Second Quantum Computing School
ICTP-SAIFR

Hackathon-UFSCarros

Eduardo Marsola
Luis Eduardo Penante
Nicolas Cenedesi
Pedro Marques Pontes

São Paulo, Brazil
17 de outubro de 2024

Sumário

1 Introduction

The purpose of this report is to present the solutions developed by the UFSCarros team for the challenges posed during the Hackathon at the Second Quantum Computing School.

Each section of this document will be organized according to the themes of each lecture, including the respective questions and challenges. Considering that there are lengthy questions, only the beginning of these questions will be stated. For the questions involving code, the solution will be available on GitHub.

2 Introduction to Applications of Quantum Computing to Quantum Chemistry (October 7-11)

2.1 Exercise 1

Consider the following Hamiltonian:

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

...

2.1.1 Solution

Available on GitHub.

2.2 Challenge 2

Ground State Energy for Molecule and Spin System with Variational Quantum Algorithms and Trotterization ...

2.2.1 Solution

Available on GitHub.

3 Bose-Einstein Condensates and the Involvement in Advances for New Technologies. (October 9-11)

3.1 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...

3.1.1 Solution

(a)

The wave number k is related to the kinetic energy of the particles by the equation:

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

where m_r is the reduced mass. In the low-energy limit, the energy E is very small, meaning that $k \to 0$.

In low-energy scattering, the wavelength associated with the wave number k is much larger than the range of the potential R, i.e.,

$$kR \ll 1.$$

This indicates that the interactions are dominated by long-range processes.

Now, regarding why the angular momentum $l = 0$ (s-wave) is the most relevant:

- When $k \to 0$, angular momentum significantly affects the efficiency of scattering. Modes with $l > 0$ (p-wave, d-wave, etc.) face a centrifugal barrier proportional to $l(l+1)/r^2$, which suppresses scattering at low energies.
- Only the mode with $l = 0$ (s-wave) has significant scattering amplitude because it does not experience this centrifugal barrier. As a result, s-wave scattering dominates at low energies.

(b)

The scattering length a is a measure of the strength of the interaction between two particles in a potential. It indicates how the effective potential deflects the particles compared to free scattering.

(c)

The Born approximation is a way to simplify the calculation of scattering by assuming that the potential is weak and that the particles approximately follow free trajectories.

The expression given for the scattering length a is:

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

This tells us that the scattering length is proportional to the volumetric integral of the potential $U(r)$.

Finding U_0

When we use a delta potential $U_{\text{eff}}(r, r') = U_0 \delta(r - r')$, we want the integral of this potential to be equivalent to that of the original potential. Thus:

$$U_0 \int d^3r \, \delta(r - r') = U_0$$

which means the integral simply gives us U_0.

To ensure that the scattering length is the same for the delta potential, we compare it with the expression from the Born approximation:

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

Thus, the constant U_0 will be:

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

3.2 Exercise 2

The Gross-Pitaevskii Equation

In undergraduate and graduate 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...

3.2.1 Solution

3.3 Challenge 3

Computational Project

To treat the dynamics of BECs, we need the time-dependent GPE,

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

Studying the dynamics of interacting systems is challenging. Fortunately, we can employ numerical methods to investigate these systems...

3.3.1 Solution

4 Prospects and Challenges for Quantum Machine Learning (October 14-16)

4.1 Exercise 1

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

4.1.1 Solution

a) $\forall a, b \in \{\mathbb{I}, \mathbf{X}\}$, $a + b = c$, with $c \in \{\mathbf{1}, \mathbf{X}\}$:

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

Here we also prove that $a \cdot b = b \cdot a$ for this group $\{\mathbb{I}, \mathbf{X}\}$.

