QNat - Analytical Solutions for the Hackathon
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Alberto Bezerra de Palhares Junior

Joab Morais Varela

Moisés da Rocha Alves

Paulo Vitor de Queiroz Ferreira

Tailan Santos Sarubi

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Abstract

This document presents the analytical solutions developed by the QNat group for the hackathon held during the Second Quantum Computing School organized by ICTP-SAIFR.

Contents

1. Bose-Einstein Condensates and the Involvement in Advances for New Technologies

> **Exercise 1: Interactions between atoms and the low-energy limit**
>
> In cold atomic clouds, it is possible to have particle separations which are one order of magnitude larger than the length scale associated with atom-atom interactions. Consequently, two-body interactions are much more relevant than higher-body interactions. Moreover, the very low temperatures (and other relevant energy scales) achieved in these systems justify employing low-energy scattering theory.
>
> In this first exercise, we will focus on two particles of mass m interacting via a two-body potential $U(r)$ of **finite** range R. Their energy in the center-of-mass frame is given by
>
> $$E = \frac{\hbar^2 k^2}{2m_r} = \frac{\hbar^2 k^2}{m},$$
>
> where m_r is the reduced mass. We may compute the angular momentum of the pair, and associate a quantum number ℓ to it.
>
> (a) What is the low-energy limit in terms of k and R? Why is the $\ell = 0$ component the most relevant one in low-energy scattering theory (the so-called s-wave scattering)?
>
> (b) What is the s-wave scattering length? Explain in one or two sentences!
>
> (c) To first order in the interaction (Born approximation), the scattering length is given by:
>
> $$a = \frac{m_r}{2\pi\hbar^2} \int d^3r\, U(\mathbf{r}).$$
>
> This is a very interesting result because it shows us that potentials with different shapes produce the same scattering length as long as their volumetric integral is the same. Use this result to create a two-body potential with scattering length a of the form:
>
> $$U_{\text{eff}}(\mathbf{r}, \mathbf{r}') = U_0 \delta(\mathbf{r} - \mathbf{r}'),$$
>
> where the two particles are situated at $\mathbf{r}$ and $\mathbf{r}'$, and U_0 is a constant you have to calculate. The potential in Eq. (7) is called a contact interaction since the potential is non-zero only if the two particles are at the same position. It presents a much simpler alternative to the true interatomic potentials (which can be quite complicated) and retains the relevant physical information.

Solution:
Author: Moisés da Rocha Alves

(a) The energy of the particles is related to the wave number k by the equation:

$$E = \frac{\hbar^2 k^2}{2m_r} = \frac{\hbar^2 k^2}{m}, \tag{1.1}$$

which can also be written as:

$$E = \frac{\hbar^2}{m\lambdabar^2}, \tag{1.2}$$

where $\lambdabar = \lambda/2\pi$ is the reduced de Broglie wavelength.

In the low-energy scattering regime, we consider solutions where the reduced wavelength is much larger than the range of the potential. Thus, we are interested in situations where $\lambdabar \gg R$, which is equivalent to the condition $kR \ll 1$, noting that $\lambdabar = 1/k$. Therefore, the low-energy limit corresponds to $kR \ll 1$.

Now, the reason why the $\ell = 0$ component is the most relevant in low-energy scattering theory $(k \to 0)$ is primarily because of the centrifugal barrier. The effective potential for a partial wave with angular momentum ℓ in the context of scattering theory is given by:

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 \ell(\ell + 1)}{2mr^2}. \tag{1.3}$$

If the energy is close to zero, the second term of this potential creates a centrifugal barrier that prevents the wave function from penetrating the scattering region unless $\ell = 0$. As a result, in the low-energy regime, only the term with $\ell = 0$ becomes relevant, making the contributions from the partial waves with $\ell > 0$ negligible.

(b) The s-wave scattering length a can be interpreted as the range in which the interaction between the particles becomes significant. It can be mathematically defined as $\lim_{k \to 0} k \cot \delta_0(k) = -\frac{1}{a}$ in the context of low-energy scattering, and can also be an indication of whether the interaction is repulsive $a < 0$ or attractive $a > 0$.

(c) We can relate the two-body potential to the scattering length through the following derivation. Using the given two-body potential, we obtain the result:

$$a = \frac{m_r}{2\pi\hbar^2} \int d^3r \, U_0 \, \delta(\mathbf{r} - \mathbf{r}'). \tag{1.4}$$

Now, noticing that the Dirac delta is constrained to satisfy the identity:

$$\int d^3r \, \delta(\mathbf{r} - \mathbf{r}') = 1, \tag{1.5}$$

we can simplify this to find:

$$a = U_0 \frac{m_r}{2\pi\hbar^2}. \tag{1.6}$$

Therefore, we have

$$U_0 = a \frac{2\pi\hbar^2}{m_r}, \tag{1.7}$$

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which gives us the desired result for the two-body potential:

$$U_{\text{eff}}(\mathbf{r}, \mathbf{r}') = a\frac{2\pi\hbar^2}{m_r}\delta(\mathbf{r} - \mathbf{r}') = a\frac{4\pi\hbar^2}{m}\delta(\mathbf{r} - \mathbf{r}'). \tag{1.8}$$

Exercise 2: The Gross-Pitaevskii equation

In Quantum Mechanics courses, we learn that Schrödinger's equation is linear. So, how is it possible that the far-from-equilibrium Bose-Einstein condensates (BECs) presented by Prof. Emanuel Henn in his lecture display non-linear features? The answer is to consider BECs in the presence of interactions. Particularly, we will consider the Gross-Pitaevskii equation (GPE), which describes zero-temperature properties of BECs when the scattering length a is much less than the mean interparticle distance.

The many-body Hamiltonian for N interacting bosons is given by:

$$H = \sum_{i=1}^{N}\left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i)\right] + U_0\sum_{i<j}\delta(\mathbf{r}_i - \mathbf{r}_j),$$

where $V(\mathbf{r}_i)$ is an external (one-body) potential, and we have made use of the result from exercise 1(c), Eq. (7), to write the interparticle interactions.

We now adopt a mean-field (or Hartree) approach and assume that the wave function is a symmetrized product of single-particle wave functions. In the fully condensed state, all particles are in the same single-particle state $\phi(\mathbf{r})$; hence the many-body wave function is given by:

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \prod_{i=1}^{N}\phi(\mathbf{r}_i).$$

The single-particle wave function is normalized to the unit,

$$\int d^3r|\phi(\mathbf{r})|^2 = 1.$$

(a) Deduce the expression for the expectation value of the Hamiltonian of Eq. (8) in the state of Eq. (9).

(b) Alternatively, we can introduce the concept of the wave function of the condensate state, $\psi(\mathbf{r}) = N^{1/2}\phi(\mathbf{r})$. Neglecting terms of order $1/N$, the solutions of (a) becomes:

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

To find the optimal $\psi(\mathbf{r})$, we have to minimize Eq. (10) with the constraint of a constant number of particles $N = \int d^3r |\psi(\mathbf{r})|^2$. This can be done conveniently using Lagrange multipliers, $\delta E - \mu \delta N = 0$, where μ is the chemical potential.

Use this procedure and consider variations with respect to $\psi^*(\mathbf{r})$ to obtain the time-independent GPE.

You will see that it resembles the Schrödinger equation, but a non-linear term takes into account the mean field produced by the other particles. Another difference is that the eigenvalue is the chemical potential, not the energy per particle, as it is for the usual Schrödinger equation. The chemical potential is equal to the energy per particle for non-interacting particles (all in the same state), but for interacting particles, it is not.

(c) What is the GPE for a uniform Bose gas?

