

October 17, 2024

(1) [Exercise] Obtaining expectation value of a Hamiltonian.

Let's work the following Hamiltonian

$$K = \frac{1}{3} \sum_{i < j} X_i X_j - \sum_{i=0}^{n-1} Z_i$$

We compute the Hamiltonian using PennyLane. We define the python's function that creates the state based on the number of qubits. The illustration of the state is shown as a circuit in Fig.1 for a number of 4 qubits.

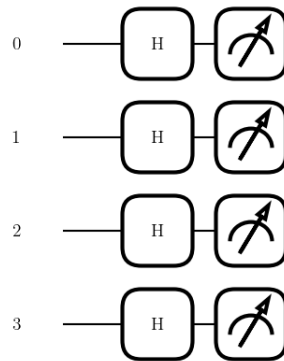


Figure 1: Circuit illustration of a state of 4 qubits obtained by using PennyLane's function `qml.draw_mpl`.

The results of the PennyLane simulation are graphed for a set of number of qubits in the Fig.2.

Let's analyze the expectation value analytically. Each qubit of the initial state starts in a ground state, so when the Hadamard gates are applied in each one the qubits are changed to the $|+\rangle$. The state ψ has the form

$$|\psi\rangle = \bigotimes_{i=1}^N H |0\rangle = \bigotimes_{i=1}^N |+\rangle$$

Then when the expectation is calculated

$$\begin{aligned} \langle \psi | K | \psi \rangle &= \bigotimes_{k=1}^N \langle + | \left(\frac{1}{3} \sum_{i < j} X_i X_j - \sum_{i=0}^{n-1} Z_i \right) \bigotimes_{k=1}^N | + \rangle \\ &= \frac{1}{3} \sum_{i < j} \bigotimes_{k=1}^N \langle + | (X_i X_j) \bigotimes_{k=1}^N | + \rangle - \sum_{i=0}^{n-1} \bigotimes_{k=1}^N \langle + | (Z_i) \bigotimes_{k=1}^N | + \rangle \end{aligned}$$

The $|+\rangle$ is an eigenvector with eigenvalue 1 of the term $X_i X_j$, and the term Z_i change the i -th state to $|-\rangle$, so the second sum will be null.

$$\langle \psi | K | \psi \rangle = \frac{1}{3} \sum_{i < j} 1 - 0 = \frac{N(N-1)}{6}$$

This result is plotted in the Fig.2. It's clear that the simulation is the same than the analytical result.

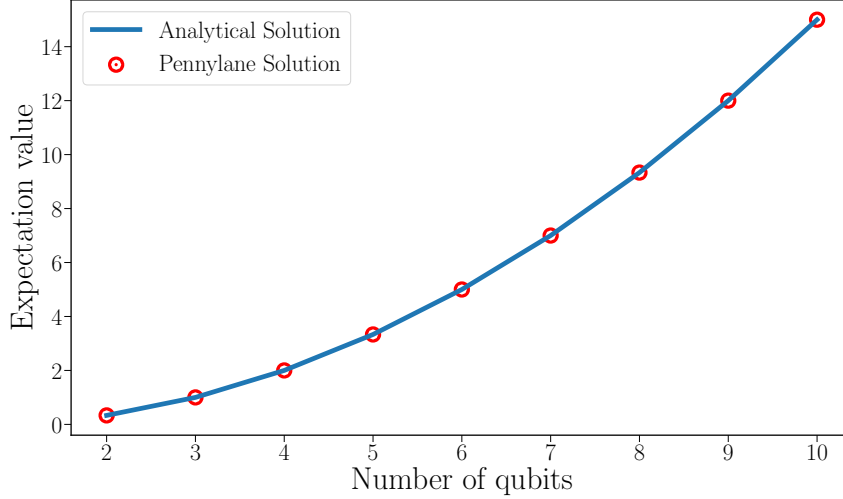


Figure 2: Expectation value in function of the number of qubits for the analytical solution (blue line) and the PennyLane's simulation (red dots)

(2) [Challenge] Ground state energy for molecule and spin system with Variational Quantum Algorithms and Trotterization.

(1) [Exercise] Interactions between atoms and the low-energy limit.

a) We have the following two body Hamiltonian

$$-\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{2m} \nabla_2^2 - V(r) = H$$

Using $r_{cm} = \frac{r_1 m_1 + r_2 m_2}{m_1 + m_2}$ and $m_r = \frac{m_1 m_2}{m_1 + m_2}$ we obtain

$$-\frac{\hbar^2}{2M_{cm}} \nabla_{cm}^2 - \frac{\hbar^2}{2m_r} \nabla_{m_r}^2 - V(r) = H$$

Which is known as the Hamiltonian of the reduced mass. The first term is a constant because the whole system conserves the kinetic energy since it is not exposed to an external potential. Then

$$\left(-\frac{\hbar^2}{m} \nabla^2 - V(r) - E \right) \psi = 0$$

The potential $V(r)$ is spherical, then

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

Then, when we make the separation of variables $\psi(r, \theta, \phi) = R(r)\Theta(\theta, \phi)$

$$\begin{aligned} \frac{\Theta(\theta, \phi)}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{R(r)}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta, \phi)}{\partial \theta} \right) + \frac{R(r)}{r^2 \sin^2 \theta} \frac{\partial^2 \Theta(\theta, \phi)}{\partial \phi^2} \\ + \frac{mV(r)}{\hbar^2} R(r)\Theta(\theta, \phi) + \frac{mE}{\hbar^2} R(r)\Theta(\theta, \phi) = 0 \end{aligned}$$

Then, we have the following differential equations

$$\begin{aligned} & \frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{m}{\hbar^2} (E + V(r)) r^2 \\ &= \frac{1}{\Theta(\theta, \phi) \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta, \phi)}{\partial \theta} \right) - \frac{1}{\Theta(\theta, \phi) \sin^2 \theta} \frac{\partial^2 \Theta(\theta, \phi)}{\partial \phi^2} = K \end{aligned}$$

The second equation has the solution of a spherical harmonic $Y_l^m(\theta, \phi)$ such that $K = l(l+1)$. Then the radial equation is

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{m}{\hbar^2} (E + V(r)) R(r) = \frac{l(l+1)}{r^2} R(r)$$

Using $u(r) = rR(r)$

$$\frac{\partial^2}{\partial r^2} u(r) + \frac{m}{\hbar^2} (E + V(r)) u(r) = \frac{l(l+1)}{r^2} u(r)$$

Then if $E = \frac{\hbar^2 k^2}{m}$

$$\left(\frac{\partial^2}{\partial r^2} + k^2 + V(r) - \frac{l(l+1)}{r^2} \right) u_l(r) = 0 \quad (1)$$

In scattering theory, the energy of the incoming particle is related to its wave number k . The wave number is related to the particle's de Broglie wavelength λ by $k = \frac{2\pi}{\lambda}$, so the lower the energy, the longer the wavelength. The low-energy limit occurs when the wavelength of the incoming particle becomes much larger than the range of the potential R .

Thus, the low-energy limit corresponds to:

$$kR \ll 1 \quad (2)$$

This means that the wave number k is much smaller than the inverse of the range of the potential, or equivalently, the particle's wavelength is much larger than the size of the potential region.