b) Associativity:

$$(\mathbb{I} \cdot \mathbb{I}) \cdot \mathbf{X} = \mathbf{X}, \quad \text{and} \quad (\mathbb{I} \cdot \mathbf{X}) \cdot \mathbb{I} = \mathbf{X},$$
$$(\mathbf{X} \cdot \mathbf{X}) \cdot \mathbb{I} = \mathbb{I} \quad \text{and} \quad \mathbf{X} \cdot (\mathbb{I} \cdot \mathbf{X}) = \mathbb{I}$$

c) Existence of identity element:

$$\forall a, \mathbf{E} \in \{\mathbb{I}, \mathbf{X}\}, \exists \mathbf{E},\ a \cdot \mathbf{E} = a \quad \text{with} \quad \mathbf{E} \in \{\mathbb{I}, \mathbf{X}\} :$$

$$\mathbb{I} \cdot \mathbf{E} = \mathbb{I} \quad (\Rightarrow \mathbf{E} = \mathbb{I}) \quad \text{and} \quad \mathbf{X} \cdot \mathbf{E} = \mathbf{X} \quad (\Rightarrow \mathbf{E} = \mathbb{I}) \quad \text{therefore is} \quad \mathbf{E} = \mathbb{I}.$$

d) Existence of inverse element:

$$\forall A, B \in \{\mathbb{I}, \mathbf{X}\}, \exists B, A \cdot B = \mathbb{I} :$$

$$\mathbf{X} \cdot \mathbf{X} = \mathbb{I},$$

$$\mathbb{I} \cdot \mathbb{I} = \mathbb{I}.$$

4.2 Exercise 2

Prove that the set of all unitary operators 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 $SU(2)$.

4.2.1 Solution

$$U^\dagger U = UU^\dagger = \mathbb{I}, \quad \det(U) = 1$$

First, given $U = e^{-i\theta_3 Y - i\theta_2 X - i\theta_1 Y}$, where we define:

$$U_3 = e^{-i\theta_3 Y}, \quad U_2 = e^{-i\theta_2 X}, \quad U_1 = e^{-i\theta_1 Y}$$

Knowing that:

$$e^{-i\alpha x} = \cos(\alpha x) - i\sin(\alpha x)$$

we have:

$$\cos(\alpha x) = \sum_{n=0}^{\infty} \frac{(-1)^n(\alpha^2)^n x^{2n}}{(2n)!}$$

$$\sin(\alpha x) = \sum_{n=0}^{\infty} \frac{(-1)^n(\alpha^2)^n x^{2n+1}}{(2n+1)!},$$

if α is a Pauli matrix

$$\alpha^{2n} = \mathbb{I}, \quad \alpha^{2n+1} = \alpha$$

Therefore:

$$e^{-i\alpha\varphi} = \mathbb{I}\cos(\varphi) - iA\sin(\varphi)$$

So:

$$U_i(A) = \mathbb{I}\cos\phi_i - iA\sin\phi_i$$

a) det$(U) = 1$

Using the property $\det(A)\cdot\det(B) = \det(A\cdot B)$, and that for $\det(U_3) = \det(U_2) = \det(U_1) = 1 \Rightarrow \det(U) = 1$.

Now, let's verify:

$$\det(U_3) = \det(\begin{pmatrix} \cos\phi_3 & 0 \\ 0 & \cos\phi_3 \end{pmatrix} - \begin{pmatrix} 0 & -\sin\phi_3 \\ \sin\phi_3 & 0 \end{pmatrix}) =$$

$$\det \begin{pmatrix} \cos\phi_3 & \sin\phi_3 \\ -\sin\phi_3 & \cos\phi_3 \end{pmatrix} = 1$$

And it is easy to see that the same applies for U_1, so :

$$\det(U_1) = \det \begin{pmatrix} \cos\phi_1 & \sin\phi_1 \\ -\sin\phi_1 & \cos\phi_1 \end{pmatrix} = 1$$

