Introduction to Applications of Quantum Computing to Quantum Chemistry

Both the Exercises and Challenge are uploaded as Jupyter notebooks.

Bose-Einstien Condensates and the Involvement in Advances for New Technologies

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

a)
Scattering is taken into account by introducing a potential $U(\mathbf{r})$ that acts on an initial state, and we obtain a final state, in a finite range ($r < R$) with hamiltonian

$$H = H_0 + U(\mathbf{r})$$

the result for the asymptotic behavior of the wave function is (for large r)

$$\psi(\mathbf{r}) \rightarrow \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{k}.\mathbf{r}} + \frac{e^{ik.r}}{r} f(\mathbf{k}, \mathbf{k}') \right]$$

where

$$f(\mathbf{k}, \mathbf{k}') = -\frac{m(2\pi)^3}{2\pi\hbar^2} \int d^3r' \langle \mathbf{k}' | \mathbf{r}' \rangle U(\mathbf{r}') \langle \mathbf{r}' | \psi \rangle$$

To obtain the last wave function, we assumed the scattering potential $U(\mathbf{r})$ to be real, finite-ranged, local, and that it is spherically symmetric. Hence, we can write $U(\mathbf{r}) = U(r)$. In the scattering region ($0 < r < R$), we can write the Schrödinger equation as

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + U(r)\psi = E\psi$$

Due to the spherical symmetry of $U(r)$ the Laplacian can be expressed in spherical coordinates

$$\left(-\frac{\hbar^2}{2m} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{L^2}{2mr^2} + U(r) \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi)$$

where L is the angular momentum operator. From the last equation we can see that the particle is subject to the action of an effective potential

$$U_{eff}(r) = U(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

where the second term on the right-hand side is a repulsive centrifugal barrier. It is absent for $l = 0$..

For low-energy scattering, in terms of k and R is:

$$kR \ll 1$$

where the reduced wavelength $\frac{\lambda}{2\pi} = \frac{1}{k}$.

If the energy is close to zero, the particle cannot overcome the centrifugal barrier and results with $l > 0$ are not important and the component with $l = 0$ is dominant to understand the low-energy scattering. Hence it is most relevant.

b) S-wave scattering length:

S-wave scattering length is the parameter that characterizes the effective range of interaction in case of the low energy limit of the incident wave, i.e., for $l = 0$ term in the partial wave analysis referred to as “s-wave”.

c) The scattering length is given by

$$a = \frac{m_r}{2\pi\hbar^2} \int U(\mathbf{r}) d^3r$$

For $U = U_0\delta(\mathbf{r}-\mathbf{r}')$:

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

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

$$a = \frac{m_r}{2\pi\hbar^2}U_0\int \delta(x-x')\delta(y-y')\delta(z-z')dxdydz$$

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

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

therefore

$$U = \frac{2\pi\hbar^2 a}{m_r}\delta(\mathbf{r}-\mathbf{r}')$$

(2) [Exercise] The Gross-Pitaevskii equation.

a) We have the Hamiltonian as

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

and the wave function as

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

Expectation value,

$$E = \int \Psi^*(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)H\Psi(\mathbf{r}_1,\mathbf{r}_2,...,\mathbf{r}_N)\prod_i d^3r_i$$

$$= \int\prod_i\left(\phi^*(r_i)\left(\sum_{i=1}^{N}[\frac{\mathbf{p}_i^2}{2m} + V(\mathbf{r}_i)\right) + U_0\sum_{j<k}\delta(\mathbf{r}_i-\mathbf{r}_j)\right)\phi(r_i)d^3r_i$$

$$\text{with } \mathbf{p}_i = i\hbar\frac{\partial}{\partial x_i} + i\hbar\frac{\partial}{\partial y_i} + i\hbar\frac{\partial}{\partial z_i}$$

$$= \prod_i\int\phi^*(\mathbf{r}_i)\left(\sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_j^2 + V(\mathbf{r}_j)\right) + U_0\sum_{j<k}\delta(\mathbf{r}_i-\mathbf{r}_j)\right)\phi(\mathbf{r}_i)d^3r_i$$

$$\text{As }\int d^3r_i|\phi(r_i)|^2 = 1 \quad \forall i$$

we get:

$$= \sum_{j=1}^{N}\int\phi^*(\mathbf{r}_j)\left(-\frac{\hbar^2}{2m}\nabla_j^2 + V(\mathbf{r}_j)\right)\phi(\mathbf{r}_j)d^3r_j$$

$$+\sum_{j=1}^{N}\sum_{j<k}\int\phi^*(\mathbf{r}_j)\phi^*(\mathbf{r}_k)U_0\delta(\mathbf{r}_j-\mathbf{r}_k)\phi(\mathbf{r}_j)\phi(\mathbf{r}_k)d^3r_jd^3r_k$$