In the low-energy limit, the solution to equation 1 indicates that the only affected part corresponds to ($l = 0$), meaning that this term contributes to the phase shift. Consequently, the terms for ($l > 0$) can be disregarded. In Fig. 3 is shown in the first column that when $kR \ll 1$ the only case where a phase shift exists is when $l = 0$ (Fig. 3(a)). On the other hand, when $l > 0$ there isn't a phase shift (Fig. 3(c,e,g)). When $kR \not\ll 1$ is shown that there are phase shifts for all the values of l (Fig. 3(b,d,f,h)). Then, it is clear that the contributions of the waves with $l > 1$ are null if $kR \ll 1$.

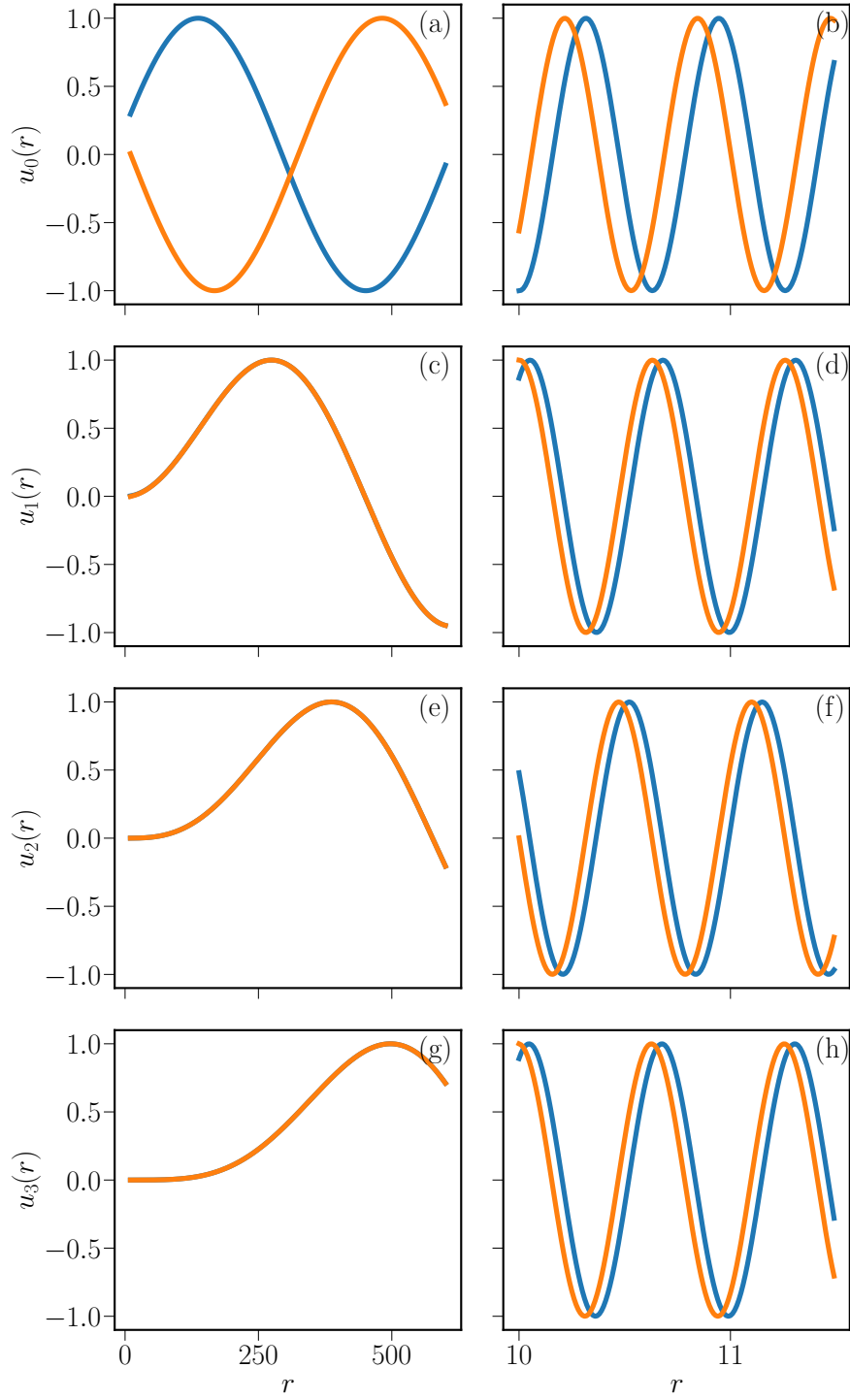


Figure 3: Numerical integration (RK4) of the $u_l(r)$ function based on the differential eq.1. The first column (a, c, e, g) shows the behavior when $kR \ll 1$. The second column (b, d, f, h) shows when $kR \ll 1$. Each row corresponds to a value of l .

b) The scattering length provides an understanding of how far particles can travel before the potential significantly alters their trajectory.

c) We need to calculate the constant U_0 . Let's substitute the given formula for the scattering length into the general formula for the scattering length in the Born approximation:

$$a = \frac{m_r}{2\pi\hbar^2} \int d^3r U_0 \delta(\mathbf{r} - \mathbf{r}') \quad (1)$$

$$a = \frac{m_r}{2\pi\hbar^2} U_0 \int d^3r \delta(\mathbf{r} - \mathbf{r}') \quad (2)$$

$$a = \frac{m_r}{2\pi\hbar^2} U_0 \quad (3)$$

So, we can solve for U_0 :

$$U_0 = a \frac{2\pi\hbar^2}{m_r} \quad (1)$$

(2) [Exercise] The Gross-Pitaevskii equation

In this problem we will considerate BEC's (Bose-Einstein Condensates) in the presence of interaction. The many-body Hamiltonian for N interacting bosons is given by:

$$H = \sum_{i=1}^N \left[\frac{p_i^2}{2m} + V(r_i) \right] + U_0 \sum_{i<j} \delta(r_i - r_j) \quad (2)$$

Where $V(r_i)$ is an external (one-body) potential, and the latter term is the interparticle interactions.

Adopting a mean-field approach, the wave function is given by:

$$\Psi(r_1, r_2, \dots, r_N) = \prod_{i=1}^N \phi(r_i) \quad (3)$$

Where we assume that all particles are in the same single-particle state $\phi(r)$. The single-particle wave functions is normalized to the unit.

$$\int d^3r |\phi(r)|^2 = 1 \quad (4)$$

1. Deduce the expression for the expectation value of the Hamiltonian of Eq. 2 in the state of Eq. 3.

The expectation value is given by:

$$E = \langle \Psi | H | \Psi \rangle \quad (5)$$

Using Eq 2, we can write:

$$\begin{aligned} E &= \langle \Psi | \sum_{i=1}^N \frac{p_i^2}{2m} + V(r_i) | \Psi \rangle + U_0 \langle \Psi | \sum_{i<j} \delta(r_i - r_j) | \Psi \rangle \\ E &= \sum_{i=1}^N \left(\langle \Psi | \frac{p_i^2}{2m} | \Psi \rangle + \langle \Psi | V(r_i) | \Psi \rangle \right) + U_0 \sum_{i<j} \langle \Psi | \delta(r_i - r_j) | \Psi \rangle \end{aligned} \quad (6)$$

Let's calculate each term, first we begin with the Kinetic contribution:

$$\langle \Psi | \frac{p_i^2}{2m} | \Psi \rangle = \frac{1}{2m} = \frac{1}{2m} (\langle \Psi | p_i | \Psi \rangle \langle p_i | \Psi \rangle) = \frac{1}{2m} \int d^3r \langle \Psi | p_i | r \rangle \langle r | p_i | \Psi \rangle = \frac{1}{2m} \int d^3r |\langle r | p_i | \Psi \rangle|^2$$

