ECE 4501/6501 Fundamentals of Computing 2023
Instructor: Prof. Avik Ghosh
HW#8
Due Sunday 19 Nov 2023
(35+25+20 = 80 points)

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On my honor as a student, I have neither given nor received unauthorized assistance on this exam.

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(sign name above)

Problem 1: Find CCNOT and CSWAP matrices.[35 points]

Listen to Lecture 12 on Quantum Gates. The CCNOT (Toffoli gate) operates on a set of 2^3 possible inputs of 3-bit numbers, $|000\rangle$ through $|111\rangle$, to generate an equal number of outputs. The truth table is easy to write down – basically you flip the third bit if and only if both the first and second bits are unity.

$$\begin{aligned} C|000\rangle &\Longrightarrow |000\rangle \\ C|001\rangle &\Longrightarrow |001\rangle \\ \ldots &\Longrightarrow \ldots \\ C|110\rangle &\Longrightarrow |111\rangle \\ C|111\rangle &\Longrightarrow |110\rangle \end{aligned} \tag{1}$$

In class, we saw that the two 1-bit input states can be written as 2×1 matrices

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{2}$$

which satisfy orthonormality

$$\langle \psi_i | \psi_j \rangle = \delta_{ij} \tag{3}$$

and completeness

$$\sum_i |\psi_i\rangle\langle\psi_i| = |0\rangle\langle 0| + |1\rangle\langle 1| = I_{2\times 2} \tag{4}$$

(a) Let us understand completeness first. Show that any ket $|R\rangle$ can be written as a superposition $|R\rangle = \sum_n R_n|\psi_n\rangle$. (Hint, left multiply by $\langle\psi|_m$).[2 points]

(b) By analogy, each of the independent 3-bit input states to the left of the CCNOT truth table can be written as a $2^3 \times 1$ vectors of the form

$$|000\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{pmatrix}, \quad |001\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \ldots \\ 0 \end{pmatrix}, \ldots, \quad |111\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \ldots \\ 1 \end{pmatrix} \tag{5}$$

Show that each 8×1 vector can be obtained by a simple kronecker product of the corresponding binary elements, e.g.

$$
\begin{aligned}
|000\rangle &= |0\rangle \otimes |0\rangle \otimes |0\rangle \\
|001\rangle &= |0\rangle \otimes |0\rangle \otimes |1\rangle \\
&\dots \\
|111\rangle &= |1\rangle \otimes |1\rangle \otimes |1\rangle
\end{aligned} \tag{6}
$$

[10 points]

(c) Now, use spectral decomposition. Verify that the basis sets above also satisfy the completeness theorem involving the 8×8 identity matrix

$$|000\rangle\langle 000| + |001\rangle\langle 001| + \ldots + |111\rangle\langle 111| = I_{8\times 8} \tag{7}$$

We can then use

$$C = CI_{8\times 8} \tag{8}$$

and replace $I_{3\times 3}$ with Eq. 7, and then replace the actions $C|000\rangle$ with $|000\rangle$ and so on from Eq. 1 to extract the final sums of ket-bras $|\ldots\rangle\langle\ldots| + |\ldots\rangle\langle\ldots| + \ldots$, and then replace with the vector assignments earlier from Eq. 5 to get the final 8×8 matrix for the CNOT operator C. [10 points]

(d) Repeat for the CSWAP (Fredkin) operator. [10 points]

(e) Verify that each matrix is unitary, ie, they satisfy

$$UU^\dagger = U^\dagger U = I \tag{9}$$

Unitarity guarantees that the quantum evolution of a vector $\{\psi\} \Longrightarrow U\{\psi\}$ is reversible in time. [3 points]

Problem 2: Spin operators [25 points]

The Pauli spin operators and the 2D identity matrices are given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{10}$$

(a) Find the eigenvalues of the four matrices. [10 points]

To recap how we do this for an arbitrary matrix M, we need to execute

$$M\{u\} = \lambda\{u\} \tag{11}$$

meaning

$$\begin{pmatrix} M_{11} - \lambda & M_{12} \\ M_{21} & M_{22} - \lambda \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{12}$$

To avoid $\{u\}$ from becoming trivially zero, we need to make sure the matrix on the left is *non-invertible*, meaning its determinant must vanish. This should give λ.

(b) Find the 2×1 eigenvectors of the 3 Pauli matrices. We do this by substituting each λ into the equation above, and finding the ratio u_1/u_2. Also note that the vector must be normalized, meaning $|u_1|^2 + |u_2|^2 = 1$.[10 points]

(c) Verify that the eigenvectors of any of the spin matrices are (a) orthonormal, ie, $\langle\psi_i|\psi_j\rangle = \delta_{ij}$, and complete, ie, $\sum_i |\psi_i\rangle\langle\psi_i| = I_{2\times 2}$. [2.5 points]

(d) As a test for completeness, show that any Hermitian matrix $\begin{pmatrix} A & B \\ B* & C \end{pmatrix}$ with A, C real, can be written as a superposition of the Pauli and identity matrices. In other words, these 4 matrices completely span the 2-D space. [2.5 points]

Problem 3: Quantum Boltzmann for spins [20 points]

Consider 3 spin 1/2 electrons on a row. Their z-spin state is given by

$$S_z = \frac{1}{2}\left[\sigma_z \otimes I_{2\times 2} \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_z \otimes I_{2\times 2} + I_{2\times 2} \otimes I_{2\times 2} \otimes \sigma_z\right] \tag{13}$$

(a) Show that the eigenvalues of this operator, which are the spin-z values, are 3/2, 1/2, -1/2, -3/2 (In general, for N spin-1/2 particles, the eigenvalues will go from $+N/2$ corresponding to all spins up, to $-N/2$ for all spins down, and all values in between separated by 1).[10 points]

(b) Apply a magnetic field hz (don't worry about units) along the z direction, a magnetic coupling J between two sets of z-directed spins, and a magnetic field hx along the x-direction as well. Use the resulting 8×8 Hamiltonian to extract the Boltzmann probability. Repeat this for Fully Quantum (ie, Boltzmann of the H matrix - use 'expm' within Matlab and trace to normalize) and Classical (drop off-diagonals of the H matrix using diag(diag(H)) before doing the expm)

Use the subplot(2,3,1)... subplot(2,3,6) commands to plot the 6 cases below on the same plot. In each case, use bar(x,diag(P),0.2,'b') to plot the bars of P with thickness 0.2 for the Quantum in blue, and on the same subplot with hold on, plot bar(x+0.2,diag(P),0.2,'r') for the classical bars in red displaced laterally for easy viewing. Here x=linspace(1,8,8).

Use
set(gca,'xticklabel',dec2bin(0:7),'fontsize',25);
legend('Quantum','Classical','fontsize',35)
to show the x-axis in terms of binary configurations, and put the legends on the plots.

Execute for the following 6 cases, and in case, explain what you are seeing.

(i) Quantum and classical for J=20 (ferromagnet), hz=0, hx=0.
(ii) J=-20 (antiferromagnet), hz=0, hx=0
(iii) J=20, hz=5, hx=0;
(iv) J=-20, hz=5, hx=0;
(v) J=20, hz=5, hx=15;
(vu) J=-20, hz=5, hx=15;

For each case, you can increase the H further (say by 20X) and see if that sharpens your results. Low temperature (high energy) is typically cleaner to look at.[10 points]