Implementation of parallel search algorithms using spatial encoding by nuclear magnetic resonance

Rangeet Bhattacharyya,[1] Ranabir Das,[1] K. V. Ramanathan,[2] and Anil Kumar[1,2,*]
[1]*Department of Physics, Indian Institute of Science, Bangalore 560012, India*
[2]*Sophisticated Instruments Facility, Indian Institute of Science, Bangalore 560012, India*
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Information storage and database search are attractive areas in the field of nuclear magnetic resonance. Among the notable works reported earlier, an implementation of a parallel search algorithm in a dipolar coupled spin cluster has gained considerable attention [A. Khitrin, V. L. Ermakov, and B. M. Fung, Phys. Rev. Lett. **89**, 277902 (2002)]. In this paper, we propose and exemplify that spatial encoding can be successfully utilized in realizing such parallel algorithms. We also introduce an improved protocol of the parallel search algorithm, which can be realized using spatial encoding. The methods have been demonstrated to perform a search operation using 215 bits.

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I. INTRODUCTION

Information storage and database search have been active areas of research in the last couple of years. It has been shown by various research groups that nuclear magnetic resonance (NMR) spectroscopy can be used to realize various aspects of information processing [1–9]. Recently, Khitrin *et al.* demonstrated that a dipolar coupled spin cluster can not only store an information array of large dimension, but can also be used to search for a specific pattern in a binary information array [10–12]. The concept of spatial encoding was proposed in the 1950s [13]; however, this technique has gained significant attention recently as a tool to enhance the acquisition speed of multidimensional NMR [14]. The use of multifrequency excitation to speed up higher-dimensional spectroscopy has also been suggested [15]. Recently, we introduced a method of NMR photography which relies on spatial encoding involving a multifrequency excitation and subsequent acquisition under a gradient [16]. Here we demonstrate that the spatial encoding technique in conjunction with the multifrequency pulses can also be useful in realizing parallel search algorithms.

The principle of spatial encoding involves radio frequency (rf) excitations at one or multiple frequencies in the presence of an inhomogeneous magnetic field, which can be realized with the help of a linear magnetic field gradient. The sample can be a small molecule that gives a single peak, such as H_2O, $CHCl_3$, or tetramethylsilane (TMS). In the presence of a linear gradient, the spectrum becomes uniformly broad. A multifrequency rf pulse, when applied under gradient, excites the regions of interest (slices) from this broad profile. The multifrequency rf pulse is a collection of harmonics whose values are chosen according to the pattern to be encoded. To encode a specific information array, the array needs to be broken down to binary form. Therefore, the entire information array is written as a series of 0's and 1's in a binary array. The multifrequency pulse is tailored according to the structure of the binary array, that is, the harmonics constituting the multifrequency pulse are chosen according to the bit values ("1" means the harmonic is present, and "0" means it is absent). Such a multifrequency pulse excites the specific slices whose arrangement encodes the entire binary array. The method of parallel search as given by Khitrin *et al.* involves the application of a series of *bit-shifted* NOT gates and an AND gate, which are realized by a set of multifrequency pulses on this encoded binary array [12]. This method along with an alternative simpler method for parallel search on a spatially encoded binary array are detailed in Sec. III.

II. SPATIAL ENCODING

We shall assume that the sample contains only one type of magnetically active nucleus. In the presence of a linear gradient, the Larmor frequency of the nucleus can be expressed as

$$\omega(z) = \gamma(B_0 + \mathcal{G}z), \quad (1)$$

where γ is the gyromagnetic ratio of the nucleus, B_0 is the static magnetic field along z direction, $\mathcal{G}$ is the magnetic field gradient strength in tesla per meter, and z is the distance of a point of the sample from the center of the sample. It is assumed that the origin of the gradient coincides with the center of the sample length. It is evident from the preceding equation that in the presence of a gradient, the spectrum becomes broad and since the frequency is a linear function of sample height, the spatial distance is mapped onto the spectrum. When a soft rf pulse is applied under a gradient it excites a specific region of the spectrum or a specific slice of the sample. The position of the slice and its width depend on the nature of the soft rf pulse. A soft pulse at ω_k frequency and of width $\Delta\omega$ excites a slice of thickness $\Delta\omega/(\gamma\mathcal{G})$ and at a distance of $(\omega_k - \gamma B_0)/(\gamma\mathcal{G})$ from the center of the sample, as follows from Eq. (1). Generalizing, one can assert that a multifrequency rf pulse applied on the sample under a gradient excites a series of slices from the sample whose positions are determined by the harmonics present in the multi-