(b) As each ϕ_i will give the same contribution to the integral, we have:

$$E = N\int\phi^*(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\phi(\mathbf{r})d^3r$$

$$+\frac{U_0N(N-1)}{2}\int\phi^*(\mathbf{r}')\phi^*(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\phi(\mathbf{r}')\phi(\mathbf{r})d^3rd^3r'$$

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

We have

$$\Psi(\mathbf{r}) = \sqrt{N} \phi(\mathbf{r})$$

so:

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

For large N, ignoring $\frac{1}{N}$ terms:

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

Using the method of Lagrange multipliers, we have to minimize the quantity $E - \mu N$, with μ being the chemical potential, and:

$$N = \int |\Psi(\mathbf{r})|^2 d^3 r$$

Seeing its variation w.r.t. $\Psi^*(\mathbf{r})$, we get:

$$\begin{aligned} &\frac{\partial}{\partial \Psi^*(\mathbf{r})} (E - \mu N) = \\ &\quad \frac{\partial}{\partial \Psi^*(\mathbf{r})} \int \Big(-\frac{\hbar^2}{2m} \Psi^*(\mathbf{r}) \nabla^2 \Psi(r) + V(\mathbf{r}) \Psi^*(r) \Psi(\mathbf{r}) + \frac{U_0}{2} \Psi^*(\mathbf{r}) \Psi(\mathbf{r}) \Psi^*(\mathbf{r}) \Psi(\mathbf{r}) \\ &\qquad\qquad - \mu |\Psi(\mathbf{r})|^2 \Big) = 0 \end{aligned}$$

$$\Rightarrow \left(-\frac{\hbar^2}{2m} \nabla^2 \Psi(\mathbf{r}) + V(\mathbf{r}) \Psi(\mathbf{r}) + U_0 |\Psi(\mathbf{r})|^2 \Psi(\mathbf{r}) - \mu \Psi(\mathbf{r}) \right) d^3 r = 0$$

Which leads to:

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + U_0 |\Psi(\mathbf{r})|^2 \right) \Psi(\mathbf{r}) = \mu \Psi(\mathbf{r})$$

This is the time-independent Gross-Pitaevskii equation.

(c) For uniform Bose gas, $\Psi(\mathbf{r})$ doesn't have a spatial dependence, so:

$$\nabla^2 \Psi(\mathbf{r}) = 0$$

Also, there is no trapping potential for a uniform Bose gas. Thus, $V(\mathbf{r}) = 0$. So the G.P.E. becomes:

$$U_0 |\Psi(\mathbf{r})|^2 = \mu$$

(3) [Challenge] Computational project.

The Challenge has been uploaded as a Jupyter notebook

Prospects and Challenges for Quantum Machine Learning

(a)[**Exercise**] We have $Id, X, \cdot$(dot product).
It's a group if :
Closure $\forall a, b \in V,\ a \cdot b \in V$
So:

$$Id \cdot X = X \quad \text{and} \quad X \cdot Id = X \quad \text{where} \quad X \in V.$$

Associativity For all $a, b, c \in V$:

$$(a \cdot b) \cdot c = a \cdot (b \cdot c)$$

Example checks for associativity:
1.) Given: $a = Id$, $b = X$, $c = Id$

$$\left.\begin{array}{l}(Id \cdot X) \cdot Id = X \cdot Id = X \\ Id \cdot (X \cdot Id) = Id \cdot X = X\end{array}\right\} \text{All are equal}$$

2.) Given: $a = Id$, $b = X$, $c = X$
We know:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = Id$$

Then:

$$\left.\begin{array}{l}(Id \cdot X) \cdot X = X \cdot X = Id \\ Id \cdot (X \cdot X) = Id \cdot Id = Id\end{array}\right\} \text{Are equal}$$

3.) Given: $a = Id$, $b = Id$, $c = Id$

$$\left.\begin{array}{l}(Id \cdot Id) \cdot Id = Id \cdot Id = Id \\ Id \cdot (Id \cdot Id) = Id \cdot Id = Id\end{array}\right\} \text{Are equal}$$

