

* Example system : The deuteron.

A pioneering calculation in the area of nuclear phy was done in

Dumitrescu et al, Phys. Rev. Lett 121, 210501
(2018)

where the authors applied VQE to determine the deuteron ground state with a quantum computer.

This was the 1st (cloud) quantum simulation of an atomic nucleus.

The deuteron is a system of one proton and one neutron - It is the only bound two-nucleon system with a binding energy:

$$E_{gs} = 2.225 \text{ MeV}$$

The deuteron wf $|1\rangle$ has quantum numbers

$$\left\{ \begin{array}{l} J=1 \quad (\text{total angular momentum}) \\ \pi=+ \quad (\text{parity}) \quad \pi=(-)^L \\ T=0 \quad (\text{isospin}) \end{array} \right. \quad \vec{J} = \vec{L} + \vec{S}$$

Because of Pauli principle the wave function of the deuteron must be antisymmetric in exch. the two nucleons

$$\Rightarrow (-)^{L+S+T} = (-)$$

$$\Rightarrow L + S + T = \text{odd}.$$

we have

$$T = +1 \Rightarrow L \text{ is even}$$

$$\Rightarrow S + T = \text{odd}$$

also $J=1 \Rightarrow \left\{ \begin{array}{l} S=0, L=1 \\ \text{or} \\ L+S \leq J \leq |L-S| \\ S=1, L=0 \\ S=1, L=2 \end{array} \right\} \Rightarrow T=0$

\Rightarrow The ground state of the deuteron is a superposition of $(L=0, S=1, T=0)$ and $(L=2, S=1, T=0)$ components.

The $L=0$ (s-wave compo) has a weight $\sim 94\%$.
The $L=2$ (d-wave comp) $\sim 6\%$.

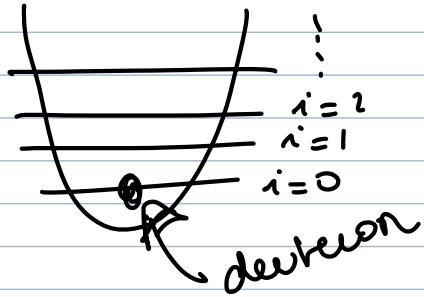
(The $L=2$ component originates from the tensor part of the nuclear force, and leads to the (small) quadrupole deformation of the deuteron)

In the paper the authors described the deuteron in a harmonic oscillator basis, and neglected the $L=2$ component.

The Hamiltonian can then be written:

$$\hat{H}_M = \sum_{i,j=0}^{N-1} \langle x_i | (\hat{T} + \hat{V}) | x_j \rangle a_i^\dagger a_j$$

where a_i^\dagger / a_i creates/annihilates a deuteron in the harmonic oscillator s-wave ($L=0$) state $|i\rangle$.



\hat{T} and \hat{V} are kinetic and potential energy operators, with matrix elements:

$$\begin{aligned} \langle x_i | T | x_j \rangle &= \frac{\hbar\omega}{2} \left[(2j+3/2) \delta_{ji} - \sqrt{j(j+1/2)} \delta_{j,i+1} \right. \\ &\quad \left. - \sqrt{(j+1)(j+3/2)} \delta_{j,i-1} \right] \end{aligned}$$

$$\langle x_i | V | x_j \rangle = V_0 \delta_{ij} \delta_{i0}$$

with $V_0 = -5.6866 \text{ meV}$, $\hbar\omega = 7 \text{ meV}$

⚠ here it is actually the kinetic energy which mixes the basis states

basis

The v states of the system are

$$|n_{M-1} \ n_{M-2} \dots \ n_0\rangle$$

where $n_i = 0, 1$

and $\sum_{i=0}^{M-1} n_i = 1$

(there is only one deuteron).

$|00\dots 1 \dots 00\rangle$ = state where the deuteron
is in state $|X_i\rangle$

• mapping the system onto qubits:

The authors used the Jordan-Wigner mapping

$$|n_{M-1} \dots \ n_0\rangle \rightarrow |\alpha_{M-1} \dots \ \alpha_0\rangle$$

where $\alpha_i = n_i$

Mapping the Hamiltonian?