Thus, for U_2,

$$\det(U_2) = \det(\begin{pmatrix} \cos\phi_2 & 0 \\ 0 & \cos\phi_2 \end{pmatrix} - \begin{pmatrix} 0 & i\sin\phi_2 \\ i\sin\phi_2 & 0 \end{pmatrix}) =$$

$$\det \begin{pmatrix} \cos\phi_2 & -i\sin\phi_2 \\ -i\sin\phi_2 & \cos\phi_2 \end{pmatrix} = 1$$

Hence, we obtain:

$$\det(U_1) \cdot \det(U_2) \cdot \det(U_3) = \det(U) = 1$$

b) $U^\dagger U = UU^\dagger = \mathbb{I}$

We recall that $U = U_3 \cdot U_2 \cdot U_1$, and using the property $(AB)^\dagger = B^\dagger A^\dagger$, we see that:

$$(U_3 U_2 U_1)^\dagger = U_1^\dagger U_2^\dagger U_3^\dagger$$

Now, we verify that:

$$UU^\dagger = U_3 U_2 U_1 U_1^\dagger U_2^\dagger U_3^\dagger$$

We calculate that:

$$U_1 = \begin{pmatrix} \cos\phi_1 & \sin\phi_1 \\ -\sin\phi_1 & \cos\phi_1 \end{pmatrix}, \quad U_2 = \begin{pmatrix} \cos\phi_2 & -i\sin\phi_2 \\ -i\sin\phi_2 & \cos\phi_2 \end{pmatrix}, \quad U_3 = \begin{pmatrix} \cos\phi_3 & \sin\phi_3 \\ -\sin\phi_3 & \cos\phi_3 \end{pmatrix}$$

and

$$U_1^\dagger = \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 \\ \sin\phi_1 & \cos\phi_1 \end{pmatrix}, \quad U_2^\dagger = \begin{pmatrix} \cos\phi_2 & i\sin\phi_2 \\ i\sin\phi_2 & \cos\phi_2 \end{pmatrix}, \quad U_3^\dagger = \begin{pmatrix} \cos\phi_3 & -\sin\phi_3 \\ \sin\phi_3 & \cos\phi_3 \end{pmatrix}$$

Finally:

$$U_1U_1^\dagger = \begin{pmatrix} \cos\phi_1 & \sin\phi_1 \\ -\sin\phi_1 & \cos\phi_1 \end{pmatrix} \begin{pmatrix} \cos\phi_1 & -\sin\phi_1 \\ \sin\phi_1 & \cos\phi_1 \end{pmatrix}$$

$$U_1U_1^\dagger = \begin{pmatrix} \cos^2\phi_1 + \sin^2\phi_1 & 0 \\ 0 & \cos^2\phi_1 + \sin^2\phi_1 \end{pmatrix}$$

$$U_1U_1^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

And it is easy to see that the same applies for U_3, so :

$$U_3U_3^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$U_2 = \begin{pmatrix} \cos\phi_2 & -i\sin\phi_2 \\ -i\sin\phi_2 & \cos\phi_2 \end{pmatrix}, \quad U_2^\dagger = \begin{pmatrix} \cos\phi_2 & i\sin\phi_2 \\ i\sin\phi_2 & \cos\phi_2 \end{pmatrix}$$

$$U_2U_2^\dagger = \begin{pmatrix} \cos^2\phi_2 + \sin^2\phi_2 & 0 \\ 0 & \cos^2\phi_2 + \sin^2\phi_2 \end{pmatrix}$$

$$U_2U_2^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Thus, we conclude that:

$$UU^\dagger = U_3U_2U_1U_1^\dagger U_2^\dagger U_3^\dagger = \mathbb{I}$$

c) Prove that σ_x and σ_y generate the Lie group.

$$\{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}$$

To prove , we just need to show that:

$$\sigma_x \cdot \sigma_x = \mathbb{I} \quad \text{and} \quad [\sigma_x, \sigma_y] = 2i\sigma_z$$

Start with the following matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

First Calculate:

$$\sigma_{\mathbf{x}} \cdot \sigma_{\mathbf{x}} = \mathbb{I}, \quad since \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