4.) Given: $a = Id$, $b = Id$, $c = X$

$$\left.\begin{array}{l}(Id \cdot Id) \cdot X = Id \cdot X = X \\ Id \cdot (Id \cdot X) = Id \cdot X = X\end{array}\right\} \text{Are equal}$$

5.) Given: $a = X$, $b = X$, $c = Id$

$$\left.\begin{array}{l}(X \cdot X) \cdot Id = Id \cdot Id = Id \\ X \cdot (X \cdot Id) = X \cdot X = Id\end{array}\right\} \text{Are equal}$$

6. Given: $a = X$, $b = X$, $c = X$

$$\left.\begin{array}{l}(X \cdot X) \cdot X = Id \cdot X = X \\ X \cdot (X \cdot X) = X \cdot Id = X\end{array}\right\} \text{Are equal}$$

7.) Given: $a = X$, $b = Id$, $c = Id$

$$\left.\begin{array}{l}(X \cdot Id) \cdot Id = X \cdot Id = X \\ X \cdot (Id \cdot Id) = X \cdot Id = X\end{array}\right\} \text{Are equal}$$

8.) Given: $a = Id$, $b = Id$, $c = X$

$$\left.\begin{array}{l}(Id \cdot Id) \cdot X = Id \cdot X = X \\ Id \cdot (Id \cdot X) = Id \cdot X = X\end{array}\right\} \text{Are equal}$$

Thus all elements are associative.
Identity Element For all $a \in V$, there exists $e \in V$ called the identity of a, such that:

$$a \cdot e = e \cdot a = a$$

1.) If a=Id Then:

$$Id \cdot Id = Id.$$

2.) If a=X Then

$$X \cdot Id = Id \cdot X = X$$

Thus $e = Id$ is the identity element of the group.
Inverse Element For all $a \in V$, there exists $b \in V$ called the inverse of a, such that:

$$a \cdot b = b \cdot a = e$$

where $e = Id$ is the identity element.
1.) If a=Id We assume that $b = Id$, thus:

$$Id \cdot Id = Id.$$

2.) If a=X We assume that $b = X$, thus:

$$X \cdot X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = Id$$

Hence this is a group.

(b)[**Exercise**] We have

$$U = e^{-i\Phi_3 Y} e^{-i\Phi_2 X} e^{-i\Phi_1 Y}$$

$$\frac{dU}{d\Phi_1}\bigg|_{\Phi=0} = -iY\, e^{-i\Phi_1 Y} e^{-i\Phi_2 X} e^{-i\Phi_3 Y}\bigg|_{\Phi=0}$$

where $\Phi = 0 \to \{\Phi_1, \Phi_2, \Phi_3\} = \{0, 0, 0\}$:

$$= -iY$$

Similarly:

$$\frac{dU}{d\Phi_2}\bigg|_{\Phi=0} = -iX$$

$$\frac{dU}{d\Phi_3}\bigg|_{\Phi=0} = -iY$$

Now we have:

$$[-iX, -iY] = -[X, Y]$$

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

$$XY = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \quad YX = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix}$$

$$[X, Y] = 2i \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = 2iZ, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$[-iX, -iY] = 2(-iZ)$$

Let:

$$C_1 = -iX, \quad C_2 = -iY, \quad C_3 = -iZ$$

$$[C_1, C_2] = 2C_3$$

Similarly:

$$[C_1, C_3] = -[X, Z]$$

$$XZ = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad ZX = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

So:

$$[C_1, C_3] = -2(-iY) = -2C_2$$

Similarly:

$$[C_2, C_3] = -[Y, Z]$$

$$YZ = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}, \quad ZY = \begin{bmatrix} 0 & -i \\ -i & 0 \end{bmatrix}$$

So:

$$[C_2, C_3] = 2(-iX) = 2C_1$$

Thus, the commutation relations are:

$$[C_i, C_j] = 2\epsilon_{ijk} C_k$$

Thus, the generators of U satisfy the same commutation relations as generators of $SU(2)$. Hence, group U is a representation of the $SU(2)$ group.

(3)[**Challenge**]

For any group g, we have:

$$R(g) \cong \bigoplus_{\lambda} I_{m_\lambda} \otimes R_\lambda(g)$$

where $R_\lambda(g)$ are the irreducible representations of group g and m_λ is their multiplicity.