Where we use that $\int d^3r |r\rangle \langle r| = \mathbb{I}$. Now we can see that $|r\rangle = |r_1, r_2, \dots, r_N\rangle$. Also, the momentum operator p_i . In three dimensions, the momentum operator takes the form of a gradient

$$\langle r | p_i | \Psi \rangle = -i\hbar \nabla_i \Psi \quad (7)$$

Where ∇_i is the gradient operator acting in the i -th coordinate. Then we can compute:

$$\langle \Psi | \frac{p_i^2}{2m} | \Psi \rangle = \frac{\hbar^2}{2m} \int d^3r |\nabla_i \Psi|^2 \quad (8)$$

Now, let's calculate the contribution of the external potential. This is direct:

$$\langle \Psi | V(r_i) | \Psi \rangle = \int d^3r \Psi^*(r) V(r_i) \Psi(r) \quad (9)$$

Finally we have to compute the interaction term. It's also direct.

$$\langle \Psi | \delta(r_i - r_j) | \Psi \rangle = \int d^3r \Psi^*(r) \delta(r_i - r_j) \Psi(r) \quad (10)$$

These are general expressions, now using that the wave function is given by Eq 3. The momentum contribution becomes:

$$\begin{aligned} \frac{\hbar^2}{2m} \int d^3r |\nabla_i \Psi|^2 &= \frac{\hbar^2}{2m} \int d^3r |\phi(r_1) \phi(r_2) \dots \nabla_i \phi(r_i) \dots \phi(r_N)|^2 \\ &= \frac{\hbar^2}{2m} \int d^3r |\phi(r_1)|^2 |\phi(r_2)|^2 \dots |\nabla_i \phi(r_i)|^2 \dots |\phi(r_N)|^2 \end{aligned}$$

Now, we can use that $d^3r = d^3r_1 d^3r_2 \dots d^3r_N$.

$$\frac{\hbar^2}{2m} \int d^3r |\nabla_i \Psi|^2 = \frac{\hbar^2}{2m} \int d^3r_1 |\phi(r_1)|^2 \int d^3r_2 |\phi(r_2)|^2 \dots \int d^3r_i |\nabla_i \phi(r_i)|^2 \dots \int d^3r_N |\phi(r_N)|^2$$

And since the wave functions are normalized, we obtain:

$$\langle \Psi | \frac{p_i^2}{2m} | \Psi \rangle = \frac{\hbar^2}{2m} \int d^3r_i |\nabla_i \phi(r_i)|^2 \quad (11)$$

On the other hand, expression (8) can be written as:

$$\begin{aligned} \int d^3r \Psi^*(r) V(r_i) \Psi(r) &= \int d^3r_1 |\phi(r_1)|^2 \int d^3r_2 |\phi(r_2)|^2 \dots \int d^3r_i \phi^*(r_i) V(r_i) \phi(r_i) \dots \int d^3r_N |\phi(r_N)|^2 \\ &= \int d^3r_i \phi^*(r_i) V(r_i) \phi(r_i) \\ &= \int d^3r_i |\phi(r_i)|^2 V(r_i) \end{aligned}$$

$$\langle \Psi | V(r_i) | \Psi \rangle = \int d^3r_i |\phi(r_i)|^2 V(r_i) \quad (12)$$

We can calculate the interaction term, noting that all the integrals evaluate to 1 except for those related to the variables i and j .

$$\begin{aligned}
\int d^3r \Psi^*(r) \delta(r_i - r_j) \Psi(r) &= \int d^3r_1 |\phi(r_1)|^2 \dots \int d^3r_i |\phi(r_i)|^2 \dots \int d^3r_j |\phi(r_j)|^2 \delta(r_i - r_j) \dots \int d^3r_N |\phi(r_N)|^2 \\
&= \int \int d^3r_i d^3r_j |\phi(r_i)|^2 |\phi(r_j)|^2 \delta(r_i - r_j) \\
&= \int d^3r_i |\phi(r_i)|^4
\end{aligned}$$

$$\langle \Psi | \delta(r_i - r_j) | \Psi \rangle = \int d^3r_i |\phi(r_i)|^4 \quad (13)$$

Then with the equations (11-13) we can compute the expectation value of the Hamiltonian with Eq 6.

$$E = \frac{\hbar^2}{2m} \sum_{i=1}^N \left(\int d^3r_i |\nabla_i \phi(r_i)|^2 \right) + \sum_i \int d^3r_i |\phi(r_i)|^2 V(r_i) + U_0 \sum_{i<j} \int d^3r_i |\phi(r_i)|^4 \quad (14)$$

Let's remember that the eigenfunction ϕ is the same for each particle, and that when integrating over d^3r_i , we are integrating over the entire space. Therefore, the subscript i is just a dummy index. Thus, we will take $d^3r_1 = d^3r$ where r is simply a variable (it is just three dimensional; it is not the same r that contained $=r_1, r_2, \dots, r_n$).

Then, we have that the sum $\sum_i = 1^N$ and $\sum_{i<j}^N$ it is summing constant terms.

$$E = \frac{\hbar^2}{2m} \sum_{i=1}^N \left(\int d^3r |\nabla \phi(r)|^2 \right) + \sum_i \int d^3r |\phi(r)|^2 V(r) + U_0 \sum_{i<j} \int d^3r |\phi(r)|^4 \quad (15)$$

Using that:

$$\sum_{i=1}^N C = NC \quad \sum_{i<j}^N C = \frac{N(N-1)}{2}$$

Where C is a constant, we can rewrite the Eq 15:

$$E = N \int d^3r \left(\frac{\hbar^2}{2m} |\nabla \phi(r)|^2 + |\phi(r)|^2 V(r) \right) + U_0 \frac{N(N-1)}{2} \int d^3r |\phi(r)|^4 \quad (16)$$

Thus obtaining an expression for the expectation value of the Hamiltonian.

2. Alternatively, we can introduce the concept of the wave function of the condensate state, $\Psi(r) = \sqrt{N} \phi(r)$. Neglecting terms of order $1/N$, obtain the time-independent GPE.

With $\phi(r) = \Psi(r)/\sqrt{N}$, we can replace in Eq 16 :

$$\begin{aligned}
E &= N \int d^3r \left[\frac{\hbar^2}{2m} \left| \nabla \frac{\Psi(r)}{\sqrt{N}} \right|^2 + \left| \frac{\Psi(r)}{\sqrt{N}} \right|^2 V(r) \right] + U_0 \frac{N(N-1)}{2} \int d^3r \left| \frac{\Psi(r)}{\sqrt{N}} \right|^4 \\
E &= \int d^3r \left[\frac{\hbar^2}{2m} |\nabla \Psi(r)|^2 + V(r) |\Psi(r)|^2 \right] + U_0 \frac{N(N-1)}{2N^2} \int d^3r |\Psi(r)|^4
\end{aligned}$$

$$E = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla \Psi(r)|^2 + V(r) |\Psi(r)|^2 \right] + \frac{U_0}{2} \left(1 - \frac{1}{N} \right) \int d^3r |\Psi(r)|^4$$

