmf.nist.gov`

The solution can be found in the chapter on orthogonal polynomials (chapter 22 in the book, or online in chapter 18). This chapter presents, in a unified way, the solutions of many second order differential equations, several of which are extremely useful in solving problems in quantum mechanics. In this exercise, our goal is to use the solutions of the harmonic oscillator problem as a basis to set up a variational calculation for a one dimension Schrödinger equation for which we do not have an analytic solution. We will use the results of this exercise in the computer assignment.

The first question is:

1a. Find a coordinate transformation, $x = \alpha y$, to rewrite the Hamiltonian as

$$\hat{H}_0 = A\left(-\frac{1}{2}\frac{\partial^2}{\partial y^2} + \frac{1}{2}y^2\right) \tag{3}$$

and determine A as a function of m and k. Note that y must be dimensionless (why?).

1b. Table 22.6 in A&S (18.8.1 online) gives the solutions of

$$[\frac{\partial^2}{\partial y^2} + (2n + 1 - y^2)]f_n(y) = 0, \tag{4}$$

where $\{f_n, n = 0, 1, 2, \ldots\}$ are Hermite polynomials times a weighting function:

$$f_n(y) = H_n(y)e^{-\frac{1}{2}y^2}. \tag{5}$$

Express the harmonic oscillator function $\phi_n(x)$ in terms of the functions $f_n(y)$.

1c. The norm and orthogonality of the Hermite polynomial H_n is given by Eq. 22.1.2 in A&S and table 22.2 as

$$\int_{-\infty}^{\infty} H_m(y)H_n(y)e^{-y^2}\,dy = \delta_{m,n}\,2^n n!\sqrt{\pi}. \tag{6}$$

Compute the normalization constant for $\phi_n(x)$.

The Hermite polynomials are defined by recursion relations in table 22.7 of A&S (18.9 online):

$$H_0(x) = 1 \tag{7}$$
$$H_1(x) = 2x \tag{8}$$
$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \quad \text{for } n = 0, 1, 2, \ldots \tag{9}$$

1d. Setup analogous recursion relations for $\phi_n(x)$, such that they are normalized.

Now that we have the analytic solutions for the harmonic oscillator, $\phi_n(x)$, and convenient recursion relations, we will use them as a basis $B = \{\phi_0(x), \phi_1(x), \ldots\}$ in a variational calculation of the anharmonic oscillator problem

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + cx^4. \tag{10}$$

We expand the solutions as

$$\Psi_j(x) = \sum_{i=1}^{n}\phi_i(x)c_{ij}. \tag{11}$$

1e. Setup the matrix eigenvalue problem needed to solve the expansion coefficients c_{ij} in a variational calculation.

To compute the matrix elements, we will need matrix elements of the kinetic energy operator and of the polynomial x^4 for the potential. We will derive them in a few steps:

1f. Use the recursion relations for $\phi_n(x)$ and the orthonormality of these functions to derive an expression for the matrix elements of the $\hat{x}$ operator

$$X_{m,n} = \langle \phi_m | x \phi_n \rangle. \tag{12}$$

1g. Use the recursion relation twice to get an expression for the matrix elements of x^2.

1h. Now use a little trick: get the matrix elements of the kinetic energy operator by writing it as $\hat{H}_0 - \frac{1}{2}kx^2$.

For matrix elements of x^4 we would have to use the recursion relation four times. That is a bit much work, so when we write the computer program, we can take the matrix representation of $\hat{x}$, and then take it to the power 4, or use the matrix representation of $\widehat{x^2}$, and then take the square of that matrix.

Question 2: Questions chapter 1

2a. Show that Hamilton's classical equations of motion for one particle in one dimension is equivalent to Newton's equation.

The Heavyside step function is defined by

$$\Theta(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0. \end{cases} \tag{13}$$

We define the following set of functions $f_n(x)$ for $n = \ldots, -2, -1, 0, 1, 2, \ldots$ as

$$f_n(x) = \Theta(x-n)[1 - \Theta(x-n-1)]. \tag{14}$$

2b. Make a sketch of $f_1(x)$, and compute the scalar products

$$\langle f_n | f_m \rangle = \int_{-\infty}^{\infty} f_n^*(x) f_m(x)\, dx. \tag{15}$$

2c. Is the set of functions f_n a complete basis set for the one-dimensional Hilbert space?

2d. Show that the scalar product defined by the integral, Eq. (1.20) in the lecture notes, indeed satisfies the properties of a scalar product [Eqs. (1.21)-(1.24)] in the lecture notes

The identity operator $\hat{I}$ is defined by

$$\hat{I} = \int_{-\infty}^{\infty} dx\, |x\rangle\langle x|. \tag{16}$$

2e. Show that

$$\langle x | \hat{I} | x' \rangle = \delta(x - x'). \tag{17}$$

Hints: use

$$\langle x | y \rangle = \delta(x - y) \tag{18}$$

and test Eq. (17) by multiplying both sides with an arbitrary function $f(x')$, and integrate over x'.

The commutator of position and momentum operators in n Cartesian dimensions is given by

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}, \quad \text{with } i, j = 1, 2, \ldots, n. \tag{19}$$

We define new position operators by a linear transformation

$$\hat{\boldsymbol{X}} = \boldsymbol{A}\boldsymbol{x} \tag{20}$$

or, in components

$$\hat{X}_i = \sum_k A_{ik} \hat{x}_k \tag{21}$$

where $\boldsymbol{A}$ is a nonsingular $n \times n$ matrix with elements A_{ij}. We define new momenta by the linear transformation

$$\hat{\boldsymbol{P}} = \boldsymbol{A}^{-T} \hat{\boldsymbol{p}}, \tag{22}$$

where the components of the vector operator $\hat{\boldsymbol{p}}$ are $\hat{p}_i$ and $\hat{P}_j$ are the components of $\hat{\boldsymbol{P}}$.

2f. Show that

$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}. \tag{23}$$