An element A of the commutant is of the form:

$$A \cong \bigoplus_{\lambda} A_{m_\lambda} \otimes I_{d_\lambda}$$

Here d_λ is the dimension of the irreps, and A_{m_λ} is an arbitrary $m_\lambda \times m_\lambda$ matrix.

For an arbitrary $m_\lambda \times m_\lambda$ matrix, we have m_λ^2 basis vectors.

For a matrix given as $A_{m_\lambda} \otimes I_{d_\lambda}$, we only require m_λ^2 basis elements as its basis will be:

$$\{\{\text{basis element of } A_{m_\lambda}\} \otimes I_{d_\lambda}\}$$

e.g., $m_\lambda = 2$, $d_\lambda = 2$, the basis elements are:

$$\left\{ \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right\}$$

Thus, for the element of the commutant A given as:

$$A = \bigoplus_{\lambda} A_{m_\lambda} \otimes I_{d_\lambda}$$

The number of basis elements or the dimension D is:

$$D = \sum_{\lambda} m_\lambda^2.$$

High Dimensional Quantum Computing with Structured Light

(1) [**Exercise**] First order Hermite-Gauss modes are given as:

$$\begin{aligned} HG_{01}(x,y) &= \frac{1}{\omega(z)\sqrt{\pi}} H_0\left(\frac{\sqrt{2}\,x}{\omega(z)}\right) H_1\left(\frac{\sqrt{2}\,y}{\omega(z)}\right) e^{-\frac{x^2+y^2}{\omega^2(z)}} e^{i\left(k\frac{(x^2+y^2)}{2R(z)}\right)} e^{-i\phi_N(z)} \\ &= \frac{\sqrt{2}}{\sqrt{\pi}} \left(\frac{y}{\omega^2(z)}\right) e^{-\frac{x^2+y^2}{\omega^2(z)}} e^{i\left(k\frac{(x^2+y^2)}{2R(z)}\right)} e^{-i\phi_N(z)} \\ HG_{10}(x,y) &= \frac{1}{\omega(z)\sqrt{\pi}} H_1\left(\frac{\sqrt{2}\,x}{\omega(z)}\right) H_0\left(\frac{\sqrt{2}\,y}{\omega(z)}\right) e^{-\frac{x^2+y^2}{\omega^2(z)}} e^{i\left(k\frac{(x^2+y^2)}{2R(z)}\right)} e^{-i\phi_N(z)} \\ &= \frac{\sqrt{2}}{\sqrt{\pi}} \left(\frac{x}{\omega^2(z)}\right) e^{-\frac{x^2+y^2}{\omega^2(z)}} e^{i\left(k\frac{(x^2+y^2)}{2R(z)}\right)} e^{-i\phi_N(z)} \end{aligned}$$

where H_0, H_1 are Hermite Polynomials.

Under a counterclockwise rotation, we have:

$$x' = \cos\theta\, x + \sin\theta\, y$$
$$y' = -\sin\theta\, x + \cos\theta\, y$$

$$HG_\theta(x,y) = HG_{10}(x',y') = \frac{\sqrt{2}}{\sqrt{\pi}} \left(\frac{x'}{\omega^2(z)}\right) e^{-\frac{x'^2+y'^2}{\omega^2(z)}} e^{i\left(k\frac{(x'^2+y'^2)}{2R(z)}\right)} e^{-i\phi_N(z)}$$

$$x'^2 + y'^2 = (x\cos\theta + y\sin\theta)^2 + (-x\sin\theta + y\cos\theta)^2$$

$$= x^2\cos^2\theta + y^2\sin^2\theta + 2\cos\theta\sin\theta\, xy + x^2\sin^2\theta + y^2\cos^2\theta - 2\cos\theta\sin\theta\, xy$$

$$= x^2 + y^2$$

Thus,

$$x'^2 + y'^2 = x^2 + y^2$$

$$HG_\theta(x,y) = \frac{\sqrt{2}}{\sqrt{\pi}\,\omega^2(z)}\,(\cos\theta\, x + \sin\theta\, y)\, e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{i\left(k\frac{x^2+y^2}{2R(z)}\right)}\, e^{-i\phi_N(z)}$$