Then, neglecting terms of order $1/N$, we obtain:

$$\boxed{E = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla \Psi(r)|^2 + V(r) |\Psi(r)|^2 + \frac{U_0}{2} |\Psi(r)|^4 \right]} \quad (17)$$

Now that we have the energy, we must minimize it to find the optimal $\Psi(r)$, subject to the constraint that the number of particles N is fixed. The number of particles is given by:

$$N = \int d^3r |\Psi(r)|^2 \quad (18)$$

This can be done conveniently using Lagrange multipliers, $\delta E \mu \delta N = 0$, where μ is the chemical potential. Then applying variational calculus we build the functional $S[\Psi]$

$$S[\Psi] = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla \Psi(r)|^2 + V(r) |\Psi(r)|^2 + \frac{U_0}{2} |\Psi(r)|^4 - \mu |\Psi(r)|^2 \right] \quad (19)$$

To obtain the optimal $\Psi(r)$ we perform the variation:

$$\delta S = S[\Psi + \delta \Psi] - S[\Psi] = 0$$

Let's compute $S[\Psi + \delta \Psi]$, neglecting $O(\delta \psi^2)$ terms.

$$S[\Psi + \delta \Psi] = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla(\Psi(r) + \delta \Psi)|^2 + V(r) |\Psi(r) + \delta \Psi|^2 + \frac{U_0}{2} |\Psi(r) + \delta \Psi|^4 - \mu |\Psi(r) + \delta \Psi|^2 \right]$$

$$S[\Psi + \delta \Psi] = \int d^3r \left[\frac{\hbar^2}{2m} |\nabla(\Psi(r) + \delta \Psi)|^2 + (V(r) - \mu) |\Psi(r) + \delta \Psi|^2 + \frac{U_0}{2} |\Psi(r) + \delta \Psi|^4 \right] \quad (20)$$

Expanding each of the terms.

$$\begin{aligned} |\nabla(\Psi(r) + \delta \Psi)|^2 &= |\nabla \Psi(r) + \nabla \delta \Psi|^2 = (\nabla \Psi^*(r) + \nabla \delta \Psi^*(r)) (\nabla \Psi(r) + \nabla \delta \Psi(r)) \\ &= |\nabla \Psi|^2 + \nabla \Psi^* \nabla \delta \Psi + \nabla \delta \Psi^* \nabla \Psi + |\nabla \delta \Psi|^2 \\ &\approx |\nabla \Psi|^2 + \nabla \Psi^* \nabla \delta \Psi + \nabla \delta \Psi^* \nabla \Psi \end{aligned} \quad (21)$$

$$\begin{aligned} |\Psi + \delta \Psi|^2 &= (\Psi^* + \delta \Psi^*)(\Psi + \delta \Psi) \\ &= |\Psi|^2 + \Psi^* \delta \Psi + \Psi \delta \Psi^* + |\delta \Psi|^2 \\ &\approx |\Psi|^2 + \Psi^* \delta \Psi + \Psi \delta \Psi^* \end{aligned} \quad (22)$$

$$\begin{aligned} |\Psi + \delta \Psi|^4 &= |\Psi + \delta \Psi|^2 |\Psi + \delta \Psi|^2 \\ &\approx (|\Psi|^2 + \Psi^* \delta \Psi + \Psi \delta \Psi^*) (|\Psi|^2 + \Psi^* \delta \Psi + \Psi \delta \Psi^*) \\ &\approx |\Psi|^4 + 2|\Psi|^2 \Psi^* \delta \Psi + 2|\Psi|^2 \Psi \delta \Psi^* + O(\delta^2) \\ &\approx |\Psi|^4 + 2|\Psi|^2 \Psi^* \delta \Psi + 2|\Psi|^2 \Psi \delta \Psi^* \end{aligned} \quad (23)$$

We can now replace the equations (21-23) and compute δS

$$\begin{aligned}
\delta S &= \int d^3r \left[\frac{\hbar^2}{2m} (|\nabla\Psi|^2 + \nabla\Psi^*\nabla\delta\Psi + \nabla\delta\Psi^*\nabla\Psi) + (V(r) - \mu)(|\Psi|^2 + \Psi^*\delta\Psi + \Psi\delta\Psi^*) \right. \\
&\quad \left. + U_0(|\Psi|^4 + 2|\Psi|^2\Psi^*\delta\Psi + 2|\Psi|^2\Psi\delta\Psi^*) - \frac{\hbar^2}{2m}|\nabla\Psi|^2 - (V(r) - \mu)|\Psi|^2 - \frac{U_0}{2}|\Psi|^4 \right] \\
\delta S &= \int d^3r \left[\frac{\hbar^2}{2m} (\nabla\Psi^*\nabla\delta\Psi + \nabla\Psi\nabla\delta\Psi^*) + (V(r) - \mu)(\Psi^*\delta\Psi + \Psi\delta\Psi^*) \right. \\
&\quad \left. + U_0(|\Psi|^2\Psi^*\delta\Psi + |\Psi|^2\Psi\delta\Psi^*) \right] \tag{24}
\end{aligned}$$

Then integrating by parts, or alternatively:

$$\begin{aligned}
\nabla \cdot (\nabla\Psi^*\delta\Psi) &= \nabla^2\Psi^*\delta\Psi + \nabla\Psi^*\nabla\delta\Psi \\
\implies \nabla\Psi^*\nabla\delta\Psi &= \nabla \cdot (\nabla\Psi^*\delta\Psi) - \nabla^2\Psi^*\delta\Psi
\end{aligned}$$

And also:

$$\nabla\Psi\nabla\delta\Psi^* = \nabla \cdot (\nabla\Psi\delta\Psi^*) - \nabla^2\Psi\delta\Psi^*$$

With the latter we can write:

$$\nabla\Psi^*\nabla\delta\Psi + \nabla\Psi\nabla\delta\Psi^* = \nabla \cdot (\nabla\Psi^*\delta\Psi + \nabla\Psi\delta\Psi^*) - \nabla^2\Psi^*\delta\Psi - \nabla^2\Psi\delta\Psi^* \tag{25}$$

Then, we can notice that

$$\begin{aligned}
\int d^3r \left[\frac{\hbar^2}{2m} (\nabla\Psi^*\nabla\delta\Psi + \nabla\Psi\nabla\delta\Psi^*) \right] &= \frac{\hbar^2}{2m} \int d^3r (\nabla \cdot (\nabla\Psi^*\delta\Psi + \nabla\Psi\delta\Psi^*) - \nabla^2\Psi^*\delta\Psi - \nabla^2\Psi\delta\Psi^*) \\
&= \frac{\hbar^2}{2m} \left[\int d^3r (-\nabla^2\Psi^*\delta\Psi - \nabla^2\Psi\delta\Psi^*) + (\nabla\Psi^*\delta\Psi + \nabla\Psi\delta\Psi^*) \Big|_{\vec{r}_b}^{\vec{r}_a} \right]
\end{aligned}$$

Where we used that $\int d^3r \nabla \cdot (f) = f|_{\vec{r}_a}^{\vec{r}_b}$. Now, if we consider fixed end points:

$$\delta\Psi(\vec{r}_a) = \delta\Psi(\vec{r}_b) = \delta\Psi^*(\vec{r}_a) = \delta\Psi^*(\vec{r}_b) = 0$$