It is useful to rewrite

$$H_{\text{TF}} = \sum_{ij} \langle X_i | T + V | X_j \rangle a_i^+ a_j^-$$

$$= \sum_{\substack{i \\ (j=i)}} \langle X_i | T + V | X_i \rangle a_i^+ a_i^-$$

$$+ \sum_{i>j} \langle X_i | T + V | X_j \rangle a_i^+ a_j^-$$

$$+ \sum_{\substack{i < j \\ i \downarrow \\ j \downarrow \\ i}} \langle X_i | T + V | X_j \rangle a_i^+ a_j^-$$

$$= \langle X_i | T | X_j \rangle$$

(rename dummy indices)

$$= \sum_i \langle X_i | T + V | X_i \rangle a_i^+ a_i^-$$

$$+ \sum_{i>j} \langle X_i | T | X_j \rangle (a_i^+ a_j^- + a_j^+ a_i^-)$$

using the Jordan-Wigner mapping

$$\left\{ \begin{array}{l} a_i^+ \rightarrow \left(\frac{\pi}{\hbar} z_k \right) \sigma_i^- \\ a_j^- \rightarrow \left(\frac{\pi}{\hbar} z_\ell \right) \sigma_j^+ \end{array} \right.$$

$$\left\{ \begin{array}{l} a_i^+ \rightarrow \left(\frac{\pi}{\hbar} z_k \right) \sigma_i^- \\ a_j^- \rightarrow \left(\frac{\pi}{\hbar} z_\ell \right) \sigma_j^+ \end{array} \right.$$

$$a_i^+ a_j^- \rightarrow \left(\prod_{k>i} z_k \right) \sigma_i^- \left(\prod_{l>j} z_l \right) \sigma_j^+$$

$$= \left(\prod_{k>i} \underbrace{z_k^2}_{d} \right) \underbrace{\sigma_i^- z_i^-}_{\sigma_i^-} \left(\prod_{i>l>j} z_l \right) \sigma_j^+$$

for $i > j$

$$= \left(\prod_{i>l>j} z_l \right) \sigma_i^- \sigma_j^+$$

Similarly

$$a_j^+ a_i^- \rightarrow \left(\prod_{l>j} z_l \right) \sigma_j^- \left(\prod_{k>i} z_k \right) \sigma_i^+$$

$$= \left(\prod_{i>l>j} z_l \right) \sigma_j^- \underbrace{z_i^- \sigma_i^+}_{\sigma_i^+}$$

$$= \left(\prod_{i>l>j} z_l \right) \sigma_i^+ \sigma_j^-$$

$$\Rightarrow a_i^+ a_j^- + a_j^+ a_i^-$$

$$\equiv \left(\prod_{i>l>j} z_l \right) (\sigma_i^- \sigma_j^+ + \sigma_i^+ \sigma_j^-)$$

J

$$\Rightarrow \alpha_i^+ \alpha_j^- + \alpha_j^+ \alpha_i^-$$

$$\equiv \begin{pmatrix} \pi & z_e \\ i\sigma_i & j\sigma_j \end{pmatrix} \frac{1}{2} (x_i x_j + y_i y_j)$$

and

$$\alpha_i^+ \alpha_i^- = \begin{pmatrix} \pi & z_e \\ i\sigma_i & j\sigma_j \end{pmatrix} \sigma_i^- - \begin{pmatrix} \pi & z_e \\ j\sigma_j & i\sigma_i \end{pmatrix} \sigma_i^+$$

$$= \begin{pmatrix} \pi & z_e^2 \\ i\sigma_i & \frac{1}{4} \end{pmatrix} \sigma_i^- \sigma_i^+$$

$$= \frac{1}{4} (x_i^- \bar{x}_i^+ y_i^-) (x_i^+ \bar{y}_i^-)$$

$$= \frac{1}{4} \left(\underbrace{x_i^2}_{1} + \underbrace{i x_i y_i}_{i/2} - \underbrace{i y_i x_i}_{-i z_i} + \underbrace{y_i^2}_{1} \right)$$

$$= \frac{1}{2} (1 - z_i^-)$$

$$\Rightarrow \boxed{\alpha_i^+ \alpha_i^- \equiv \frac{1}{2} (1 - z_i^-)}$$

Notes :

- $\begin{cases} z \sigma^\pm = \pm \sigma^\pm \\ \sigma^\pm z = \mp \sigma^\pm \end{cases}$

- qubit operators acting on \neq qubits commute.

$$H_{\text{eff}} \rightarrow H_{\text{qubits}}^{\text{JW}} = \frac{1}{2} \sum_{i=0}^{n-1} \langle i | T+V | i \rangle (z_i - z_i)$$

$$+ \frac{1}{2} \sum_{\substack{i,j=0 \\ i>j}}^{n-1} \left(\langle i | T | z_j \rangle \right) V_{ij} (x_i x_j + y_i y_j)$$

The authors of the study considered

$$M = 1, 2, 3$$

- Case $M=1$ \rightarrow 1 qubit state $|X_0\rangle$

$$H_1 = \langle X_0 | T+V | X_0 \rangle a_0^\dagger a_0$$

$$= \left[\frac{\hbar\omega}{2} \times \frac{3}{2} + V_0 \right] a_0^\dagger a_0.$$

\leadsto mapping onto 1 qubit is trivial

$$H_1 = \left(\frac{3\hbar\omega}{4} + V_0 \right) \times \frac{1}{2} (z_0 - z_0).$$

$$|n_0\rangle = |0\rangle, |1\rangle \rightarrow |x_0\rangle = |0\rangle, |1\rangle$$

due to preservation of particle #
 (we have one electron) the 2 states
 do not mix

$|x_0\rangle = |0\rangle$ is unphysical
(state with no deuteron).