Solution:
Authors: Paulo Vitor de Queiroz Ferreira and Moisés da Rocha Alves

(a) We want to deduce the expectation value of the Hamiltonian given by the exercise, thus

$$\langle H \rangle = \langle H_0 \rangle + \langle U \rangle, \tag{1.9}$$

where $\langle H_0 \rangle$ and $\langle U \rangle$ are given by:

$$\langle H_0 \rangle = \left\langle \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right] \right\rangle,$$

$$\langle U \rangle = \left\langle U_0 \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j) \right\rangle.$$

First, we calculate the expectation value of $\langle H_0 \rangle$. Using the mean-field approximation, we can express the expectation value in terms of the expectation value of just one particle, multiplied by the N particles that reside in the same state. Consequently, the expectation value of the Hamiltonian $\langle H_0 \rangle$ can be expressed as follows:

$$\langle H_0 \rangle = \int \Psi^*(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i) \right] \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) d^3r_1 \, d^3r_2 \, \ldots \, d^3r_N, \tag{1.10}$$

which simplifies to:

$$\langle H_0 \rangle = \frac{-N\hbar^2}{2m} \int \phi^*(\mathbf{r}) \nabla^2 \phi(\mathbf{r}) \, d^3r + N \int \phi^*(\mathbf{r}) V(\mathbf{r}) \phi(\mathbf{r}) \, d^3r. \tag{1.11}$$

We are first interested in solving the integral on the left side of the above equation. To this end, we utilize the following property:

$$\nabla \cdot (\phi^*(\mathbf{r})\nabla\phi(\mathbf{r})) = \nabla\phi^*(\mathbf{r}) \cdot \nabla\phi(\mathbf{r}) + \phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r}),$$
$$-\phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r}) = \nabla\phi^*(\mathbf{r}) \cdot \nabla\phi(\mathbf{r}) - \nabla \cdot (\phi^*(\mathbf{r})\nabla\phi(\mathbf{r})). \tag{1.12}$$

By integrating over the entire space on both sides of the above equation, we obtain:

$$-\int \phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r})d^3r = \int \nabla\phi^*(\mathbf{r}) \cdot \nabla\phi(\mathbf{r})d^3r - \int \nabla \cdot (\phi^*(\mathbf{r})\nabla\phi(\mathbf{r}))d^3r. \tag{1.13}$$

Using Gauss's theorem,

$$\int_v \nabla \cdot \mathbf{A}d\tau = \oint_s \mathbf{A} \cdot d\mathbf{S}, \tag{1.14}$$

we will obtain

$$-\int \phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r})d^3r = \int |\nabla\phi(\mathbf{r})|^2 d^3r - \oint_s \phi^*(\mathbf{r})\nabla\phi(\mathbf{r}) \cdot d\mathbf{S}. \tag{1.15}$$

By imposing a localization condition for the function $\phi(\mathbf{r})$, i.e., it decays rapidly at infinity, the second term on the right-hand side of the equation vanishes and we get

$$-\int \phi^*(\mathbf{r})\nabla^2\phi(\mathbf{r})d^3r = \int |\nabla\phi(\mathbf{r})|^2 d^3r, \tag{1.16}$$

giving us the desired result

$$\langle H_0 \rangle = \frac{N\hbar^2}{2m}\int |\nabla\phi(\mathbf{r})|^2 d^3r + N\int V(\mathbf{r})|\phi(\mathbf{r})|^2 d^3r. \tag{1.17}$$

Now, we need to calculate the expectation value $\langle U \rangle$. Thus,

$$\langle U \rangle = U_0 \sum_{i<j}^{N} \langle \delta(\mathbf{r}_i - \mathbf{r}_j) \rangle$$
$$= U_0 \sum_{i<j}^{N} \int \Psi^*(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)\delta(\mathbf{r}_i - \mathbf{r}_j)\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)d^3r_1 \ldots d^3r_N. \tag{1.18}$$

Using mean-field approximation, we get

$$\langle U \rangle = U_0 \sum_{i<j}^{N} \int \prod_{k=1}^{N} |\phi(\mathbf{r}_k)|^2 \delta(\mathbf{r}_i - \mathbf{r}_j)d^3r_1 \ldots d^3r_N, \tag{1.19}$$

and since $\int d^3r_k|\phi(\mathbf{r}_k)|^2 = 1$, we will obtain,

$$\langle U \rangle = U_0 \sum_{i<j}^{N} \int d^3r_i d^3r_j |\phi(\mathbf{r}_i)|^2 |\phi(\mathbf{r}_j)|^2 \delta(\mathbf{r}_i - \mathbf{r}_j). \tag{1.20}$$

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Using the filtering property of the Dirac delta function,

$$\langle U \rangle = U_0 \sum_{i<j}^{N} \int d^3 r_i |\phi(\mathbf{r}_i)|^4. \tag{1.21}$$

Since the summation gives $\binom{N}{2}$ terms, we use the binomial coefficient to compute the combinations of pairs in the summation, such that:

$$\binom{N}{2} = \frac{N!}{2!(N-2)!} = \frac{N(N-1)(N-2)!}{2(N-2)!} = \frac{N(N-1)}{2}. \tag{1.22}$$

Therefore, the result for $\langle U \rangle$ is

$$\langle U \rangle = U_0 \frac{N(N-1)}{2} \int d^3 r |\phi(\mathbf{r})|^4. \tag{1.23}$$

Thus, the expected value of the Hamiltonian has the following form

$$\langle H \rangle = \frac{N\hbar^2}{2m} \int |\nabla \phi(\mathbf{r})|^2 d^3 r + N \int V(\mathbf{r})|\phi(\mathbf{r})|^2 d^3 r + U_0 \frac{N(N-1)}{2} \int d^3 r |\phi(\mathbf{r})|^4. \tag{1.24}$$

If we use the wave function of the condensate state, $\psi(\mathbf{r}) = N^{1/2}\phi(\mathbf{r})$ and neglect the term of order $1/N$, the solution becomes the equation given in (b),

$$\langle H \rangle = \int d^3 r \left[\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{1}{2} U_0 |\psi(\mathbf{r})|^4 \right]. \tag{1.25}$$

(b) We aim to minimize the function $E(\psi)$, which depends on the wave function $\psi(\mathbf{r})$, while imposing the constraint on the number of particles $N = \int d^3 r |\psi(\mathbf{r})|^2$, which must remain constant. To do this, we will use the method of Lagrange multipliers,

$$\delta E - \mu \delta N = 0, \tag{1.26}$$

where μ is the Lagrange multiplier, which in this context corresponds to the chemical potential.

Now we create a new energy function that takes into account the constraint on the number of particles.

$$f(\psi) = E(\psi) - \mu \left(\int d^3 r |\psi(\mathbf{r})|^2 - N \right), \tag{1.27}$$

which can be written as

$$f(\psi) = \int d^3 r \left[\frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2 + V(\mathbf{r})|\psi(\mathbf{r})|^2 + \frac{1}{2} U_0 |\psi(\mathbf{r})|^4 - \mu |\psi(\mathbf{r})|^2 \right]. \tag{1.28}$$

We can ignore the term $+\mu N$, since this term in the new function $f(\psi)$ will not affect the result when we perform the minimization. By minimizing the new function $f(\psi)$, we will not only be minimizing the energy $E(\psi)$, but also ensuring that the wave function $\psi(\mathbf{r})$ remains normalized with the particle number N.

The next step for our solution is to perform the minimization, which consists of deriving the function $f(\psi)$ with respect to the term we want to minimize and setting it to zero. In this case, the term we will vary is $\psi^*(\mathbf{r})$.

$$\frac{\partial f(\psi)}{\partial \psi^*(\mathbf{r})} = 0 \tag{1.29}$$

To make the solution clearer throughout the calculations, we will take each part of the function $f(\psi)$ individually.