Then we will have:

$$\int d^3r \left[\frac{\hbar^2}{2m} (\nabla\Psi^*\nabla\delta\Psi + \nabla\Psi\nabla\delta\Psi^*) \right] = -\frac{\hbar^2}{2m} \int d^3r (\nabla^2\Psi^*\delta\Psi + \nabla^2\Psi\delta\Psi^*) \tag{26}$$

Finally we can compute δS

$$\begin{aligned}
\delta S &= \int d^3r \left[\frac{-\hbar^2}{2m} (\nabla^2\Psi^*\delta\Psi + \nabla^2\Psi\delta\Psi^*) + (V(r) - \mu)(\Psi^*\delta\Psi + \Psi\delta\Psi^*) \right. \\
&\quad \left. + U_0(|\Psi|^2\Psi^*\delta\Psi + |\Psi|^2\Psi\delta\Psi^*) \right]
\end{aligned}$$

$$\begin{aligned}\delta S = \int d^3r \left[\frac{-\hbar^2}{2m} \nabla^2 \Psi^* + (V(r) - \mu) \Psi^* + U_0 |\Psi|^2 \Psi^* \right] \delta \Psi \\ + \int d^3r \left[\frac{-\hbar^2}{2m} \nabla^2 \Psi + (V(r) - \mu) \Psi + U_0 |\Psi|^2 \Psi \right] \delta \Psi^* = 0\end{aligned}\quad (27)$$

This relation must hold for all $\delta \Psi$ and $\delta \Psi^*$ then, we obtain the following equations:

$$\frac{-\hbar^2}{2m} \nabla^2 \Psi^* + (V(r) - \mu) \Psi^* + U_0 |\Psi|^2 \Psi^* = 0 \quad (28)$$

$$\frac{-\hbar^2}{2m} \nabla^2 \Psi + (V(r) - \mu) \Psi + U_0 |\Psi|^2 \Psi = 0 \quad (29)$$

We can rewrite both equations to obtain de GPE-Equations for the $\Psi^*(r)$ and for $\Psi(r)$.

$$\boxed{\frac{-\hbar^2}{2m} \nabla^2 \Psi^* + V(r) \Psi^* + U_0 |\Psi|^2 \Psi^* = \mu \Psi^*} \quad (30)$$

$$\boxed{\frac{-\hbar^2}{2m} \nabla^2 \Psi + V(r) \Psi + U_0 |\Psi|^2 \Psi = \mu \Psi} \quad (31)$$

We can see that resembles de Schrodinger equation but with a nonlinear term that takes account the mean field produced by the other particles. Also, the eigenvalue in this equation its not the energy but the chemical potential.

3. What is the GPE for a uniform Bose gas?

For a uniform Bose gas, we can consider that $|\Psi(r)|^2 = n_0$ (then $\nabla_i \Psi(r) = 0$) and also that happens in a box potential, so we fix the external potential $V(r)=0$ inside the box and $V(r) = \infty$ outside the box. Taking this into account the GPE-equation for a uniform Bose gas is:

$$\begin{aligned}\frac{-\hbar^2}{2m} \nabla^2 \Psi + V(r) \Psi + U_0 |\Psi|^2 \Psi = \mu \Psi \\ U_0 |\Psi|^2 \Psi = U_0 n_0 \Psi = \mu \Psi \\ \boxed{U_0 n_0 = \mu}\end{aligned}\quad (32)$$

Then, the GPE for a uniform bose gas has a very simple form. Also we can notice that for the uniform Bose gas, the energy [17](#) is:

$$E = \frac{U_0}{2} \int d^3r |\Psi|^4 = \frac{U_0}{2} n^2 \int d^3r$$

If we assume that the box has volume V then:

$$E = \frac{U_0}{2} n^2 V \quad (33)$$

Taking the partial derivative respect to N .

$$\frac{\partial E}{\partial N} = \frac{\partial E}{\partial n} \frac{\partial n}{\partial N} = \frac{U_0}{2} 2nV \frac{1}{V} = nU_0 \quad (34)$$

With this, we demonstrate that the equations are consistent with the thermodynamic relations because with 33 and 34.

$$\boxed{\frac{\partial E}{\partial N} = \mu} \quad (35)$$

Computational Project: Analytical Results

First, let us consider one-dimensional non interacting case. The dimensionless equation is:

$$H\Psi(x, t) = i \frac{\partial \Psi(x, t)}{\partial t} \quad (36)$$

$$H = \frac{-1}{2} \frac{\partial^2 \Psi}{\partial x^2} + V(x) \quad (37)$$

If we consider a separation into real and imaginary parts.

$$\Psi(x, t) = R(x, t) + iI(x, t) \quad (38)$$

Replacing in the Schrodinger equation:

$$HR + iHI = i\dot{R} - \dot{I} \quad (39)$$

Then, we obtain 2 equations:

$$\frac{dR}{dt} = HI \quad \frac{dI}{dt} = -HR \quad (40)$$

Now if we consider an Harmonic trap $V(x) = \frac{1}{2}x^2$. The eigenfunctions of this problem are given by:

$$\phi_n = \frac{1}{\sqrt{2^n n!}} \left(\frac{1}{\pi} \right)^{\frac{1}{4}} e^{\frac{-x^2}{2}} H_n(x) \quad (41)$$

Where $H_n(x)$ are the Hermite Polynomials. And the eigenvalues.

$$E_n = n + \frac{1}{2} \quad (42)$$

Then for the initial condition $\Psi(x, t=0) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} e^{\frac{-x^2}{2}} = \phi_0$. We can note that the probability density it will maintain constant this because:

$$\Psi(x, t) = \Psi_0 e^{-iHt} = \phi_0 e^{iE_0 t}$$

Then, the exponential term its only a phase:

$$\implies \boxed{|\Psi|^2 = |\phi|^2}$$

Now for the second initial condition given by:

$$\Psi(x, 0) = \left(\frac{2}{\pi}\right)^{1/4} e^{-x^2} \quad (43)$$

We can find the evolution of this if we write the initial condition as a lineal combination of eigenfunctions:

$$\Psi(x, 0) = \sum_n c_n \phi_n \quad (44)$$

$$\Psi = \sum_n c_n \phi_n e^{-iHt} = \sum_n c_n \phi_n e^{-iE_n t} \quad (45)$$

Then we can see that in this case, the probability density will vary with time.

Finally we will study the interaction case. If we consider the term $U_0 = -2$ and $V = 0$ we would obtain the Non Linear Schrodinger equation (NLSE) adimensional given by (for the Time-independent equation):

$$-\frac{1}{2} \frac{\partial^2 \Psi}{\partial x^2} - 2|\Psi|^2 \Psi = \mu \Psi \quad (46)$$

We now that one of the eigenfunction of the above equation its given by:

$$\phi = \frac{1}{\sqrt{2} \cosh x} \quad (47)$$

Then, the time-evolution is:

$$\Psi(x, t) = \Psi(x, 0) \exp(-iHt) \quad (48)$$

And the initial condition is a eigenfunction of the problem. Then, the evolution it would be

$$\Psi(x, t) = \phi e^{-i\mu t} \quad (49)$$

Like in the first case, the probability density it would mantain constant in time!

$$|\Psi|^2 = |\phi|^2 \quad (50)$$

(1) [Exercise] Let $V = \mathbb{C}^2$ be the Hilbert space of a single qubit. Then, consider the set of objects $\{\mathbb{I}, X\}$, where \mathbb{I} is the 2×2 identity matrix and X the Pauli-x matrix. Show that these objects, which represent bit-flips, form a group.

