Quantum Computing for Nuclear Physics

Nuclear Talent course

June 16-July 4, 2025

Project suggestion

The aim of this project is to study the so-called Lipkin model (which is a simplified Hamiltonian) using the VQE algorithm. The total score is 100 points. You can answer each exercise in a sequential way or write a scientific report. Each exercise is given a final score. If you plan to write a report, you could use the article in the Physical Review C, volume 106, see https://journals.aps.org/prc/pdf/10.1103/PhysRevC.106.024319 as a template for your report.

Part a) (score 10pt)

Write a function which sets up a one-qubit basis and apply the various Pauli matrices to these basis states. Apply the Hadamard and Phase gates to the same one-qubit basis states and study their actions on these states. Define also Bell states and write a code where you implement a Hadamard gate and thereafter a **CNOT** gate on one of the Bell states of your choice. Perform thereafter a measurement on the first qubit and thereafter on the second qubit. The measurements should be performed several times and it is the average results of these measurements which should be discussed and presented.

Compare your code with the results obtained using for example software like **Qiskit**.

Part b) (score 10pt)

We define a symmetric matrix $H \in \mathbb{R}^{2\times2}$

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix},$$

We let $H = H_0 + H_I$, where

$$H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix},$$

is a diagonal matrix. Similarly,

$$H_I = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix},$$

where V_{ij} represent various interaction matrix elements. We can view H_0 as the non-interacting solution

$$H_0|0\rangle = E_1|0\rangle, \tag{1}$$

and

$$H_0|1\rangle = E_2|1\rangle, \tag{2}$$

where we have defined the orthogonal computational one-qubit basis states $|0\rangle$ and $|1\rangle$.

We rewrite H (and H_0 and H_I) via Pauli matrices

$$H_0 = \mathcal{E}I + \Omega\sigma_z, \quad \mathcal{E} = \frac{E_1 + E_2}{2}, \ \Omega = \frac{E_1 - E_2}{2},$$

and

$$H_I = c\boldsymbol{I} + \omega_z\sigma_z + \omega_x\sigma_x,$$

with $c = (V_{11} + V_{22})/2$, $\omega_z = (V_{11} - V_{22})/2$ and $\omega_x = V_{12} = V_{21}$. We let our Hamiltonian depend linearly on a strength parameter λ

$$H = H_0 + \lambda H_\mathrm{I},$$

with $\lambda \in [0, 1]$, where the limits $\lambda = 0$ and $\lambda = 1$ represent the non-interacting (or unperturbed) and fully interacting system, respectively. The model is an eigenvalue problem with only two available states.

Here we set the parameters $E_1 = 0$, $E_2 = 4$, $V_{11} = -V_{22} = 3$ and $V_{12} = V_{21} = 0.2$.

The non-interacting solutions represent our computational basis. Pertinent to our choice of parameters, is that at $\lambda \geq 2/3$, the lowest eigenstate is dominated by $|1\rangle$ while the upper is $|0\rangle$. At $\lambda = 1$ the $|0\rangle$ mixing of the lowest eigenvalue is 1% while for $\lambda \leq 2/3$ we have a $|0\rangle$ component of more than 90%. The character of the eigenvectors has therefore been interchanged when passing $z = 2/3$. The value of the parameter V_{12} represents the strength of the coupling between the two states..

Solve **by standard eigenvalue solvers** (either numerically or analytically) the above eigenvalue problem. Find the two eigenvalues as function of the interaction strength λ. Study the behavior of these eigenstates as functions of the interaction strength λ. Comment your results.

Part c) (score 10pt)

Implement now the variational quantum eigensolver (VQE) for the above Hamiltonian and set up the circuit(s) which is(are) needed in order to find the eigenvalues of this system. Discuss the results and compare these with those from part b). Feel free to use either **Qiskit** or your own code (based on the setup from part a)) or both approaches. Discuss your results.

Part d) (score 15pt)

Extend part c) to a two-qubit system with the following computational basis states and Hamiltonian matrix written out in terms of Pauli spin matrices.