Starting with the kinetic part of our function, $K = \int d^3 r \frac{\hbar^2}{2m} |\nabla \psi(\mathbf{r})|^2$:

$$\frac{\partial K}{\partial \psi^*(\mathbf{r})} = \frac{\partial}{\partial \psi^*(\mathbf{r})} \left\{ \int d^3 r' \frac{\hbar^2}{2m} \nabla \psi^*(\mathbf{r}') \cdot \nabla \psi(\mathbf{r}') \right\}. \tag{1.30}$$

We will use the result of equation Eq. (1.16) to simplify our calculations. Since it is the same wave function, it must satisfy the same boundary conditions.

$$\begin{aligned}
\frac{\partial K}{\partial \psi^*(\mathbf{r})} &= \frac{\partial}{\partial \psi^*(\mathbf{r})} \left\{ -\int d^3 r' \frac{\hbar^2}{2m} \psi^*(\mathbf{r}') \nabla^2 \psi(\mathbf{r}') \right\} \\
&= \left\{ -\int d^3 r' \frac{\hbar^2}{2m} \frac{\partial \psi^*(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \nabla^2 \psi(\mathbf{r}') + \psi^*(\mathbf{r}') \frac{\partial}{\partial \psi^*(\mathbf{r})} \left(\nabla^2 \psi(\mathbf{r}') \right) \right\}.
\end{aligned} \tag{1.31}$$

The second term that arises from the product rule is zero, since the function does not depend on $\psi^*(\mathbf{r})$. The term $\frac{\partial \psi^*(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} = \delta(\mathbf{r}' - \mathbf{r})$ arises because we are differentiating with respect to $\psi^*(\mathbf{r})$, and we need the evaluated point $\mathbf{r}'$ to coincide with $\mathbf{r}$.

$$\frac{\partial K}{\partial \psi^*(\mathbf{r})} = -\int d^3 r' \frac{\hbar^2}{2m} \delta(\mathbf{r}' - \mathbf{r}) \nabla^2 \psi(\mathbf{r}'). \tag{1.32}$$

Considering the delta function's filtering property, we finally obtain the kinetic part of our equation:

$$\frac{\partial K}{\partial \psi^*(\mathbf{r})} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}). \tag{1.33}$$

Moving to the external potential term, $P = \int d^3 r V(\mathbf{r}) |\psi(\mathbf{r})|^2$, we want to calculate $\frac{\partial P}{\partial \psi^*(\mathbf{r})}$. Thus,

$$\frac{\partial P}{\partial \psi^*(\mathbf{r})} = \frac{\partial}{\partial \psi^*(\mathbf{r})} \left[\int d^3r' V(\mathbf{r}') \psi^*(\mathbf{r}') \psi(\mathbf{r}') \right]$$

$$= \int d^3r' V(\mathbf{r}') \left[\frac{\partial \psi^*(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \psi(\mathbf{r}') + \psi^*(\mathbf{r}') \frac{\partial \psi(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \right] \qquad (1.34)$$

$$= \int d^3r' V(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}) \psi(\mathbf{r}')$$

$$= V(\mathbf{r}) \psi(\mathbf{r}).$$

The penultimate term from Eq. (1.28) corresponds to the interaction potential, $I = \int d^3r \frac{1}{2} U_0 |\psi(\mathbf{r})|^4$, and we want to find $\frac{\partial I}{\partial \psi^*(\mathbf{r})}$. Therefore,

$$\frac{\partial I}{\partial \psi^*(\mathbf{r})} = \frac{\partial}{\partial \psi^*(\mathbf{r})} \left[\int d^3r' \frac{1}{2} U_0 \left(\psi^*(\mathbf{r}') \psi(\mathbf{r}') \right)^2 \right]$$

$$= \int d^3r' \frac{1}{2} U_0 \left(2\psi^*(\mathbf{r}') \frac{\partial \psi^*(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \psi(\mathbf{r}')^2 + \psi^*(\mathbf{r}')^2 \frac{\partial \psi(\mathbf{r}')^2}{\partial \psi^*(\mathbf{r})} \right)$$

$$= \int d^3r' \frac{1}{2} U_0 \left(2\psi^*(\mathbf{r}') \delta(\mathbf{r}' - \mathbf{r}) \psi(\mathbf{r}')^2 \right) \qquad (1.35)$$

$$= \frac{1}{2} U_0 2\psi^*(\mathbf{r}) \psi(\mathbf{r})^2$$

$$= U_0 |\psi(\mathbf{r})|^2 \psi(\mathbf{r}).$$

Lastly, for the term containing the constraint, $\Lambda = -\mu |\psi(\mathbf{r})|^2$, we need to find $\frac{\partial \Lambda}{\partial \psi^*(\mathbf{r})} = \frac{\partial \Lambda}{\partial \psi^*(\mathbf{r})}$, giving us:

$$\frac{\partial \Lambda}{\partial \psi^*(\mathbf{r})} = \frac{\partial}{\partial \psi^*(\mathbf{r})} \left[\int d^3r' \mu \psi^*(\mathbf{r}') \psi(\mathbf{r}') \right]$$

$$= \int d^3r' \mu \left[\frac{\partial \psi^*(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \psi(\mathbf{r}') + \psi^*(\mathbf{r}') \frac{\partial \psi(\mathbf{r}')}{\partial \psi^*(\mathbf{r})} \right] \qquad (1.36)$$

$$= \mu \psi(\mathbf{r}).$$

Combining everything into a single minimization equation, we have:

$$\frac{\partial f(\psi)}{\partial \psi^*(\mathbf{r})} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) + U_0 |\psi(\mathbf{r})|^2 \psi(\mathbf{r}) - \mu \psi(\mathbf{r}) = 0, \qquad (1.37)$$

or, written in a more convenient form,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + U_0 |\psi(\mathbf{r})|^2 \right] \psi(\mathbf{r}) = \mu \psi(\mathbf{r}). \qquad (1.38)$$

Thus, the Gross-Pitaevskii Equation (GPE) obtained has the chemical potential as its eigenvalue, as indicated in the statement.

(c) A uniform Bose gas refers to a system where the gas has no external potential acting on it and is uniformly distributed throughout space. The Hamiltonian for such a system corresponds to the one studied in the previous sections, but now disregarding the external potential term. This results in a simplified Hamiltonian as follows:

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\nabla_i^2 + U_0 \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j). \tag{1.39}$$

We will proceed with a similar treatment to what was done in the previous sections. First, we are interested in the expectation value of this Hamiltonian:

$$\langle H \rangle = \left\langle -\frac{\hbar^2}{2m}\nabla_i^2 + U_0 \sum_{i<j} \delta(\mathbf{r}_i - \mathbf{r}_j) \right\rangle. \tag{1.40}$$

If we compare this to the result from section (a), we can simply ignore the external potential term, and we will have the corresponding expectation value, which is given by:

$$\langle H \rangle = \int d^3r \left[\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r},t)|^2 + \frac{1}{2}U_0|\psi(\mathbf{r},t)|^4 \right]. \tag{1.41}$$

From this, we can derive the GPE using the variational principle, as was done in section (b). Let's take a step back and look at the action. The action is the fundamental object in the variational principle and is given by the integral of the Lagrangian over time:

$$\mathbf{S}(\psi, \psi^*) = \int dt \mathcal{L}(\psi, \psi^*), \tag{1.42}$$

where, for quantum systems, the Lagrangian is given by

$$\mathcal{L}(\psi, \psi^*) = \int d^3r \left(i\hbar\psi^*(\mathbf{r},t)\frac{\partial\psi(\mathbf{r},t)}{\partial t} - \mathcal{H}(\psi, \psi^*) \right), \tag{1.43}$$

where,

$$\mathcal{H}(\psi, \psi^*) = \left[\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r},t)|^2 + \frac{1}{2}U_0|\psi(\mathbf{r},t)|^4 \right]. \tag{1.44}$$

Now, we apply the derivative of the action with respect to $\psi^*(\mathbf{r}, t)$, such that:

$$\frac{\delta\mathbf{S}(\psi, \psi^*)}{\delta\psi^*(\mathbf{r},t)} = 0. \tag{1.45}$$

