# Macroscopic Binary Entropy in the Initialization of NMR Computers

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**Abstract.** There has been continuous development in the compression schemes for mixed quantum states. However, the schemes for the initialization of NMR quantum computers have not been precisely evaluated. According to our simulation, the compression down to von Neumann entropy for the thermal equilibrium mixed state cannot be realized in polynomial time even for a large number of qubits when the circuit is designed by referring only to the macroscopic spin polarizations. The main cause of this phenomenon is the growth in the macroscopic entropy, namely the total of the binary entropies of the macroscopic spins.

**Keywords:** macroscopic entropy, initialization, NMR computer

## 1 Compression as the initialization of NMR computers

Data compressions are applicable to any physical state as well as to usual bit streams. The comprehensive description of them is the compression of mixed quantum states. Much work has been done on the theory of quantum compression [1, 2]. Some practical compression schemes to generate quantum circuits for the ensemble of quantum states were developed [1, 3, 4, 5]. Initialization of [3, 4, 5] NMR quantum computers [6, 7] is one of the important applications of them. Suppose that the initial state is the thermal equilibrium state: there are $n$ spins-$\frac{1}{2}$ and their initial biases (polarizations) are $\varepsilon_1, \ldots, \varepsilon_n$; a microscopic $i$-th spin is in $|0\rangle \equiv |\uparrow\rangle$ with the probability $(1+\varepsilon_i)/2$ and in $|1\rangle \equiv |\downarrow\rangle$ with the probability $(1-\varepsilon_i)/2$. Then after quantum operations, we have to extract the final state which corresponds to a specific initial state from the mixture of the bases $|0\rangle, \ldots, |2^n-1\rangle$ with respective populations $c_0, \ldots, c_{2^n-1}$. Since the original population of basis $|0\rangle^{\otimes n}$ is very small for large $n$, the initialization is required, which prepares the basis with a large population as the initial state for a quantum computation. Data compressions can be used for the initialization within the resources increasing polynomially in $n$ [3]. These compressions are those which redistribute the biases to create two different blocks of macroscopic spins: one with very large biases which is used as the initialized qubits and the other with very small biases. This can be done by gathering 0s into one side in the bases with large populations and gathering 1s into the same side in those with small populations.

Schulman and Vazirani's boosting scheme [3, 4] is one of such schemes. Their scheme makes use of the basic circuits as shown in Fig. 1. When these quantum circuits are applied to three qubits $a$ , $b$ and $c$ with positive biases $\varepsilon_a$, $\varepsilon_b$ and $\varepsilon_c$ respectively, suppose each of these qubits are not correlated to the others, then the bias of the first qubit $a$ becomes

$$\varepsilon'_a = \frac{1}{2}\left(\varepsilon_a + \varepsilon_b + \varepsilon_c - \varepsilon_a\varepsilon_b\varepsilon_c\right). \tag{1}$$

This equation shows that the bias is enhanced under the

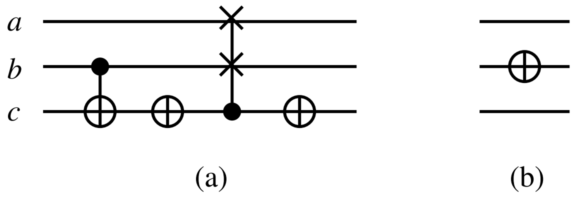


Figure 1: The basic circuits used in Schulman-Vazirani scheme [4]. (a) is the circuit for boosting the bias of bit $a$ and (b) is that for inverting the bias of $b$ when it becomes negative after the circuit (a).

condition $\varepsilon_a < \frac{\varepsilon_b+\varepsilon_c}{1+\varepsilon_b\varepsilon_c}$ for the positive biases in the absence of the correlations. In their scheme, only the biases are referred to in generating the compression circuit, which decreases the efficiency of the initialization as described in the rest of this Paper.

## 2 Total macroscopic binary entropy

Here we have to note that the spins to compress are macroscopic ones which are determined only by the corresponding biases $\varepsilon_i$. As we have proposed in Ref. [8], the entropy measure of importance in the compression of ensemble states is the total of the binary entropy of each macroscopic bit:

$$S_b = -\sum_{i=1}^{n}\left(\frac{1+\varepsilon_i}{2}\log_2\frac{1+\varepsilon_i}{2} + \frac{1-\varepsilon_i}{2}\log_2\frac{1-\varepsilon_i}{2}\right), \tag{2}$$

where $\varepsilon_i$ is the bias of the $i$-th qubit at time step $t$ in the scheme, given by

$$\varepsilon_i = -1 + 2\sum_{k|i-th\ bit\ is\ 0} c_k. \tag{3}$$

This $S_b$ is the lower bound for the length of the compressed macroscopic string at the step $t$.