This system can be thought of as composed of two subsystems A and B. Each subsystem has computational basis states

$$|0\rangle_{A,B} = \begin{bmatrix} 1 & 0 \end{bmatrix}^T \qquad |1\rangle_{A,B} = \begin{bmatrix} 0 & 1 \end{bmatrix}^T.$$

The subsystems could represent single particles or composite many-particle systems of a given symmetry. This leads to the many-body computational basis states

$$|00\rangle = |0\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 1 & 0 & 0 & 0 \end{bmatrix}^T,$$

and

$$|01\rangle = |0\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 1 & 0 & 0 \end{bmatrix}^T,$$

and

$$|10\rangle = |1\rangle_A \otimes |0\rangle_B = \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^T,$$

and finally

$$|11\rangle = |1\rangle_A \otimes |1\rangle_B = \begin{bmatrix} 0 & 0 & 0 & 1 \end{bmatrix}^T.$$

These computational basis states define also the eigenstates of the non-interacting Hamiltonian

$$H_0|00\rangle = \epsilon_{00}|00\rangle,$$
$$H_0|10\rangle = \epsilon_{10}|10\rangle,$$
$$H_0|01\rangle = \epsilon_{01}|01\rangle,$$

and

$$H_0|11\rangle = \epsilon_{11}|11\rangle.$$

The interacting part of the Hamiltonian H_I is given by the tensor product of two σ_x and σ_z matrices, respectively, that is

$$H_I = H_x \sigma_x \otimes \sigma_x + H_z \sigma_z \otimes \sigma_z,$$

where H_x and H_z are interaction strength parameters. Our final Hamiltonian matrix is given by

$$\boldsymbol{H} = \begin{bmatrix} \epsilon_{00} + H_z & 0 & 0 & H_x \\ 0 & \epsilon_{10} - H_z & H_x & 0 \\ 0 & H_x & \epsilon_{01} - H_z & 0 \\ H_x & 0 & 0 & \epsilon_{11} + H_z \end{bmatrix}.$$

The four eigenstates of the above Hamiltonian matrix can in turn be used to define density matrices. As an example, the density matrix of the first eigenstate (lowest energy E_0) Ψ_0 is

$$\rho_0 = \left(\alpha_{00}|00\rangle\langle 00| + \alpha_{10}|10\rangle\langle 10| + \alpha_{01}|01\rangle\langle 01| + \alpha_{11}|11\rangle\langle 11| \right),$$

where the coefficients α_{ij} are the eigenvector coefficients resulting from the solution of the above eigenvalue problem.

We can then in turn define the density matrix for the subsets A or B as

$$\rho_A = \mathrm{Tr}_B(\rho_0) = \langle 0|\rho_0|0\rangle_B + \langle 1|\rho_0|1\rangle_B,$$

or

$$\rho_B = \mathrm{Tr}_A(\rho_0) = \langle 0|\rho_0|0\rangle_A + \langle 1|\rho_0|1\rangle_A.$$

The density matrices for these subsets can be used to compute the so-called von Neumann entropy, which is one of the possible measures of entanglement. A pure state has entropy equal zero while entangled state have an entropy larger than zero. The von-Neumann entropy is defined as

$$S(A,B) = -\mathrm{Tr}\left(\rho_{A,B} \log_2(\rho_{A,B})\right).$$

You can select parameter values (or other of your choice)

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Hx = 2.0
Hz = 3.0
# H_0
Energiesnoninteracting = [0.0, 2.5, 6.5, 7.0]
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Compute the eigenvalues **using standard eigenvalue solvers** as functions of the interaction strength λ and study the role of entanglement. Compute thereafter the Von Neumann entropy for one of the subsystems using the denisty matrix of the lowest two-body state . Comment your results.

The example here shows the above von Neumann entropy based on the density matrix for the lowest many-body state. We see clearly a jump in the entropy around the point where we have a level crossing. At interaction strenght $\lambda = 0$ we have many-body states purely defined by their computational basis states. As we switch on the interaction strength, we obtain an increased degree of mixing and the entropy increases till we reach the level crossing point where we see an additional and sudden increase in entropy. Similar behaviors are observed for the other states. The most important result from this example is that entanglement is driven by the Hamiltonian itself and the strength of the interaction matrix elements and the non-interacting energies.