For the Hilbert space $V = \mathbb{C}^2$, consider the objects $\{\mathbb{I}, X\}$, where

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

For a set G form a group, the elements must comply with the following properties

- 1) **Closure:** For all $g_i, g_j \in G$, $g_i \circ g_j \in G$.
- 2) **Identity element:** there exist an element $e \in G$ such that for all $g_i \in G$ $e \circ g_i = g_i \circ e = g_i$.
- 3) **Inverse element:** For each $g_i \in G$ there exist an element $g_i^{-1} \in G$ such that $g_i g_i^{-1} = g_i^{-1} g_i = e$.
- 4) **Associativity:** For all $g_i, g_j, g_k \in G$, $(g_i \circ g_j) \circ g_k = g_i \circ (g_j \circ g_k)$.

In our case, we will use as binary operation the matrix multiplication. Then, all possible multiplications between elements of the group are

$$\begin{aligned}\mathbb{I}.\mathbb{I} &= \mathbb{I}, \\ \mathbb{I}.X &= X, \\ X.\mathbb{I} &= X, \\ X.X &= \mathbb{I}.\end{aligned}$$

All these products satisfy the **(1) Closure** relation. Moreover, as $g_j.\mathbb{I} = \mathbb{I}.g_j = g_j$, we have that the **(2) identity element** of the group is the identity matrix $e = \mathbb{I}$. Note that, $X^{-1} = X$ and $\mathbb{I}^{-1} = \mathbb{I}$. Therefore, the **(3) inverse element** property is achieved. Now, For the **(4) Associativity** property simply note that the matrix multiplication is associative by definition.

With all the exposed above, we can conclude that the set $\{\mathbb{I}, X\}$ satisfies all necessary conditions to be a group.

(2) [Exercise] Proves that the set of all unitaries of the form $U = e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y}$ constitutes a representation of the unitary Lie group $SU(2)$ group.

We start from statetment for definition of $SU(2) = \{A \in \mathbb{C}^{2 \times 2} : AA^\dagger = A^\dagger A = \mathbb{I}, \det A = 1\}$. Then, we have

$$U^\dagger = e^{i\phi_1 Y} e^{i\phi_2 X} e^{i\phi_3 Y}.$$

Therefore,

$$UU^\dagger = e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y} e^{i\phi_1 Y} e^{i\phi_2 X} e^{i\phi_3 Y} = \mathbb{I}.$$

Next, we will calculate the determinant. Note that

$$\begin{aligned}\det(U) &= \det\left(e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y}\right) \\ &= \det\left(e^{-i\phi_3 Y}\right) \det\left(e^{-i\phi_2 X}\right) \det\left(e^{-i\phi_1 Y}\right). \\ &= e^{-i\phi_3 \det(Y)} e^{-i\phi_2 \det(X)} e^{-i\phi_1 \det(Y)}.\end{aligned}$$

Moreover, for $A \in \mathbb{C}^{n \times n} \det(A) = \prod_{i=1}^n \lambda_i(A)$ where $\lambda_i(A)$ is the i -th eigenvalue of A . Applying this property, we obtain

$$\begin{aligned}\det(U) &= \exp\left(-i\phi_3 \prod_{i=1}^2 \lambda_i(Y)\right) \exp\left(-i\phi_2 \prod_{i=1}^2 \lambda_i(X)\right) \exp\left(-i\phi_1 \prod_{i=1}^2 \lambda_i(Y)\right) \\ &= \exp\left(-i\phi_3 \sum_{i=1}^2 \lambda_i(Y)\right) \exp\left(-i\phi_2 \sum_{i=1}^2 \lambda_i(X)\right) \exp\left(-i\phi_1 \sum_{i=1}^2 \lambda_i(Y)\right)\end{aligned}$$

As the eigenvalues of the Pauli matrices are ± 1 , we have:

$$\det(U) = e^0 = 1$$

Now we need to proof that U are actually a representation of $SU(2)$. For this, we state the Lie algebra for this group,

$$su(2) = \{A \in \mathbb{C}^{2 \times 2} : A^\dagger = -A, \text{tr}(A) = 0\}$$

We can use the Pauli matrices $\{X, Y, Z\}$ multiplied by a factor i as generator for this algebra. Moreover, a fundamental property of Lie groups is that any element of the group can be written as an exponentiation of a linear combination from the generator for the Lie algebra associated to the group. For $su(2)$ we have that for any $U \in SU(2)$

$$U = e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y}$$

If we use the Baker–Campbell–Hausdorff formula given by

$$e^A e^B = e^C$$

with $C = (A + B + \frac{1}{2}[A, B] + \frac{1}{12}[A[A, B]] - \frac{1}{12}[B[B, A]] \dots)$. For our case, the commutation relation is $[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$. In that sense, any nested commutator will be of the form

$$[(ia)\sigma_i[\dots[(ia)\sigma_i, (ib)\sigma_j]]] = iK\sigma_\ell, \quad i \neq j, a, b \in \mathcal{R}$$

where $K \in \mathbb{R}$ and $\sigma_\ell \in \{X, Y, Z\}$. For example,

$$[(i\phi_2)X, [(i\phi_2)X, (i\phi_1)Y]] = 2(\phi_2)^2(\phi_1)[X, Z] = -4i(\phi_2)^2(\phi_1)Y$$

Therefore, matrix U can be represented by

$$U = e^{i(\alpha X + \beta Y + \gamma Z)}$$

That is an exponentiation of a linear combination of the generators of the $su(2)$ Lie algebra, proving that U is a representation of the $SU(2)$ group.

(3) [Challenge] Show that the dimension D of the commutant $C(k)(G)$, outlined in Definition 8 of the lecture notes, is determined by $D = \sum_\lambda m_\lambda^2$

For this challenge, we start by stating what is an irreducible representation for a group. *A representation R of a group G (with algebra g) over V is called reducible if there exists a nontrivial invariant subspace $W \subseteq V$. If the only invariant subspaces are the trivial subspaces 1 and V , then, V is called irreducible.* Moreover, invariant subspaces are closely connected to simultaneous block diagonalization and direct sums.

In this sense, *Let R be a representation of G (resp. g) on a vector space V . Then V is called completely reducible if there exists a direct sum decomposition of V into subspaces W_1, \dots, W_k , $V = W_1 \oplus W_2 \oplus \dots \oplus W_k$, where each W_j is an R invariant subspace such that the restriction $R_j := R|_{W_j}$ is irreducible.*

If R is a completely completely reducible representation on V , there exists a basis of V such that we have simultaneous block diagonalization:

$$R(g) \simeq \begin{pmatrix} R_1(g) & 0 & 0 & \dots & 0 \\ 0 & R_2(g) & 0 & \dots & 0 \\ 0 & 0 & \ddots & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & R_k(g) \end{pmatrix}$$

For all $g \in G$. A more compact representation is

$$R(g) \simeq \bigoplus_\lambda \mathbb{I}_{m_\lambda} \otimes R_\lambda(g) \quad \text{for all } g \in G. \quad (51)$$

Where, λ label a irreducible representation and \mathbb{I}_{m_λ} is the $m_\lambda \times m_\lambda$ identity matrix, with m_λ called the multiplicity.