\Rightarrow the ground state is simply

$|4\rangle = |x_0=1\rangle$ with energy

$$\langle 4 | H_1 | 4 \rangle = \left(\frac{3\hbar\omega}{4} + V_0 \right) \times \underbrace{\frac{1}{2} \langle 1 | 1 - z_0 | 1 \rangle}_{1+1}$$

$$= \left(\frac{3\hbar\omega}{4} + V_0 \right)$$

- Case $H=2$ 2 deuteron states
 $i=0, 1.$

~~$\sum_{i=1}^2$~~

$$H_2 = \sum_{i=0,1} \langle \chi_i | T + V | \chi_i \rangle a_i^\dagger a_i + \langle \chi_1 | T | \chi_0 \rangle (a_1^\dagger a_0 + a_0^\dagger a_1)$$

with basis states

$$|n_1 n_0\rangle = \underbrace{|00\rangle, |01\rangle, |10\rangle}_{\text{unphysical}} , |11\rangle \underbrace{|11\rangle}_{\text{unphysical}} \quad (0 \text{ deuteron}) \quad (2 \text{ deuterons})$$

→ mapping onto 2 qubits:

$$|n_1 n_0\rangle \equiv |x_1 x_0\rangle$$

$$H_2 \equiv \sum_{i=0,1} \langle x_i | T + V | x_i \rangle \frac{1}{2} (d - z_i)$$

$$+ \frac{1}{2} \langle x_i | T | x_0 \rangle (x_i x_0 + y_i y_0)$$

$$\approx 5.91 d + 0.22 z_0 - 6.13 z_1 \\ - 2.14 (x_i x_0 + y_i y_0)$$

Hence

$$H_2^{\text{JW}} = \frac{1}{2} (d - z_0) \langle x_0 | H_2 | x_0 \rangle \\ + \frac{1}{2} (d - z_1) \langle x_1 | H_2 | x_1 \rangle$$

$$+ \frac{1}{2} (x_i x_0 + y_i y_0) \langle x_0 | H_2 | x_1 \rangle$$

$$= \boxed{\frac{1}{2} (H_2^{\infty} + H_2'')} d$$

$$5.9067 = \boxed{-\frac{1}{2} (H_2^{\infty})} z_0 \quad \boxed{-\frac{1}{2} H_2''} z_1 \\ 0.2829 = -6.125$$

$$+ \boxed{\frac{1}{2} H_2'} (x x + y y)$$

$$- 2.1433$$

The ground state of this Hamiltonian can be found using, for example, VQE with an general ansatz for the (real) two-qubit state as seen previously -

We see, however, that due to particle number conservation (we have exactly 1 deuteron) only 2 basis states $|\alpha_1 \alpha_2\rangle = |10\rangle$ and $|01\rangle$ are relevant and will contribute to the ground state (the others $|00\rangle, |11\rangle$ will have zero amplitude)

This can be seen easily ^{see} from the matrix

$$H_2^{\text{JW}} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \begin{array}{|cc|} -0.44 & -4.28 \\ -4.28 & 12.26 \end{array} & 0 \\ 0 & \begin{array}{|cc|} 0 & 0 \end{array} & 11.82 \end{pmatrix} \begin{array}{l} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{array} \text{ rep:}$$

only this part is relevant.

(The states $|00\rangle$ & $|11\rangle$ do not couple to anything)

\Rightarrow In fact this system can be mapped to 1 qubit only:

$$|\eta_1 \eta_0\rangle = |01\rangle \rightarrow |0\rangle$$

$$= |10\rangle \rightarrow |1\rangle .$$

$$\text{with } 1\text{-qubit Hami:} = \begin{pmatrix} -0.44 & -4.28 \\ -4.28 & 12.26 \end{pmatrix}$$

$$= \alpha_1 + \beta x + \gamma y + \delta z$$

\parallel \parallel
 -4.28 0

$$\begin{aligned} \alpha + \delta &= -0.44 \\ \alpha - \delta &= 12.26 \end{aligned} \quad \left. \right\} \Rightarrow \begin{aligned} \alpha &\approx 5.91 \\ \delta &\approx -6.35 \end{aligned}$$

This is an example of how symmetries (here particle number) can be used to solve problems more efficiently with QC).