Part e) (score 15 pt)

Compute now the eigenvalues of this system using the VQE method and set up the circuits needed to find the lowest state. Compare these results with those from the previous part. Feel free again to either use your own code for the circuit and your VQE code or use the functionality of Qiskit, or both.

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Part f) (score 20 pt)

We introduce now the Lipkin Hamiltonian and study this for the 3×3 matrix case with total spin $J = 1$ and the 5×5 matrix for the $J = 2$ case. We will follow closely the article in the Physical Review C, volume 106, see https://journals.aps.org/prc/pdf/10.1103/PhysRevC.106.024319.

The Hamiltonian in second quantization is given by

$$H = H_0 + H_1 + H_2,$$

with

$$H_0 = \frac{1}{2}\varepsilon \sum_{p\sigma} \sigma a_{p\sigma}^\dagger a_{p\sigma},$$

and

$$H_1 = \frac{1}{2}V \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p'\sigma}^\dagger a_{p'-\sigma} a_{p-\sigma},$$

and

$$H_2 = \frac{1}{2}W \sum_{p,p',\sigma} a_{p\sigma}^\dagger a_{p'-\sigma}^\dagger a_{p'\sigma} a_{p-\sigma}.$$

We can rewrite this Hamiltonian in terms of the so-called quasispin operators leading to

$$H_0 = \varepsilon J_z, \tag{3}$$

and

$$H_1 = \frac{1}{2}V \left(J_+^2 + J_-^2 \right). \tag{4}$$

$$H_2 = \frac{1}{2}W \left(-N + J_+ J_- + J_- J_+ \right). \tag{5}$$

We start here with a simpler case, namely the $J = 1$ case and we set $W = 0$. Show that Hamiltonian matrix is then given by

$$H_{J=1} = \begin{pmatrix} -\epsilon & 0 & -V \\ 0 & 0 & 0 \\ -V & 0 & \epsilon \end{pmatrix} \tag{6}$$

To solve the above hamiltonian problem on a quantum computer we need to rewrite the Hamiltonian in terms of the Pauli spin matrices. Rewrite the above $J = 1$ Hamiltonian (with $N = 2$ particles) in terms of the Pauli matrices and the identity matrix.

For $J = 2$ we have a 5×5 matrix given by

$$H_{J=2} = \begin{pmatrix} -2\varepsilon & 0 & \sqrt{6}V & 0 & 0 \\ 0 & -\varepsilon + 3W & 0 & 3V & 0 \\ \sqrt{6}V & 0 & 4W & 0 & \sqrt{6}V \\ 0 & 3V & 0 & \varepsilon + 3W & 0 \\ 0 & 0 & \sqrt{6}V & 0 & 2\varepsilon \end{pmatrix} \tag{7}$$

Find also the $J = 2$ Hamiltonian ($N = 4$ particles) in terms of the same matrices (still with $W = 0$).

Challenge: Set up the Hamiltonian with the W term as well in terms of the Pauli spin matrices.

Diagonalize thereafter, using classical methods, the above Hamiltonian matrices and find the eigenvalues as functions of the strength of the interaction V while keeping the single-particle energies fixed. Comment your results. Feel free to add the Hartree-Fock results as discussed in the lectures.

Part g) (score 20 pt)

Use now the VQE method to find the same eigenvalues as in part f) and set up the circuits and simulations which are needed. Compare your results with those from part f) and comment your results.

The preferred format for the report is a PDF file. You can also use DOC or postscript formats or as an ipython notebook file. As programming language we prefer that you choose between C/C++, Fortran2008 or Python. The following prescription should be followed when preparing the report:

- Send us an email in order to hand in your projects with a link to your GitHub/Gitlab repository.

- In your GitHub/GitLab or similar repository, please include a folder which contains selected results. These can be in the form of output from your code for a selected set of runs and input parameters.

Finally, we encourage you to collaborate. Optimal working groups consist of 2-3 students. You can then hand in a common report.