We only need to calculate the variation in the first term of the action, as the other derivatives have already been obtained in section (b),

$$\frac{\partial}{\partial\psi^*(\mathbf{r},t)} \left(i\hbar\psi^*(\mathbf{r},t)\frac{\partial\psi(\mathbf{r},t)}{\partial t} \right) = i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}. \tag{1.46}$$

Combining it with the results obtained in Eq. (1.33) and Eq. (1.35), we can write the action minimization as:

$$\frac{\delta \mathbf{S}(\psi, \psi^*)}{\delta \psi^*(\mathbf{r}, t)} = 0,$$

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} + \left(\frac{\hbar^2}{2m} \nabla^2 - U_0 |\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t) = 0, \qquad (1.47)$$

$$i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t} = - \left(\frac{\hbar^2}{2m} \nabla^2 + U_0 |\psi(\mathbf{r}, t)|^2 \right) \psi(\mathbf{r}, t),$$

such that this corresponds to our GPE for a uniform Bose gas. We can consider a stationary solution, assuming a wave function of the form:

$$\psi(\mathbf{r}, t) = \psi_0(\mathbf{r}) e^{-i\mu t/\hbar}. \qquad (1.48)$$

In this case, μ corresponds to the chemical potential, which indicates the conservation of the number of particles. Applying this wave function directly into equation Eq. (1.47), we obtain:

$$\mu \psi_0(\mathbf{r}) = \left(\frac{\hbar^2}{2m} \nabla^2 + U_0 |\psi_0(\mathbf{r})|^2 \right) \psi_0(\mathbf{r}). \qquad (1.49)$$

Considering a uniform Bose gas, the condensate density is the same everywhere, and therefore $\nabla^2 \psi_0(\mathbf{r}) = 0$. This simplifies the time-independent GPE to:

$$\mu = U_0 |\psi_0(\mathbf{r})|^2. \qquad (1.50)$$

This tells us that the chemical potential in the case of a uniform condensate is proportional to the condensate density $|\psi_0(\mathbf{r})|^2$.

2. Prospects and Challenges for Quantum Machine Learning

Exercise 1

Let $V = \mathbb{C}_2$ be the Hilbert space of a single qubit. Then, consider the set of objects $\{\mathbb{1}, X\}$, where $\mathbb{1}$ is the 2×2 identity matrix and X the Pauli-x matrix. Show that these objects, which represent bit-flips, form a group.

Solution:
Authors: Tailan Santos Sarubi and Moisés da Rocha Alves

In this exercise, we need to prove that $\{\mathbb{1}, X\}$ forms a group under matrix multiplication. Before getting into our solution, we need to state what a group is.

Definition 2.1. A *group* is a non-empty set G equipped with a binary operation $* : G \times G \to G$ satisfying the following axioms:

- (i) Closure: if $a, b \in G$, then $a * b \in G$.

- (ii) Associativity: $a * (b * c) = (a * b) * c$ for all $a, b, c \in G$.

- (iii) Identity: there is an element $e \in G$, such that $a * e = e * a = a$ for all $a \in G$.

- (iv) Inverse: for each element $a \in G$, there is an element $b \in G$ such that $a * b = e = b * a$.

First, we will prove that $\{\mathbb{1}, X\}$ satisfies the closure axiom. One can verify that the following expressions hold,

$$\mathbb{1}\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \quad (2.1) \qquad X\mathbb{1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X \quad (2.3)$$

$$\mathbb{1}X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = X \quad (2.2) \qquad XX = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbb{1} \quad (2.4)$$

and, therefore, the closure axiom is satisfied.

Using the same expressions, one can verify that the identity and inverse axioms are also satisfied. The identity axiom follows from Eq. (2.1), Eq. (2.2) and Eq. (2.3), where $\mathbb{1} \in \{\mathbb{1}, X\}$ is the neutral element of the group. The inverse axiom is satisfied by Eq. (2.1) and Eq. (2.4), with $\mathbb{1}$ and X being their own inverses.

And last but not least, we can see, using all the equations above, that the following expressions are also true:

$$\mathbb{1}(\mathbb{1}\mathbb{1}) = (\mathbb{1}\mathbb{1})\mathbb{1} = \mathbb{1} \qquad (2.5)$$

$$\mathbb{1}(\mathbb{1}X) = (\mathbb{1}\mathbb{1})X = X \qquad (2.6)$$

$$\mathbb{1}(X\mathbb{1}) = (\mathbb{1}X)\mathbb{1} = X \qquad (2.7)$$

$$X(\mathbb{1}\mathbb{1}) = (X\mathbb{1})\mathbb{1} = X \qquad (2.8)$$

$$\mathbb{1}(XX) = (\mathbb{1}X)X = \mathbb{1} \qquad (2.9)$$

$$X(X\mathbb{1}) = (XX)\mathbb{1} = \mathbb{1} \qquad (2.10)$$

$$X(\mathbb{1}X) = (X\mathbb{1})X = \mathbb{1} \qquad (2.11)$$

$$X(XX) = (XX)X = X \qquad (2.12)$$

Therefore, we have proven that $\{\mathbb{1}, X\}$ satisfies the associativity axiom.

If $\{\mathbb{1}, X\}$ satisfies all the axioms stated in Definition 2.1, then it forms a group under matrix multiplication, as we have shown.

Exercise 2

Prove 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 $SU(2)$.

Solution:
Author: Tailan Santos Sarubi

The unitary Lie group $SU(2)$ consists of all unitary 2×2 matrices with determinant 1. First of all, let's prove that U is unitary and has determinant equals to 1.

A matrix is unitary if and only if $U^\dagger U = \mathbb{1}$, therefore

$$U^\dagger U = e^{i\phi_1 Y} e^{i\phi_2 X} e^{i\phi_3 Y} e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y} = \mathbb{1},$$

which proves the unitarity of U. For the determinant, we can use the property $\det\left(e^A\right) = e^{\operatorname{tr}(A)}$. Therefore, using the determinant product rule,

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

and noticing that all Pauli matrices have zero trace:

$$\det U = e^{-i\phi_3 \operatorname{tr}(Y)} e^{-i\phi_2 \operatorname{tr}(X)} e^{-i\phi_1 \operatorname{tr}(Y)} = 1,$$

as we wanted.

The next step is to show that U can represent all matrices of $SU(2)$. A generic element of $SU(2)$ can be expressed as:

$$U = \begin{pmatrix} a & -b^* \\ b & a^* \end{pmatrix}, \quad \text{with} \quad |a|^2 + |b|^2 = 1, \qquad (2.13)$$

where a and b are complex numbers. This condition ensures that U is unitary and has determinant 1.

For the element U given in the statement, X and Y are the generators of the Lie algebra of $SU(2)$. These generators represent the rotation operators around the x- and y-axes. Explicitly, we have:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

These operators satisfy the commutation relations of the Lie algebra of $SU(2)$:

$$[X, Y] = 2iZ, \quad [Y, Z] = 2iX, \quad [Z, X] = 2iY,$$

where Z is the generator around the z-axis, given by:

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We can interpret the expression $U = e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y}$ as a sequence of rotations. These are exactly the Euler rotations used to parametrize elements of the group $SU(2)$. Therefore, the given expression for U is consistent with the expected structure for elements of $SU(2)$:

$$U = R_y(2\Phi_3) R_x(2\Phi_2) R_y(2\Phi_1).$$

The rotation matrices associated with the generators X and Y are:

$$e^{-i\phi Y} = \cos\left(\frac{\phi}{2}\right) \mathbb{1} - i \sin\left(\frac{\phi}{2}\right) Y = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) & -\sin\left(\frac{\phi}{2}\right) \\ \sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) \end{pmatrix},$$

and

$$e^{-i\phi X} = \cos\left(\frac{\phi}{2}\right) \mathbb{1} - i \sin\left(\frac{\phi}{2}\right) X = \begin{pmatrix} \cos\left(\frac{\phi}{2}\right) & -i\sin\left(\frac{\phi}{2}\right) \\ -i\sin\left(\frac{\phi}{2}\right) & \cos\left(\frac{\phi}{2}\right) \end{pmatrix}.$$