Now, we introduce the notion of k -th order commutant of a group. *Given some representation R of a group G , its k -th order commutant, denoted as $\mathcal{C}^{(k)}(G)$, to be the vector subspace of the space of bounded linear operators on $\mathcal{H}^{\otimes k}$ that commutes with $R(g)^{\otimes k}$ for all $g \in G$. That is .*

$$\mathcal{C}^{(k)}(G) = \left\{ A \in \mathcal{B}(\mathcal{H}^{\otimes k}) \mid [A, R(g)^{\otimes k}] = 0, \forall g \in G \right\}$$

According to equation (51), a representation R of a group G can be written as the direct sum of its irreducible representations. Moreover, Schur's lemma says that is $R_\lambda(g) \forall g \in G$ is an irreducible representation of G , then, an operator T that commutes with all $R_\lambda(g)$ must be multiple of identity $T = \alpha \mathbb{I}$. Therefore, all elements of the commutant $\mathcal{C}^{(k)}(G)$ must be of the form

$$A = \bigoplus_{\lambda} A_{m_\lambda} \otimes \mathbb{I}_{d_\lambda}, \quad (52)$$

where A_{m_λ} is an arbitrary $m_\lambda \times m_\lambda$ matrix and $d_\lambda = \dim(R_\lambda(g))$. As the matrix is A_{m_λ} is arbitrary, for a given λ it has m_λ^2 degrees of freedom and therefore $D_\lambda = m_\lambda^2$. Then, the dimension of the commutant is the sum over λ .

$$D = \sum_{\lambda} D_\lambda = \sum_{\lambda} m_\lambda^2 \quad (53)$$

(1) [Exercise] Let $HG_\theta(x, y)$ be the first order Hermite-Gauss mode rotated counterclockwise by θ . Show that

a $HG_\theta(x, y) = \cos(\theta)HG_{01}(x, y) + \sin(\theta)HG_{10}(x, y)$

1. The Hermite-Gaussian modes are given by the product of a Gaussian mode, a Hermite polynomial in direction x and a Hermite polynomial in direction y

$$HG_{n_x, n_y} = A_G \times H_{n_x}(x) \times H_{n_y}(y).$$

Then,

$$HG_{1,0} = A_G H_1(x) H_0(y)$$

Moreover, the Hermite polynomials $H_0(x) = 1$ and $H_1(x) = 2x$

$HG_\theta(x, y)$ it can be defined as the $HG_{10}(x', y')$ mode evaluated in a rotated frame of reference. If we apply a rotation matrix $R(\theta)$ to the cartesian basis, the new coordinates it would be given by:

$$x' = x \cos \theta + y \sin \theta \quad (54)$$

$$y' = -x \sin \theta + y \cos \theta \quad (55)$$

Then

$$HG_{10}(x', y') = A_G H_{10} \left(\frac{\sqrt{2}x'}{\omega} \right) e^{-\frac{(x'^2 + y'^2)}{w}} \quad (56)$$

Now we can note that

$$\begin{aligned} x'^2 + y'^2 &= (x \cos \theta + y \sin \theta)^2 + (-x \sin \theta + y \cos \theta)^2 \\ &= x^2 \cos^2 \theta + y^2 \sin^2 \theta + 2xy \cos \theta \sin \theta + x^2 \sin^2 \theta + y^2 \cos^2 \theta - 2xy \cos \theta \sin \theta \\ &= x^2 + y^2 \end{aligned} \quad (57)$$

This result is expected since the rotation does not change the magnitude of the vector (x, y) . i.e. $|(x, y)|^2 = |(x', y')|^2$.

Now we can use the equations 54 and 57 to compute $HG_{10}(x', y')$.

$$\begin{aligned}
HG_{10}(x', y') &= A_G 2\sqrt{2} \frac{x'}{\omega} e^{-\frac{(x^2+y^2)}{\omega}} \\
&= A_G \frac{2\sqrt{2}}{\omega} (x \cos \theta + y \sin \theta) e^{-\frac{(x^2+y^2)}{\omega}} \\
&= A_G \left(H_1 \left(\frac{\sqrt{2}x}{\omega} \right) \cos \theta + H_1 \left(\frac{\sqrt{2}y}{\omega} \right) \sin \theta \right) e^{-\frac{(x^2+y^2)}{\omega}} \\
&= A_G H_1 \left(\frac{\sqrt{2}x}{\omega} \right) e^{-\frac{(x^2+y^2)}{\omega}} \cos \theta + A_G H_1 \left(\frac{\sqrt{2}y}{\omega} \right) e^{-\frac{(x^2+y^2)}{\omega}} \sin \theta \\
HG_{10}(x', y') &= H_{10} \cos \theta + H_{01} \sin \theta
\end{aligned} \tag{58}$$

Where we used the fact that $H_1(x) = 2x$ and $H_0(x) = 1$. Finally, since $HG_\theta(x, y) = HG_{10}(x', y')$, we conclude that:

$$\boxed{HG_\theta(x, y) = H_{10} \cos \theta + H_{01} \sin \theta} \tag{59}$$

2. Let $u_{nm}(x, y)$ be a basis set of the square integrable functions in R2. Show that

$$\sum_{n,m=0}^{\infty} u_{nm}(x, y) u_{nm}^*(x, y) = \delta(x - x') \delta(y - y') \tag{60}$$

Proof:

We can write the functions $u_{nm}(x, y)$ in Bra-ket notation with

$$u_{nm} = \langle x, y | u_{nm} \rangle \quad u_{nm}^* = \langle u_{nm} | x, y \rangle \tag{61}$$

If we replace the latter in Eq 60:

$$\sum_{n,m=0}^{\infty} \langle x, y | u_{nm} \rangle \langle u_{nm} | x, y \rangle = \langle x, y | \left(\sum_{n,m=0}^{\infty} |u_{nm}\rangle \langle u_{nm}| \right) | x, y \rangle$$

And since the functions $u_{nm}(x, y)$ form a complete basis, it follows that:

$$\sum_{n,m=0}^{\infty} |u_{nm}\rangle \langle u_{nm}| = \mathbb{I} \tag{62}$$

Then, Eq2 reduces to:

$$\sum_{n,m=0}^{\infty} u_{nm}(x, y) u_{nm}^*(x, y) = \langle x, y | x', y' \rangle = \langle x | x' \rangle \langle y | y' \rangle$$

Finally using the fact that the space kets forms a complete basis. We have:

$$\langle x | x' \rangle = \delta(x - x') \quad \langle y | y' \rangle = \delta(y - y') \quad (63)$$

With this, we can conclude that

$$\boxed{\sum_{n,m=0}^{\infty} u_{nm}(x, y) u_{nm}^*(x, y) = \delta(x - x') \delta(y - y')} \quad (64)$$

(3) [Challenge] Consider the linear polarization unit vectors rotated counter-clockwise by $\hat{\theta}$:

$$\hat{e}_{\theta} = \cos \theta \hat{e}_H + \sin \theta \hat{e}_V \quad (20)$$

- Show that the vector structures used for alignment-free quantum communication,

$$\Psi_{\theta}(x, y) = HG_{\theta}(x, y) \hat{e}_{\theta} + HG_{\theta+\pi/2}(x, y) \hat{e}_{\theta+\pi/2}, \quad (21)$$

$$\Psi_{\theta}(x, y) = HG_{\theta}(x, y) \hat{e}_{\theta+\pi/2} + HG_{\theta+\pi/2}(x, y) \hat{e}_{\theta}, \quad (22)$$

are rotation invariant.