Now, calculate $[\sigma_x, \sigma_y]$:

$$\sigma_x\sigma_y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_z$$

$$\sigma_y\sigma_x = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z$$

Thus:

$$[\sigma_x, \sigma_y] = \sigma_x\sigma_y - \sigma_y\sigma_x = 2i\sigma_z$$

4.3 Challenge 3

Show that the dimension D of the commutant $C^{(k)}(G)$, outlined in Definition 8 of the lecture notes, is determined by

$$D = \lambda m^2 \lambda.$$

4.3.1 Solution

5 High Dimensional Quantum Communication with Structured Light (October 14, 16-17)

5.1 Exercise 1

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

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

- $\int HG^*_\theta(x,y) HG_\theta(x,y)\, dx\, dy = 1$
- $\int HG^*_\theta(x,y) HG_\theta + \frac{\pi}{2}(x,y)\, dx\, dy = 0$
- $LG\pm(r,\phi) = \frac{1}{\sqrt{2}}\left[HG_{10}(x,y) + iHG_{01}(x,y)\right]$

5.1.1 Solution

We have:

$$\int HG^*(x,y) H_G(x,y) dxdy = 1$$

Now, let's expand the terms:

$$\int \cos\theta\left(HG_{10}{}^*(x,y) + \sin\theta HG_{01}{}^*(x,y)\right)\left(\cos\theta HG_{10}(x,y) + \sin\theta HG_{01}(x,y)\right) dxdy$$

$$= \int \cos^2\theta HG_{10}{}^*(x,y) HG_{10}(x,y) + \sin\theta\cos\theta\left(HG_{10}{}^*(x,y) HG_{01}(x,y) + HG_{01}{}^*(x,y) HG_{10}(x,y)\right)$$

$$+ \sin^2\theta HG_{01}{}^*(x,y) HG_{01}(x,y) dxdy$$

Since:

$$\int HG_{10}{}^*(x,y) HG_{01}(x,y) dxdy = 0$$

we obtain:

$$\cos^2\theta + \sin^2\theta = 1$$

For the second part:

$$\int (HG_{10}{}^* \cos\theta + HG_{01}{}^* \sin\theta) \left(HG_{10} \cos(\theta + \frac{\pi}{2}) + HG_{01} \sin(\theta + \frac{\pi}{2})\right) dxdy =$$

regarding:

$$\cos(\theta + \frac{\pi}{2}) = -\sin(\theta) \quad , \quad \sin(\theta + \frac{\pi}{2}) = \cos(\theta)$$

We get:

$$= \int -\cos\theta \sin\theta HG_{10}{}^* HG_{10} + \sin\theta \cos\theta HG_{01}{}^* HG_{01} dxdy +$$

$$+ \int \cos^2\theta HG_{10}{}^* HG_{01} - \sin^2\theta HG_{10}{}^* HG_{01} dxdy$$

Thus, we conclude:

$$-\cos\theta \sin\theta(1) + \cos\theta \sin\theta(1) + \cos^2\theta(0) - \sin^2\theta(0) = 0$$

5.2 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 $u_{nm}(x, y) = \langle x, y | u_{nm} \rangle$.

5.2.1 Solution

Given:

$$\langle a|b\rangle^* = \langle b|a\rangle$$

We also have:

$$u_{n,m} = \langle x, y | u_{n,m} \rangle$$

Thus:

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

$$= \sum_{n,m} \langle x, y | u_{n,m} \rangle \langle u_{n,m} | x', y' \rangle \quad \Rightarrow \quad \sum_{n,m} |u_{n,m}\rangle \langle u_{n,m}| = \mathbb{I}$$

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

5.3 Challenge 3

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

$$\hat{e}_\theta = \cos\theta \, \hat{e}_H + \sin\theta \, \hat{e}_V \tag{20}$$

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

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

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

are rotation invariant.

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

5.3.1 Solution