We will now multiply these matrices in the order $e^{-i\phi_3 Y} e^{-i\phi_2 X} e^{-i\phi_1 Y}$. Multiplying $e^{-i\phi_2 X}$ and $e^{-i\phi_1 Y}$:

$$e^{-i\phi_2 X} e^{-i\phi_1 Y} = \begin{pmatrix} \cos\left(\frac{\phi_2}{2}\right) & -i\sin\left(\frac{\phi_2}{2}\right) \\ -i\sin\left(\frac{\phi_2}{2}\right) & \cos\left(\frac{\phi_2}{2}\right) \end{pmatrix} \begin{pmatrix} \cos\left(\frac{\phi_1}{2}\right) & -\sin\left(\frac{\phi_1}{2}\right) \\ \sin\left(\frac{\phi_1}{2}\right) & \cos\left(\frac{\phi_1}{2}\right) \end{pmatrix}$$

Performing the multiplication gives:

$$e^{-i\phi_2 X} e^{-i\phi_1 Y} = \begin{pmatrix} \cos\left(\frac{\phi_1}{2}\right)\cos\left(\frac{\phi_2}{2}\right) - i\sin\left(\frac{\phi_1}{2}\right)\sin\left(\frac{\phi_2}{2}\right) & -\sin\left(\frac{\phi_1}{2}\right)\cos\left(\frac{\phi_2}{2}\right) - i\cos\left(\frac{\phi_1}{2}\right)\sin\left(\frac{\phi_2}{2}\right) \\ \sin\left(\frac{\phi_1}{2}\right)\cos\left(\frac{\phi_2}{2}\right) - i\cos\left(\frac{\phi_1}{2}\right)\sin\left(\frac{\phi_2}{2}\right) & \cos\left(\frac{\phi_1}{2}\right)\cos\left(\frac{\phi_2}{2}\right) + i\sin\left(\frac{\phi_1}{2}\right)\sin\left(\frac{\phi_2}{2}\right) \end{pmatrix}.$$

Now, if we multiply this result for $e^{-i\phi_3 Y}$, we will get as a final result, after some simplification:

$$U = \begin{pmatrix} -i\sin\left(\frac{\phi_2}{2}\right)\sin\left(\frac{\phi_1+\phi_3}{2}\right) + \cos\left(\frac{\phi_2}{2}\right)\cos\left(\frac{\phi_1+\phi_3}{2}\right) & -i\sin\left(\frac{\phi_2}{2}\right)\cos\left(\frac{\phi_1+\phi_3}{2}\right) - \sin\left(\frac{\phi_1+\phi_3}{2}\right)\cos\left(\frac{\phi_2}{2}\right) \\ -i\sin\left(\frac{\phi_2}{2}\right)\cos\left(\frac{\phi_1+\phi_3}{2}\right) + \sin\left(\frac{\phi_1+\phi_3}{2}\right)\cos\left(\frac{\phi_2}{2}\right) & i\sin\left(\frac{\phi_2}{2}\right)\sin\left(\frac{\phi_1+\phi_3}{2}\right) + \cos\left(\frac{\phi_2}{2}\right)\cos\left(\frac{\phi_1+\phi_3}{2}\right) \end{pmatrix},$$

where we can identify in Eq. (2.13):

$$a = -i \sin\left(\frac{\phi_2}{2}\right) \sin\left(\frac{\phi_1 + \phi_3}{2}\right) + \cos\left(\frac{\phi_2}{2}\right) \cos\left(\frac{\phi_1 + \phi_3}{2}\right), \qquad (2.14)$$

and

$$b = -i \sin\left(\frac{\phi_2}{2}\right) \cos\left(\frac{\phi_1 + \phi_3}{2}\right) + \sin\left(\frac{\phi_1 + \phi_3}{2}\right) \cos\left(\frac{\phi_2}{2}\right), \qquad (2.15)$$

which are parametrized by (ϕ_1, ϕ_2, ϕ_3), and thus representing all $SU(2)$ matrices.

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

Solution:
Author: Moisés da Rocha Alves

First of all, we need to describe the exact definition of the commutant $C(k)(G)$, as stated in the lecture notes.

Definition 2.2. Given some representation R of G, we define 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,

$$\mathcal{C}^{(k)}(G) = \{A \in \mathcal{B}(\mathcal{H}^{\otimes k}) \mid [A, R(g)^{\otimes k}] = 0, \ \forall g \in G\}. \qquad (2.16)$$

As already stated in Eq. 9 of the lecture notes, notice that if $R(g)^{\otimes k}$ is a completely reducible representation, then it can be described as having a block diagonal structure of irreducible representations as

$$R(g)^{\otimes k} \simeq \bigoplus_\lambda \mathbb{1}_{m_\lambda} \otimes R_\lambda(g) \quad \text{for all } g \in G, \qquad (2.17)$$

where λ labels the irreducible representations, and m_λ is the multiplicity factor (which indicates how many times the irreducible representations appear in the block diagonal structure).

As also stated in Eq. 17 of the lecture notes, the operator A, described in Definition 2.2, must be written as

$$A \simeq \bigoplus_\lambda A_\lambda \otimes \mathbb{1}_{d_\lambda} \qquad (2.18)$$

in order to commute with $R(g)^{\otimes k}$, where A_λ is an arbitrary $m_\lambda \times m_\lambda$ matrix, and $d_\lambda = \dim(R_\lambda)$.

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With all these definitions set, notice that the Hilbert space can then be described by

$$\mathcal{H}^{\otimes k} = \bigoplus_\lambda \mathbb{C}^{m_\lambda} \otimes \mathbb{C}^{d_\lambda}, \tag{2.19}$$

where $\mathbb{C}^{m_\lambda}$ is the multiplicity space, and $\mathbb{C}^{d_\lambda}$ is the space where the irreducible representation R_λ acts.

Using Schur's lemma, notice that A can only act in the multiplicity space in order to commute with $R(g)^{\otimes k}$, as the latter has a block diagonal structure, and thus A must have the structure of Eq. (2.18) as a direct consequence of Schur's lemma. In this case, the dimension of the commutant $\mathcal{C}^{(k)}(G)$ is related to the degrees of freedom of all A_λ matrices that appear in Eq. (2.18).

Since A_λ is an arbitrary $m_\lambda \times m_\lambda$ matrix and can act freely in the multiplicity space, it will have m_λ^2 entries. Thus, the dimension D of the commutant is simply the sum of all contributions from the A_λ matrices, or

$$D = \sum_\lambda m_\lambda^2, \tag{2.20}$$

as we wanted.

3. High Dimensional Quantum Communication with Structured Light

> **Exercise 1**
>
> Let $HG_\theta(x, y)$ be the first order Hermite-Gauss mode rotated counter-clockwise by θ. Show that:
>
> - $HG_\theta(x, y) = \cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y)$
>
> - $\int HG_\theta^*(x, y)HG_\theta(x, y)\, dx\, dy = 1$
>
> - $\int HG_\theta^*(x, y)HG_{\theta+\pi/2}(x, y)\, dx\, dy = 0$
>
> - $LG_\pm(r, \phi) = \frac{1}{\sqrt{2}}\left[HG_{10}(x, y) \pm iHG_{01}(x, y)\right]$

Solution:
Author: Moisés da Rocha Alves

Before answering the exercise, it is necessary to define the Hermite-Gaussian modes mathematically. The Hermite-Gaussian modes are defined as follows:

$$HG_{mn}(x, y) = \frac{A_{mn}}{w(z)} H_m\left(\frac{\sqrt{2}x}{w(z)}\right) H_n\left(\frac{\sqrt{2}y}{w(z)}\right) \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)}, \tag{3.1}$$

where A_{mn} is a normalization constant, H_m and H_n are the Hermite polynomials of orders m and n, respectively, $w(z)$ is the beam waist as a function of the propagation distance z, $R(z)$ is the radius of curvature of the beam's wavefront and $\phi_N(z) = (N + 1)\arctan(z/z_R)$ is the Gouy phase, where $N = m + n$. The Hermite-Gaussian modes also obey the following property,

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} HG_{mn}(x, y)HG_{m'n'}^*(x, y)\, dx\, dy = \delta_{mm'}\delta_{nn'}, \tag{3.2}$$

which makes them an orthonormal set of functions. This relation is guaranteed by the orthonormality condition of the Hermite polynomials, and the normalization constant A_{mn} ensures that this condition is properly maintained.