Using the definitions above, we can write $\Psi_{\theta}(x, y)$:

$$\begin{aligned} \Psi_{\theta}(x, y) = & (\cos \theta HG_{10}(x, y) + \sin \theta HG_{01}(x, y)) (\cos \theta \hat{e}_H + \sin \theta \hat{e}_V) \\ & + (-\sin \theta HG_{10}(x, y) + \cos \theta HG_{01}(x, y)) (-\sin \theta \hat{e}_H + \cos \theta \hat{e}_V) \end{aligned}$$

$$\begin{aligned} \Psi_{\theta}(x, y) = & \cos^2 \theta HG_{10} \hat{e}_H + \cos \theta \sin \theta HG_{10} \hat{e}_V + \sin \theta \cos \theta HG_{01} \hat{e}_H + \sin^2 \theta HG_{01} \hat{e}_V \\ & + \sin^2 \theta HG_{10} \hat{e}_H - \sin \theta \cos \theta HG_{10} \hat{e}_V - \sin \theta \cos \theta HG_{01} \hat{e}_H + \cos^2 \theta HG_{01} \hat{e}_V \end{aligned}$$

Then using the trigonometric identity $\cos^2 \theta + \sin^2 \theta = 1$.

$$\boxed{\Psi_{\theta}(x, y) = HG_{10} \hat{e}_H + HG_{01} \hat{e}_V} \quad (65)$$

b)

For the second part, we will use a more mathematical approach!

Given

$$\Psi_{\theta}^1 = HG_{\theta} \hat{e}_{\theta} + HG_{-\theta} \hat{e}_{-\theta} \quad (1)$$

and

$$\Psi_{\theta}^2 = HG_{-\theta} \hat{e}_{\theta} + HG_{\theta} \hat{e}_{-\theta} \quad (1)$$

vector structures used for describing polarization modes in the \mathbb{R}^2 polarized space. We already show that Ψ_{θ}^1 is invariant under rotations. It is easy to proof that the set $\{\Psi_{\theta}^1, \Psi_{\theta}^2\}$ forms an Orthogonal Basis.

Proof:

$$\langle \Psi_{\theta}^1 | \Psi_{\theta}^2 \rangle = \int_{\mathbb{R}^2} (HG_{\theta} \hat{e}_{\theta} + HG_{-\theta} \hat{e}_{-\theta})^* \cdot (HG_{-\theta} \hat{e}_{\theta} + HG_{\theta} \hat{e}_{-\theta}) \quad (1)$$

$$= \int_{\mathbb{R}^2} HG_{\theta}^* HG_{-\theta} dA + \int_{\mathbb{R}^2} HG_{-\theta}^* HG_{\theta} dA = 0 \quad (1)$$

where we occupied the ortogonal relationship of the HG_{θ} basis.

And by taking the inner product of each vector:

$$\langle \Psi_{\theta}^1 | \Psi_{\theta}^1 \rangle = \int_{\mathbb{R}^2} (HG_{\theta} \hat{e}_{\theta} + HG_{-\theta} \hat{e}_{-\theta})^* \cdot (HG_{\theta} \hat{e}_{\theta} + HG_{-\theta} \hat{e}_{-\theta}) = 2 \quad (1)$$

$$\langle \Psi_{\theta}^2 | \Psi_{\theta}^2 \rangle = \int_{\mathbb{R}^2} (HG_{-\theta} \hat{e}_{\theta} + HG_{\theta} \hat{e}_{-\theta})^* \cdot (HG_{-\theta} \hat{e}_{\theta} + HG_{\theta} \hat{e}_{-\theta}) = 2 \quad (1)$$

so we have proof that the set $\{\Psi_{\theta}^1, \Psi_{\theta}^2\}$ forms indeed an ONB, up to a scalar multiplication. And now, how the rotations group action under the \mathbb{R}^2 polarized vector space, leaves invariant to one Ψ_{θ}^1 , the another element of the basis must remain the same. And therefore, Ψ_{θ}^2 is leaved invariant under rotations.

Stokes Parameters

Lets compute the first Stoke parameter

$$S_1 = \frac{I_H - I_V}{I_{tot}}$$

Where $I_j = \sum_k \left| \hat{e}_j^* \int \phi_k^* \psi dr^2 \right|$

Considering the state

$$\psi = HG_{\theta} \hat{e}_{\theta} + HG_{-\theta} \hat{e}_{-\theta} = HG_{\theta}(\cos \theta \hat{e}_H + \sin \theta \hat{e}_V) + HG_{-\theta}(-\sin \theta \hat{e}_H + \cos \theta \hat{e}_V) \quad (2)$$

Invariant under rotations

$$\psi = HG_{\theta} \hat{e}_{-\theta} + HG_{-\theta} \hat{e}_{\theta} = HG_{\theta}(-\sin \theta \hat{e}_H + \cos \theta \hat{e}_V) + HG_{-\theta}(\cos \theta \hat{e}_H + \sin \theta \hat{e}_V) \quad (3)$$

Let's compute I_H with eq.8

$$\begin{aligned} I_H &= \sum_k \left| \hat{e}_H \cdot \int \phi^*(r) (HG_{\theta}(\cos \theta \hat{e}_H + \sin \theta \hat{e}_V) + HG_{-\theta}(-\sin \theta \hat{e}_H + \cos \theta \hat{e}_V)) dr^2 \right|^2 \\ &= \sum_k \left| \int \phi^*(r) (HG_{\theta} \cos \theta - HG_{-\theta} \sin \theta) dr^2 \right|^2 \end{aligned}$$

Now considering I_V with eq.8

$$\begin{aligned} I_V &= \sum_k \left| \hat{e}_V \cdot \int \phi_k^* (HG_{\theta}(\cos \theta \hat{e}_H + \sin \theta \hat{e}_V) + HG_{-\theta}(-\sin \theta \hat{e}_H + \cos \theta \hat{e}_V)) dr^2 \right|^2 \\ &= \sum_k \left| \int \phi_k^* (HG_{\theta} \sin \theta + HG_{-\theta} \cos \theta) dr^2 \right|^2 \end{aligned}$$

For very large areas ($r^2 dr d\theta$) we are integrating over all the space, so the change of variables $\theta \rightarrow -\theta$ compute the same integral

$$I_H = \sum_k \left| \int \phi_k^* (HG_{-\theta} \sin(-\theta) + HG \cos(-\theta)) dr^2 \right|^2$$

and then

$$I_H = I_V \rightarrow S_1 = 0$$

By considering the $\{\hat{e}_\theta, \hat{e}_{-\theta}\}$ basis and eq.8

$$\begin{aligned} I_\theta &= \sum_k \left| \hat{e}_\theta \cdot \int \phi_k^* (HG_\theta \hat{e}_\theta + HG_{-\theta} \hat{e}_{-\theta}) dr^2 \right|^2 \\ &= \sum_k \left| \hat{e}_\theta \cdot \int \phi_k^* HG_\theta dr^2 \right|^2 \end{aligned}$$

Now I_θ and eq.9

$$\begin{aligned} I_{-\theta} &= \sum_k \left| \hat{e}_{-\theta} \int \phi_k^* (HG_\theta \hat{e}_{-\theta} + HG_{-\theta} \hat{e}_\theta) dr^2 \right| \\ &= \sum_k \left| \int \phi_k^* HG_\theta dr^2 \right| \end{aligned}$$

and then

$$I_\theta = I_{-\theta} \rightarrow S_3 = 0$$