• Case ... $\gamma = 3$ 3 deuteron states X_i ($i=0,1,2$)

$$\sum_{i=0}^2$$

$$H_3 = \sum_{i=0,1,2} \langle X_i | T + V | X_i \rangle a_i^\dagger a_i$$

$$+ \langle X_2 | T | X_1 \rangle (a_2^\dagger a_1 + a_1^\dagger a_2)$$

$$+ \langle X_2 | T | X_0 \rangle (a_2^\dagger a_0 + a_0^\dagger a_2)$$

$$+ \langle X_1 | T | X_0 \rangle (a_1^\dagger a_0 + a_0^\dagger a_1)$$

mapping onto 3 qubits :

$$\Rightarrow H_3^{JW} = H_2^{JW} + 9.6 (d - z_2) - 3.91 (x_2 x_1 + y_2 y_1).$$

Similarly the dimensionality of the problem can also be reduced since only 3 basis states:

$$|n_2 n_1 n_0\rangle = |001\rangle, |010\rangle, |100\rangle$$

relevant, and thus 2 qubits are enough, for ex, one could adopt the mapping

$$|n_2 n_1 n_0\rangle$$

$$|001\rangle$$

$$|z_1 z_0\rangle$$

$$\longrightarrow |00\rangle$$

$$|010\rangle \longrightarrow |01\rangle$$

$$|100\rangle \longrightarrow |10\rangle.$$

(with one state
|11⟩ unused)

VQE simulations :

n -qubit states can be generally parameterized with a # of angles which grows $\exp(n)$.

The authors of the study used an approx ansatz which scales better with increasing number of qubits -

This type of ansatz is known as unitary coupled cluster (UCC) ansatz, and is based on exponentials of particle-excitation operators.

$$|\Psi\rangle = U(\vec{\theta}) |\Phi_0\rangle$$

simple tensor-product state with correct particle #. (cphat-basis state).

For ex : 0 for $\eta=2$ (2 qubits) they have

$$|14\rangle = U(0) |01\rangle$$

with $U(\theta) = e^{-\theta(a_1^+ a_0 - a_0^+ a_1)}$

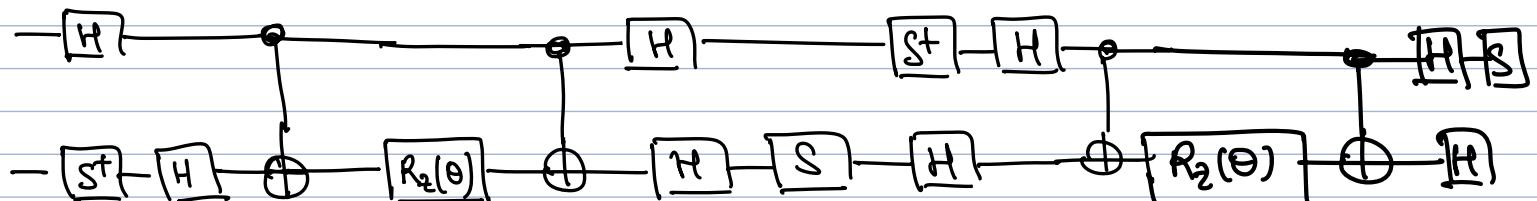
$a_0^+ a_1 - a_1^+ a_0$ maps onto (with JW mapping)

$$\mapsto \sigma_1^- \sigma_0^+ - \sigma_1^+ \sigma_0^-$$

$$= \frac{i}{2} [x_1 y_0 - y_1 x_0] - \frac{i\theta}{2} (x_1 y_0 - y_1 x_0)$$

$$U(\theta)_{JW} = e^{-\frac{i\theta}{2} x_1 y_0} e^{-\frac{i\theta}{2} y_1 x_0}$$

which be implemented, for ex by the stoicce algorithm:



(which can be further simplified as shown in the paper)

• For $\eta = 3$ they take

$$U(\eta, \Theta) = e^{-\eta(a_1^+ a_0 - hc)} - e^{-\Theta(a_2^+ a_0 - hc)}$$

$$\approx e^{-\eta(a_1^+ a_0 - hc)} e^{-\Theta(a_2^+ a_0 - hc)}$$

LO Trotter

where "hc" = hermitian conjugate

$$\Rightarrow U(\eta, \Theta)_{JW} \approx e^{\frac{-i\eta}{2}(x_1 y_0 - y_1 x_0)} e^{-i\frac{\Theta}{2}(x_2 z_0 - z_2 x_0)}$$

These UCC ansatz are approx but they require a # of angles that scales polynomially with # of qubits.

The results of the VQE simulations are shown in the paper.