Since we are dealing with first order Hermite-Gauss modes, we can describe them following the definition of Eq. (3.1). Since $H_1(x) = 2x$ and $H_0(x) = 1$, for the first-order mode in the x-direction:

$$HG_{10}(x, y) = \frac{A_{10}}{w(z)} \cdot \frac{2\sqrt{2}x}{w(z)} \cdot \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)}. \tag{3.3}$$

Following the same argument, for the first-order mode in the y-direction:

$$HG_{01}(x, y) = \frac{A_{01}}{w(z)} \cdot \frac{2\sqrt{2}y}{w(z)} \cdot \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)}. \tag{3.4}$$

Now, let's prove the first property stated in the exercise. Following the result of Eq. (3.3), we want to rotate it counter-clockwise. Thus,

$$HG_\theta(x, y) = HG_{10}(x', y') \quad \text{with} \quad \begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}, \tag{3.5}$$

which gives us,

$$\begin{aligned} HG_\theta(x, y) = &\frac{A_{10}}{w(z)} \frac{2\sqrt{2}(x\cos\theta + y\sin\theta)}{w(z)} \\ &\exp\left(-\frac{(x\cos\theta + y\sin\theta)^2 + (-x\sin\theta + y\cos\theta)^2}{w^2(z)}\right) \\ &\exp\left(ik\frac{(x\cos\theta + y\sin\theta)^2 + (-x\sin\theta + y\cos\theta)^2}{2R(z)}\right) e^{-i\phi_N(z)} \end{aligned} \tag{3.6}$$

that can be simplified to

$$HG_\theta(x, y) = \frac{A_{10}}{w(z)} \cdot \frac{2\sqrt{2}(x\cos\theta + y\sin\theta)}{w(z)} \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)}. \tag{3.7}$$

Now, notice that both HG_{10} and HG_{01} should have the same normalization constant, since they are both first-order modes, which means that $A_{10} = A_{01}$. This final step gives us the desired result,

$$\begin{aligned} HG_\theta(x, y) = &\frac{A_{10}}{w(z)} \cdot \frac{2\sqrt{2}x\cos\theta}{w(z)} \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)} \\ &+ \frac{A_{01}}{w(z)} \cdot \frac{2\sqrt{2}y\sin\theta}{w(z)} \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\phi_N(z)}, \end{aligned} \tag{3.8}$$

where we can recognize HG_{10} and HG_{01} from Eq. (3.3) and Eq. (3.4), thus giving

$$HG_\theta(x, y) = \cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y). \tag{3.9}$$

Now that we have proven the first identity, we can prove the second and third identities using this result. Let's first prove the second one. If we calculate the integral in the exercise and use the first identity, we get

$$\begin{aligned} \int HG_\theta^* \, HG_\theta \, dx\, dy &= \int \left[\cos\theta\, HG_{10}^* + \sin\theta\, HG_{01}^*\right] \left[\cos\theta\, HG_{10} + \sin\theta\, HG_{01}\right] \, dx\, dy \\ &= \cos^2\theta \int HG_{10}^* \, HG_{10} dx dy + \cos\theta\sin\theta \int HG_{10}^* \, HG_{01} dx dy \\ &\quad + \sin\theta\cos\theta \int HG_{01}^* \, HG_{10} dx dy + \sin^2\theta \int HG_{01}^* \, HG_{01} dx dy. \end{aligned} \tag{3.10}$$

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Using Eq. (3.2), one can see that the second and third integrals vanish, and the first and last integrals equal to one, implying that

$$\int HG_\theta^*(x,y)\, HG_\theta(x,y)\, dx\, dy = \cos^2\theta + \sin^2\theta = 1, \tag{3.11}$$

as we wanted.

For the third identity, we can use the same approach. Notice that

$$HG_{\theta+\pi/2}(x,y) = \cos(\theta + \pi/2)\, HG_{10}(x,y) + \sin(\theta + \pi/2)\, HG_{01}(x,y), \tag{3.12}$$

and since $\cos(\theta + \pi/2) = -\sin\theta$ and $\sin(\theta + \pi/2) = \cos\theta$, this gives us

$$HG_{\theta+\pi/2}(x,y) = -\sin\theta\, HG_{10}(x,y) + \cos\theta\, HG_{01}(x,y). \tag{3.13}$$

Now, we calculate the integral,

$$\begin{aligned}
\int HG_\theta^*\, HG_{\theta+\pi/2}\, dx\, dy &= \int [\cos\theta\, HG_{10}^* + \sin\theta\, HG_{01}^*]\, [-\sin\theta\, HG_{10} + \cos\theta\, HG_{01}]\, dx\, dy \\
&= -\cos\theta\sin\theta \int HG_{10}^*\, HG_{10}\, dx dy + \cos^2\theta \int HG_{10}^*\, HG_{01}\, dx dy \\
&\quad - \sin^2\theta \int HG_{01}^*\, HG_{10}\, dx dy + \cos\theta\sin\theta \int HG_{01}^*\, HG_{01}\, dx dy.
\end{aligned} \tag{3.14}$$

Again, using Eq. (3.2), we should be left with the following result

$$\int HG_\theta^*(x,y)\, HG_{\theta+\pi/2}(x,y)\, dx\, dy = \cos\theta\sin\theta - \cos\theta\sin\theta = 0. \tag{3.15}$$

To conclude, we want to prove the last property. For this purpose, we shall introduce the Laguerre-Gaussian modes:

$$LG_{pl}(r,\phi) = \frac{B_{pl}}{w(z)} \left(\frac{\sqrt{2}r}{w(z)}\right)^{|l|} L_p^{|l|}\left(\frac{2r^2}{w^2(z)}\right) \exp\left(-\frac{r^2}{w^2(z)}\right) \exp\left(ik\frac{r^2}{2R(z)}\right) e^{-i\psi_N(z)} e^{il\phi}, \tag{3.16}$$

where again B_{pl} is a normalization constant, $L_p^{|l|}$ is the generalized Laguerre polynomial, and $\phi_N(z) = (N+1)\arctan(z/z_R)$ is the Gouy phase, with $N = 2p + |l|$.