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

(a)

$$\int HG^*_\theta(x,y)\, HG_\theta(x,y)\, dx\, dy = \int \Big(\cos^2\theta\, HG_{10}(x,y)^2 + \sin^2\theta\, HG_{01}(x,y)^2 + 2\sin\theta\cos\theta\, HG_{10}(x,y)\, HG_{01}(x,y)\Big)\, dx\, dy$$

$$\int HG_{01}(x,y)\, HG_{10}(x,y)\, dx\, dy$$

$$= \frac{1}{\pi\,\omega^2(z)}\left[\int \left(H_0\left(\frac{\sqrt{2}\,x}{\omega(z)}\right)\right)^2 e^{-\frac{x^2}{\omega^2(z)}}\, dx \int \left(H_1\left(\frac{\sqrt{2}\,y}{\omega(z)}\right)\right)^2 e^{-\frac{y^2}{\omega^2(z)}}\, dy\right]$$

$$\frac{\sqrt{2}\,x}{\omega(z)} \to x \quad \text{and} \quad \frac{\sqrt{2}\,y}{\omega(z)} \to y$$

$$dx \to \frac{\omega(z)}{\sqrt{2}}\, dx \quad \text{and} \quad dy \to \frac{\omega(z)}{\sqrt{2}}\, dy$$

$$\int (HG_{10}(x,y))^2\, dx\, dy = \frac{1}{2\pi}\int H_0(x)\, H_0(x)\, e^{-x^2}\, dx \int H_1(y)\, H_1(y)\, e^{-y^2}\, dy$$

Hermite polynomials have the property:

$$\int H_n(x)\, H_m(x)\, e^{-x^2}\, dx = \sqrt{\pi}\, 2^n\, n!\, \delta_{nm}$$

Using this, we get:

$$\int (H_0(x))^2\, e^{-x^2}\, dx = \sqrt{\pi}$$

$$\int (H_1(x))^2\, e^{-x^2}\, dx = \sqrt{\pi}\, 2$$

Thus

$$\int (HG_{10}(x,y))^2\, dx\, dy = 1$$

Similarly:

$$\int (HG_{01}(x,y))^2\, dx\, dy = 1$$

$$\int HG_{01}(x,y)\, HG_{10}(x,y)\, dx\, dy = \frac{1}{\pi\,\omega^2(z)}\left[\int H_0\left(\frac{\sqrt{2}\,x}{\omega(z)}\right) H_1\left(\frac{\sqrt{2}\,x}{\omega(z)}\right) e^{-\frac{2x^2}{\omega^2(z)}}\, dx\right] \times \left[\int H_1\left(\frac{\sqrt{2}\,y}{\omega(z)}\right) H_0\left(\frac{\sqrt{2}\,y}{\omega(z)}\right) e^{-\frac{2y^2}{\omega^2(z)}}\, dy\right]$$

$$= \frac{1}{2\pi} \int H_0(x)\, H_1(x)\, e^{-x^2}\, dx \int H_1(y)\, H_0(y)\, e^{-y^2}\, dy$$

$$= 0$$

Thus:

$$\int HG^*_\theta(x,y)\, HG_\theta(x,y)\, dx\, dy = \cos^2\theta + \sin^2\theta = 1$$

(b)

$$\int HG^*_\theta(x,y)\, HG_{\theta+\pi/2}(x,y)\, dx\, dy$$

$$= \int \left(\cos\theta\, HG_{10}(x,y) + \sin\theta\, HG_{01}(x,y)\right)\left(-\sin\theta\, HG_{10}(x,y) + \cos\theta\, HG_{01}(x,y)\right)\, dx\, dy$$

$$= \int \Big[-\cos\theta\sin\theta\, HG_{10}(x,y)^2 + \cos^2\theta\sin^2\theta\, HG_{01}(x,y)^2 + (\cos^2\theta - \sin^2\theta)\, HG_{01}(x,y)\, HG_{10}(x,y)\Big]\, dx\, dy$$

Using previous results:

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

(c)

$$LG_{0,\pm1}(r,\varphi) = \frac{1}{\sqrt{2\pi}\,\omega(z)} \left(\frac{\sqrt{2}\,(x^2+y^2)}{\omega(z)}\right) L_0\left(\frac{2(x^2+y^2)}{\omega^2(z)}\right) e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{i\left(k\frac{x^2+y^2}{2R(z)}\right)} e^{-i\phi_N(z)} e^{\pm il\varphi}$$

$$= \frac{x^2+y^2}{\sqrt{\pi}\,\omega(z)} e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{\left(ik\frac{x^2+y^2}{2R(z)}\right)} e^{-i\phi_0(z)} e^{i\ell\varphi}$$