Generally, it is believed to be possible to generate a circuit to compress the macroscopic string down to von Neumann entropy $S_{vN} = -\mathrm{Tr}(\rho\log_2\rho)$ within the depth of the circuit increasing polynomially in $n$, where $\rho$ is the density operator of the ensemble. Nevertheless, this would not be true for the compression schemes which utilize only the macroscopic information, *e.g.*, biases. This

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would be clear when we rewrite $S_b$ by using partial traces. The partial trace which represents the $i$-th macroscopic spin can be written as

$$\tilde{\rho}_i = \sum_{k=0}^{2^{n-1}-1} \langle \psi_k^i | \rho | \psi_k^i \rangle, \tag{4}$$

where $\{\psi_k^i\}$ is the set of complete orthonormal bases:

$$\begin{aligned} \{|\psi_0^i\rangle &= |0_1 \cdots 0_{i-1} 0_{i+1} \cdots 0_n\rangle, \\ |\psi_1^i\rangle &= |0_1 \cdots 0_{i-1} 0_{i+1} \cdots 1_n\rangle, \\ &\vdots \qquad\qquad\qquad , \\ |\psi_{2^{n-1}-1}^i\rangle &= |1_1 \cdots 1_{i-1} 1_{i+1} \cdots 1_n\rangle\}. \end{aligned} \tag{5}$$

Then $S_b$ is represented as

$$S_b = \sum_{i=1}^{n} S_{vN}(\tilde{\rho}_i). \tag{6}$$

From this notation, it is clear that

$$S_b - S_{vN} = S(\rho | \tilde{\rho}_1 \otimes \cdots \otimes \tilde{\rho}_n), \tag{7}$$

where $S(\rho | \tilde{\rho}_1 \otimes \cdots \otimes \tilde{\rho}_n)$ is the relative entropy of $\rho$ with respect to $\tilde{\rho}_1 \otimes \cdots \otimes \tilde{\rho}_n$. Hence $S_b - S_{vN}$ is the measure of the total correlation of the $n$ macroscopic qubits. When the total correlation grows during the compression, the length of the compressed string can be much larger than $S_{vN}$.

For the evaluation of the schemes, the maximal efficiency of an initialization of the macroscopic string is useful, which is given by:

$$r = \frac{n - S_b}{n - S_{vN}}. \tag{8}$$

This is the ratio of the maximal number of initialized qubits achieved by the scheme to the one expected from the von Neumann entropy. Similarly, the maximal efficiency of a compression is given by $S_{vN}/S_b$.

## 3 Simulation, results and conclusion

The molecular simulation has been conducted by using a virtual molecular system which consists of $N$ molecules composed of $n$ binary digits to verify the Schulman-Vazirani scheme. Since $S_b$ becomes much larger than $S_{vN}$ as shown in Fig. 2, the scheme gives large increase in the total classical correlation. From the plot of the maximal initialization efficiency shown in Fig. 3, it is obvious that the scheme is inefficient unless the initial mean bias is very large. One can conclude that the efficient compression schemes for the macroscopic string must be those which generate the circuits according to the more faithful information, namely the populations $\{c_k\}$, rather than the macroscopic biases.

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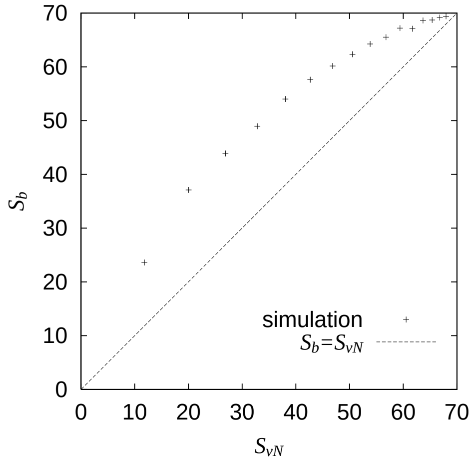


Figure 2: The relation between total binary entropy $S_b$ and von Neumann entropy $S_{vN}$ at max(depth) = 100 for $n = 70$. The simulation of the bias boosting makes use of $1.0 \times 10^8$ virtual molecules. The pluses are data from the simulation.

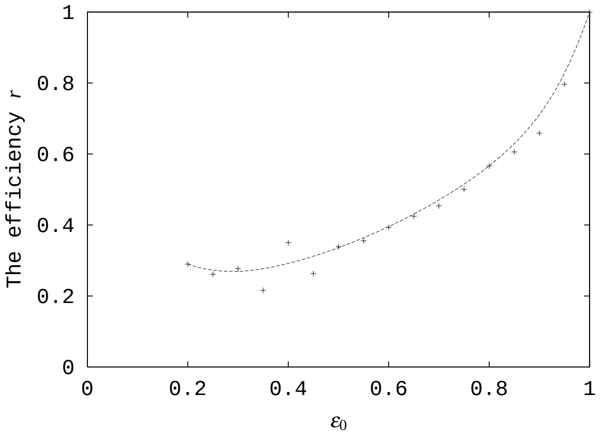


Figure 3: The maximal efficiency $r = (n - S_b)/(n - S_{vN})$ against the initial bias $\varepsilon_0$. Plots are done by the molecular simulation for $n = 70, N = 1.0 \times 10^8$ at max(depth) = 100. The spins are uniformly polarized originally.

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