In this context, $LG_+(r,\phi)$ and $LG_-(r,\phi)$ are shorthands for Laguerre-Gaussian modes with $l = \pm 1$, which correspond to different signs of the azimuthal index. Let's choose $p = 0$, which is the fundamental radial mode. Then, we can describe them as

$$LG_\pm(r,\phi) = LG_{0,\pm 1}(r,\phi) = \frac{B_{0,\pm 1}}{w(z)} \frac{\sqrt{2}r}{w(z)} \exp\left(-\frac{r^2}{w^2(z)}\right) \exp\left(ik\frac{r^2}{2R(z)}\right) e^{-i\psi_N(z)} e^{\pm i\phi}, \tag{3.17}$$

since $L_0^{|l|} = 1$. Notice now that $re^{\pm i\phi} = r(\cos\phi \pm i\sin\phi) = x \pm iy$. Writing $r^2 = x^2 + y^2$, we shall get

$$LG_\pm(r,\phi) = \frac{B_{0,\pm 1}}{w(z)} \frac{\sqrt{2}(x \pm iy)}{w(z)} \exp\left(-\frac{x^2 + y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2 + y^2}{2R(z)}\right) e^{-i\psi_N(z)}. \tag{3.18}$$

Now, to conclude our result, we need to know the relation between the two constants of normalization. For instance, the constant B_{pl} can be written as

$$B_{pl} = \sqrt{\frac{2p!}{\pi(p+|l|)!}}, \tag{3.19}$$

so $B_{0,\pm 1} = \sqrt{2/\pi}$. For the constant in Eq. (3.1), we have

$$A_{mn} = \sqrt{\frac{2}{\pi 2^{m+n}m!n!}}, \tag{3.20}$$

which gives us $A_{10} = A_{01} = \sqrt{1/\pi}$. Using these two relations, gives us

$$B_{0,\pm 1} = \sqrt{2}A_{10} = \sqrt{2}A_{01}. \tag{3.21}$$

We can now substitute these relations into Eq. (3.18), multiply it by $\sqrt{2}/\sqrt{2}$, and get

$$
\begin{aligned}
LG_{\pm}(r,\phi) = \frac{1}{\sqrt{2}} & \left[\frac{A_{10}}{w(z)} \frac{2\sqrt{2}x}{w(z)} \exp\left(-\frac{x^2+y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2+y^2}{2R(z)}\right) e^{-i\psi_N(z)} \right] \\
\pm i & \left[\frac{A_{01}}{w(z)} \frac{2\sqrt{2}y}{w(z)} \exp\left(-\frac{x^2+y^2}{w^2(z)}\right) \exp\left(ik\frac{x^2+y^2}{2R(z)}\right) e^{-i\psi_N(z)} \right].
\end{aligned}
\tag{3.22}
$$

From this expression, we can recognize HG_{10} and HG_{01} from Eq. (3.3) and Eq. (3.4), thus giving

$$LG_{\pm}(r,\phi) = \frac{1}{\sqrt{2}} \left[HG_{10}(x,y) \pm iHG_{01}(x,y) \right], \tag{3.23}$$

which concludes our proof.

Exercise 2

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

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

Hint: Use bra-ket notation to write $u_{nm}(x,y) = \langle x,y|u_{nm}\rangle$.

Solution:
Author: Moisés da Rocha Alves

Using bra-ket notation, we can observe that the following is true,

$$
\begin{aligned}
\sum_{n,m=0}^{\infty} u_{nm}(x,y)u_{nm}^*(x',y') &= \sum_{n,m=0}^{\infty} \langle x,y|u_{nm}\rangle\langle u_{nm}|x',y'\rangle, \\
&= \langle x,y| \left[\sum_{n,m=0}^{\infty} |u_{nm}\rangle\langle u_{nm}| \right] |x',y'\rangle.
\end{aligned}
\tag{3.24}
$$

Notice that the set of functions $\{|u_{nm}\rangle\}$ does not necessarily form an orthonormal basis, but since it spans the Hilbert space of square-integrable functions on $\mathbb{R}^2$, it forms a complete basis set, and thus obeys a completeness relation:

$$\sum_{n,m=0}^{\infty} |u_{nm}\rangle\langle u_{nm}| = \mathbb{1}. \tag{3.25}$$

With that in mind, we can substitute this expression into Eq. (3.24) and get the result

$$\sum_{n,m=0}^{\infty} u_{nm}(x,y)u_{nm}^*(x',y') = \langle x,y|x',y'\rangle, \tag{3.26}$$

and since the position eigenstates $\{|x,y\rangle\}$ are orthonormal, we shall have $\langle x,y|x',y'\rangle = \delta(x-x')\delta(y-y')$, proving the desired result:

$$\sum_{n,m=0}^{\infty} u_{nm}(x,y)u_{nm}^*(x',y') = \delta(x-x')\delta(y-y'). \tag{3.27}$$

Challenge

Consider the linear polarization unit vectors rotated counter-clockwise by θ:

$$\hat{e}_\theta = \cos\theta\,\hat{e}_H + \sin\theta\,\hat{e}_V$$

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

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

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

are rotation invariant.

- Show that the polarization Stokes parameters for these vector structures are all equal to zero, if measured with large area detectors.

Solution:
Authors: Moisés da Rocha Alves and Paulo Vitor de Queiroz Ferreira

- Let's begin by demonstrating the first part of the challenge. Firstly, we want to prove that the first vector structure,

$$\Psi_\theta(x,y) = HG_\theta(x,y)\hat{e}_\theta + HG_{\theta+\pi/2}(x,y)\hat{e}_{\theta+\pi/2}, \tag{3.28}$$

is rotation invariant. The way we want to show it is by using Eq. (3.9) and Eq. (3.13), as well as

$$\hat{e}_{\theta+\pi/2} = \cos(\theta + \pi/2)\hat{e}_H + \sin(\theta + \pi/2)\hat{e}_V$$
$$= -\sin\theta\,\hat{e}_H + \cos\theta\,\hat{e}_V, \tag{3.29}$$

and substitute directly in the expression for $\Psi_\theta(x, y)$ to show its rotation invariance. With these relations in mind, we can write:

$$\begin{aligned} \Psi_\theta(x, y) =&[\cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y)](\cos\theta\hat{e}_H + \sin\theta\hat{e}_V) \\ &+ [-\sin\theta\, HG_{10}(x, y) + \cos\theta\, HG_{01}(x, y)](-\sin\theta\hat{e}_H + \cos\theta\hat{e}_V), \end{aligned} \tag{3.30}$$

which results in

$$\begin{aligned} \Psi_\theta(x, y) =&[HG_{10}(x, y)(\cos^2\theta + \sin^2\theta) + HG_{01}(x, y)(\sin\theta\cos\theta - \cos\theta\sin\theta)]\,\hat{e}_H \\ &+ [HG_{01}(x, y)(\cos^2\theta + \sin^2\theta) + HG_{10}(x, y)(\cos\theta\sin\theta - \sin\theta\cos\theta)]\,\hat{e}_V, \end{aligned} \tag{3.31}$$

thus giving,

$$\Psi_\theta(x, y) = HG_{10}(x, y)\hat{e}_H + HG_{01}(x, y)\hat{e}_V. \tag{3.32}$$

As $\Psi_\theta(x, y)$ is no longer dependent on θ, this shows that regardless of the angle we choose, its value remains unchanged, and therefore, we can say it is rotation invariant.

Now we want to do the same for the second expression:

$$\Psi_\theta(x, y) = HG_\theta(x, y)\hat{e}_{\theta+\pi/2} + HG_{\theta+\pi/2}(x, y)\hat{e}_\theta. \tag{3.33}$$

Let's take the same approach:

$$\begin{aligned} \Psi_\theta(x, y) =&[\cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y)](-\sin\theta\hat{e}_H + \cos\theta\hat{e}_V) \\ &+ [-\sin\theta\, HG_{10}(x, y) + \cos\theta\, HG_{01}(x, y)](\cos\theta\hat{e}_H + \sin\theta\hat{e}_V), \end{aligned} \tag{3.34}$$

which results in

$$\begin{aligned} \Psi_\theta(x, y) =&\hat{e}_H[HG_{10}(x, y)(-2\sin\theta\cos\theta) + HG_{01}(x, y)(\cos^2\theta - \sin^2\theta)] \\ &+ \hat{e}_V[HG_{10}(x, y)(\cos^2\theta - \sin^2\theta) + HG_{01}(x, y)(2\sin\theta\cos\theta)]. \end{aligned} \tag{3.35}$$

Now, we can use the fact that $\sin(2\theta) = 2\sin(\theta)\cos(\theta)$ and $\cos(2\theta) = \cos^2\theta - \sin^2\theta$. Thus,

$$\begin{aligned} \Psi_\theta(x, y) =&[-\sin(2\theta)HG_{10}(x, y) + \cos(2\theta)HG_{01}(x, y)]\hat{e}_H \\ &+ [\cos(2\theta)HG_{10}(x, y) + \sin(2\theta)HG_{01}(x, y)]\hat{e}_V. \end{aligned} \tag{3.36}$$