with $x = r\cos\varphi$ and $y = r\sin\varphi$, we get:

$$= \frac{1}{\sqrt{\pi}\,\omega(z)^2} \left(r\cos\varphi + ir\sin\varphi\right) e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{\left(ik\frac{x^2+y^2}{2R(z)}\right)} e^{-i\phi_N(z)}$$

$$= \frac{1}{\sqrt{2}} \Bigg[\frac{\sqrt{2}}{\sqrt{\pi}\,\omega(z)^2} x\, e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{\left(ik\frac{x^2+y^2}{2R(z)}\right)} e^{-i\phi_N(z)} + \frac{\sqrt{2}}{\sqrt{\pi}\,\omega(z)^2} iy\, e^{-\frac{x^2+y^2}{\omega^2(z)}}\, e^{\left(ik\frac{x^2+y^2}{2R(z)}\right)} e^{-i\phi_N(z)} \Bigg]$$

$$= \frac{HG_{10} + i\, HG_{01}}{\sqrt{2}}$$

(2) [**Exercise**]:

$$\sum_{n,m=-\infty}^{\infty} u_{n,m}(x,y)\, u^*_{n,m}(x',y') = \sum_{n,m} \langle x,y|u_{n,m}\rangle\langle u_{n,m}|x',y'\rangle = \langle x,y| \left(\sum_{n,m} |u_{n,m}\rangle\langle u_{n,m}|\right) |x',y'\rangle$$

Since $u_{n,m}$ is a basis set, it is complete. Hence:

$$\sum_{n,m} |u_{n,m}\rangle\langle u_{n,m}| = I$$

Thus, we get:

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

$\{x, y\}$ also form a complete orthogonal basis in $\mathbb{R}^2$. Thus:

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

Hence:

$$\sum_{n,m} u_{n,m}(x, y)\, u^*_{n,m}(x', y') = \delta(x - x')\, \delta(y - y')$$

(3)[**Challenge**]

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

$$= HG_\theta(x, y)\, (\cos\theta\, \hat{e}_H + \sin\theta\, \hat{e}_V) + HG_{\frac{\pi}{2}+\theta}(x, y)\, (-\sin\theta\, \hat{e}_H + \cos\theta\, \hat{e}_V)$$

$$= \left(\cos\theta\, HG_\theta(x, y) - \sin\theta\, HG_{\frac{\pi}{2}+\theta}(x, y)\right) \hat{e}_H + \left(\sin\theta\, HG_\theta(x, y) + \cos\theta\, HG_{\frac{\pi}{2}+\theta}(x, y)\right) \hat{e}_V$$

$$= [\cos\theta\, (\cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y)) - \sin\theta\, (-\sin\theta\, HG_{10}(x, y) + \cos\theta\, HG_{01}(x, y))]\, \hat{e}_H$$

$$+ [\sin\theta\, (\cos\theta\, HG_{10}(x, y) + \sin\theta\, HG_{01}(x, y)) + \cos\theta\, (-\sin\theta\, HG_{10}(x, y) + \cos\theta\, HG_{01}(x, y))]\, \hat{e}_V$$

$$= HG_{10}(x, y)\, \hat{e}_H + HG_{01}(x, y)\, \hat{e}_V$$

Hence, it remains invariant under rotation.

Similarly:

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

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

$$- (-\sin\theta\, HG_{10}(x, y) + \cos\theta\, HG_{01}(x, y))\, (\cos\theta\, \hat{e}_H + \sin\theta\, \hat{e}_V)$$

$$= \hat{e}_H \left[-\sin\theta\cos\theta\, HG_{10}(x, y) - \sin^2\theta\, HG_{01}(x, y) + \sin\theta\cos\theta\, HG_{10}(x, y) - \cos^2\theta\, HG_{01}(x, y)\right]$$

$$+ \hat{e}_V \left[\cos^2\theta\, HG_{10}(x, y) + \cos\theta\sin\theta\, HG_{01}(x, y) + \sin^2\theta\, HG_{10}(x, y) - \sin\theta\cos\theta\, HG_{01}(x, y)\right]$$

$$= -\,(HG_{01}(x, y)\, \hat{e}_H - HG_{10}(x, y)\, \hat{e}_V)$$

Hence, this is also rotationally invariant up to a global phase.

(b) We have from (a):

$$\begin{aligned} \Psi(x, y) &= HG_\theta(x, y)\, \hat{e}_\theta + HG_{\frac{\pi}{2}+\theta}(x, y)\, \hat{e}_{\frac{\pi}{2}+\theta} \\ &= HG_{10}(x, y)\, \hat{e}_H + HG_{01}(x, y)\, \hat{e}_V \end{aligned}$$

$$I_H = \int |\hat{e}^*_H \cdot \Psi(x, y)|^2\, dx\, dy = \int |HG_{10}|^2\, dx\, dy = \int HG_{10}^2\, dx\, dy = 1$$

$$I_V = \int |\hat{e}^*_V \cdot \Psi(x, y)|^2\, dx\, dy = \int |HG_{01}|^2\, dx\, dy = \int HG_{01}^2\, dx\, dy = 1$$

$$\hat{e}_H = \frac{\hat{e}_0 + \hat{e}_A}{\sqrt{2}}, \quad \hat{e}_V = \frac{\hat{e}_0 - \hat{e}_A}{\sqrt{2}}$$

$$\Psi_\theta(x, y) = \frac{(HG_{10} + HG_{01})}{\sqrt{2}}\, \hat{e}_0 + \frac{(HG_{10} - HG_{01})}{\sqrt{2}}\, \hat{e}_A$$

$$I_D = \int \left| \frac{HG_{10} + HG_{01}}{\sqrt{2}} \right|^2 dx\, dy = \frac{1}{2} \int \left(HG_{10}^2 + HG_{01}^2 + 2\, HG_{10}\, HG_{01}\right) dx\, dy$$

$$= \frac{1}{2}\left[1+1+0\right] = 1$$

$$I_A = \int \left|\frac{HG_{10} - HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = \frac{1}{2}\int \left(HG_{10}^2 + HG_{01}^2 - 2\,HG_{10}\,HG_{01}\right)\,dx\,dy$$

$$= \frac{1}{2}\left[1+1-0\right] = 1$$

$$\hat{e}_H = \frac{\hat{e}_L + i\hat{e}_R}{\sqrt{2}}, \quad \hat{e}_V = \frac{\hat{e}_L - i\hat{e}_R}{\sqrt{2}}$$

$$\Psi_\theta(x,y) = \frac{(HG_{10} + i\,HG_{01})}{\sqrt{2}}\,\hat{e}_L + \frac{(HG_{10} - i\,HG_{01})}{\sqrt{2}}\,\hat{e}_R$$

$$I_L = \int \left|\frac{HG_{10} + i\,HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = \frac{1}{2}\int \left(HG_{10}^2 + HG_{01}^2\right)\,dx\,dy = 1$$

$$I_R = \int \left|\frac{HG_{10} - i\,HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = \frac{1}{2}\int \left(HG_{10}^2 + HG_{01}^2\right)\,dx\,dy = 1$$

The polarisation Stokes parameters are thus

$$S_1 = \frac{I_H - I_V}{I_{Tot}} = 0, \quad S_2 = \frac{I_D - I_A}{I_{Tot}} = 0, \quad S_3 = \frac{I_L - I_R}{I_{Tot}} = 0$$

all zero.

The large detectors are required so the whole beam of light can be covered. Thus, integration over the whole space can be done to use Hermite-Gauss polynomial's orthogonality properties.

Similarly for:

$$\Psi_\theta(x,y) = HG_\theta(x,y)\,\hat{e}_{\frac{\pi}{2}+\theta} - HG_{\frac{\pi}{2}+\theta}(x,y)\,\hat{e}_\theta$$
$$= -HG_{01}\,\hat{e}_H + HG_{10}\,\hat{e}_V$$

Similarly to previous cases:

$$I_H = \int HG_{10}^2\,dx\,dy = 1, \quad I_V = \int HG_{01}^2\,dx\,dy = 1$$

$$I_D = \int \left|\frac{HG_{10} + HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = 1, \quad I_A = \int \left|\frac{HG_{10} - HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = 1$$

$$I_L = \int \left|\frac{HG_{10} - i\,HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = 1, \quad I_R = \int \left|\frac{HG_{10} + i\,HG_{01}}{\sqrt{2}}\right|^2 dx\,dy = 1$$

Thus again we have the polarisation Stokes parameters

$$S_1 = \frac{I_H - I_V}{I_{Tot}} = 0, \quad S_2 = \frac{I_D - I_A}{I_{Tot}} = 0, \quad S_3 = \frac{I_L - I_R}{I_{Tot}} = 0$$

to be zero