Notice that we can regroup this expression in terms of $HG_{10}(x, y)$ and $HG_{01}(x, y)$:

$$\begin{aligned} \Psi_\theta(x, y) =&HG_{10}(x, y)[-\sin(2\theta)\hat{e}_H + \cos(2\theta)\hat{e}_V] \\ &+ HG_{01}(x, y)[\cos(2\theta)\hat{e}_H + \sin(2\theta)\hat{e}_V], \end{aligned} \tag{3.37}$$

where we can recognize $\hat{e}_{2\theta+\pi/2} = -\sin(2\theta)\hat{e}_H + \cos(2\theta)\hat{e}_V$ and $\hat{e}_{2\theta} = \cos(2\theta)\hat{e}_H + \sin(2\theta)\hat{e}_V$ and write:

$$\Psi_\theta(x, y) = HG_{10}(x, y)\hat{e}_{2\theta+\pi/2} + HG_{01}(x, y)\hat{e}_{2\theta}. \tag{3.38}$$

Since $\hat{e}_{2\theta+\pi/2}$ and $\hat{e}_{2\theta}$ always form an orthogonal basis regardless of the value of θ (i.e., $\hat{e}_{2\theta+\pi/2} \cdot \hat{e}_{2\theta} = 0$), the components of the vector $\Psi_\theta(x, y)$ do not change with θ. Thus, this vector it is also rotation invariant.

- Now we move to the second part of the challenge. Let's first state the polarization stokes parameters S_1, S_2 and S_3:

$$S_1 = |E_H|^2 - |E_V|^2, \tag{3.39}$$

$$S_2 = 2\mathrm{Re}(E_H E_V^*), \tag{3.40}$$

$$S_3 = 2\mathrm{Im}(E_H E_V^*), \tag{3.41}$$

where E_H and E_V are the components of the electric field along the horizontal (H) and vertical (V) polarization directions, respectively.

A large-area detector integrates over the spatial coordinates x, y, effectively summing over the entire spatial profile of the fields. Thus, the relevant integrals for the Stokes parameters involve the integrals of $E_H(x, y)$ and $E_V(x, y)$ over all space:

$$S_1 = \int \left(|E_H(x, y)|^2 - |E_V(x, y)|^2 \right) dx\, dy, \tag{3.42}$$

$$S_2 = 2 \int \mathrm{Re}(E_H(x, y) E_V^*(x, y)) dx\, dy, \tag{3.43}$$

$$S_3 = 2 \int \mathrm{Im}(E_H(x, y) E_V^*(x, y)) dx\, dy. \tag{3.44}$$

Now, let's use the first vector structure in these expressions. Using the result of Eq. (3.32) one can recognize that $E_H(x, y) = HG_{10}(x, y)$ and $E_V(x, y) = HG_{01}(x, y)$ in this case. Therefore,

$$S_1 = \int \left(|HG_{10}(x, y)|^2 - |HG_{01}(x, y)|^2 \right) dx\, dy, \tag{3.45}$$

$$S_2 = 2 \int \mathrm{Re}(HG_{10}(x, y) HG_{01}^*(x, y)) dx\, dy, \tag{3.46}$$

$$S_3 = 2 \int \mathrm{Im}(HG_{10}(x, y) HG_{01}^*(x, y)) dx\, dy. \tag{3.47}$$

To prove these results are zero, we can just look at Eq. (3.2). For S_1 we will have

$$S_1 = \int (HG_{10}(x, y) HG_{10}^*(x, y) - HG_{10}(x, y) HG_{01}^*(x, y)) dx\, dy, = 1 - 1 = 0.$$

For S_2 and S_3, since HG_{10} and HG_{01} are orthogonal, as stated in Eq. (3.2) (the Hermite polynomials are orthogonal), we will also have $S_2 = 0$ and $S_3 = 0$. Therefore, for the first vector structure, all polarization Stokes parameters will be equal to zero.

Now what is left is proving the same for the second vector structure. For this purpose, we are going to use the expression in Eq. (3.36). From this expression, we can recognize that

$$E_H(x, y) = -\sin(2\theta)HG_{10}(x, y) + \cos(2\theta)HG_{01}(x, y)$$

and

$$E_V(x, y) = \cos(2\theta)HG_{10}(x, y) + \sin(2\theta)HG_{01}(x, y).$$

Thus, the polarization Stokes parameters will be

$$S_1 = \int \left\{ |-\sin(2\theta)HG_{10}(x, y) + \cos(2\theta)HG_{01}(x, y)|^2 \right. \tag{3.48}$$
$$\left. - |\cos(2\theta)HG_{10}(x, y) + \sin(2\theta)HG_{01}(x, y)|^2 \right\} dx\,dy,$$

$$S_2 = 2\int \mathrm{Re}\left\{ \left[-\sin(2\theta)HG_{10}(x, y) + \cos(2\theta)HG_{01}(x, y) \right] \right. \tag{3.49}$$
$$\left. \left[\cos(2\theta)HG_{10}(x, y) + \sin(2\theta)HG_{01}(x, y) \right]^* \right\} dx\,dy,$$

$$S_3 = 2\int \mathrm{Im}\left\{ \left[-\sin(2\theta)HG_{10}(x, y) + \cos(2\theta)HG_{01}(x, y) \right] \right. \tag{3.50}$$
$$\left. \left[\cos(2\theta)HG_{10}(x, y) + \sin(2\theta)HG_{01}(x, y) \right]^* \right\} dx\,dy.$$

For S_1, we'll have:

$$S_1 = \int \left\{ \left[-\sin(2\theta)HG_{10} + \cos(2\theta)HG_{01} \right]\left[-\sin(2\theta)HG_{10} + \cos(2\theta)HG_{01} \right]^* \right.$$
$$\left. - \left[\cos(2\theta)HG_{10} + \sin(2\theta)HG_{01} \right]\left[\cos(2\theta)HG_{10} + \sin(2\theta)HG_{01} \right]^* \right\} dx\,dy. \tag{3.51}$$

Since all contributions from terms with $HG_{10}HG_{01}^*$ and $HG_{01}HG_{10}^*$ will be zero, as they are orthogonal, we will be left with:

$$S_1 = \int \left\{ [\sin^2(2\theta) - \cos^2(2\theta)]HG_{10}HG_{10}^* - [\sin^2(2\theta) - \cos^2(2\theta)]HG_{01}HG_{01}^* \right\} dx\,dy. \tag{3.52}$$

Noticing again that $\int HG_{10}HG_{10}^* dx dy = HG_{01}HG_{01}^* dx dy = 1$:

$$S_1 = [\sin^2(2\theta) - \cos^2(2\theta)] - [\sin^2(2\theta) - \cos^2(2\theta)] = 0, \tag{3.53}$$

which concludes the result for S_1.

For S_2 and S_3, we can use the same argument (contributions from terms with $HG_{10}HG_{01}^*$ and $HG_{01}HG_{10}^*$ will be zero) and get

$$S_2 = 2 \int \text{Re}\left\{\left[-\sin(2\theta)\cos(2\theta)HG_{10}HG_{10}^*+\sin(2\theta)\cos(2\theta)HG_{01}HG_{01}^*\right.\right\}dx\,dy, \quad (3.54)$$

$$S_3 = 2 \int \text{Im}\left\{\left[-\sin(2\theta)\cos(2\theta)HG_{10}HG_{10}^*+\sin(2\theta)\cos(2\theta)HG_{01}HG_{01}^*\right.\right\}dx\,dy, \quad (3.55)$$

and we can see that these contributions should cancel out, since the integrals with $HG_{10}HG_{10}^*$ and $HG_{01}HG_{01}^*$ will give the same value. Thus, finally, $S_2 = S_3 = 0$, concluding our proof.