*Electronic address: anilnmr@physics.iisc.ernet.in

frequency pulse. The slice intensities are proportional to the amplitudes of the harmonics constituting the pulse. To generate a multifrequency pulse, a certain shape (for example, Gaussian) was modulated with a number of harmonics with the same amplitude and phase, so that all excited slices are also in the same phase. The following equation was used to generate a specific shape $g(t)$:

$$g(t) = \sum_{k=1}^{N} A e^{-Bt^2} e^{-i\omega_k t}, \qquad (2)$$

where A is the common amplitude or weighing factor for all the harmonics, and B represents the width of the Gaussian. The set of frequencies $\{\omega_k\}$ is chosen in the following way. The pattern to be encoded and to be used as an unsorted database has been written as a binary string. In this paper, we have selected the phrase `the quick brown fox jumps over the lazy dog` as the information array. Each letter of this string was assigned a decimal number. For simplicity, we assigned `a`=1 and `b`=2,…,`z`=26 and zero for blank spaces. The string, then, in decimal notation can be translated as `[20 8 5 0 17 21 9 3 11 0 2 18 15 23 14 0 6 15 24 0 10 21 13 16 19 0 15 22 5 18 0 20 8 5 0 12 1 26 25 0 4 15 7]`.

This string in binary form is given by

$$\mathbb{A} = [\texttt{10100 01000 00101 00000 10001 10101 01001 00011 01011 00000 00010 10010 01111 10111 01110 00000 00110 01111 11000 00000 01010 10101 01101 10000 10011 00000 01111 10110 00101 10010 00000 10100 01000 00101 00000 01100 00001 11010 11001 00000 00100 01111 00111}], \qquad (3)$$

which is a pattern of 215 bits, and is named as $\mathbb{A}$ for further reference. The multifrequency pulse was generated using uniformly spaced frequency values, with zero amplitude for zero bits and finite equal amplitudes for all nonzero bits.

The multifrequency rf pulses used for the pattern encoding were calibrated to have an 18° flip angle for each of the harmonics. The duration of these multifrequency pulses was kept constant in order to ensure the uniformity of the width of the excited slice. The duration of each multifrequency pulse was 20 ms. The spectrum, in which the aforementioned pattern ($\mathbb{A}$) was encoded, is shown in Fig. 1(A) and the total number of 128 transients were acquired with eight dummy scans. Further experimental details are provided in (Sec. IV) and in the figure captions.

III. PARALLEL SEARCH ALGORITHM

The search problem can be contemplated as the problem of searching for a particular letter in a sequence of letters. The letters are encoded in a series of bits as mentioned previously. The classical algorithm based on the Turing machine would take up each value of each register, check whether it corresponds to the desired one, and then move onto the next. Another approach is to perform a parallel search, where the algorithm addresses each register simultaneously. In this section, we describe two different search algorithms. The first method (method A) proposed by Khitrin *et al.* [12], will be referred to here as the NOT-shift-AND search algorithm. We introduce a second method (method B), which is referred to as the XOR search algorithm.

A. Method A: NOT-shift-AND search algorithm

This method is based on a parallel search algorithm suggested by Khitrin *et al.* [12]. To search for a single letter or a pattern of five bits, whose binary code is $\alpha\beta\gamma\delta\epsilon$, the algorithm involves the following five search steps.

(1) $\mathrm{NOT}^{\alpha}\mathbb{A}$, where $\mathbb{A}$ is the original bit of string corresponding to the phrase, which in our case is `the quick brown fox jumps over the lazy dog`. If $\alpha=0$, then the original multifrequency pulse corresponding to $\mathbb{A}$ is applied, whereas if $\alpha=1$, then the multifrequency pulse is changed such that the harmonics corresponding to 0's are present and the harmonics corresponding to 1's are absent.

(2) $\mathrm{NOT}^{\beta}\mathrm{L}\mathbb{A}$, where $\mathrm{L}\mathbb{A}$ is the same array $\mathbb{A}$ but now left shifted by one register or one bit. In experiment this corresponds to shifting the frequency of the multifrequency pulse by a unit of the frequency difference between two adjacent slices. A NOT operation will have to be applied depending on the value of β.

(3) $\mathrm{NOT}^{\gamma}\mathrm{L}^2\mathbb{A}$, where $\mathrm{L}^2\mathbb{A}$ corresponds to two frequency shifts.

(4) $\mathrm{NOT}^{\delta}\mathrm{L}^3\mathbb{A}$.

(5) $\mathrm{NOT}^{\epsilon}\mathrm{L}^4\mathbb{A}$.

The operations can be written in the following manner:

$$\mathbb{B} = [(\mathrm{NOT})^{\alpha}\mathbb{A}]\mathrm{OR}[(\mathrm{NOT})^{\beta}\mathrm{L}\mathbb{A}]\mathrm{OR}[(\mathrm{NOT})^{\gamma}\mathrm{L}^2\mathbb{A}] \\ \mathrm{OR}[(\mathrm{NOT})^{\delta}\mathrm{L}^3\mathrm{A}]\mathrm{OR}[(\mathrm{NOT})^{\epsilon}\mathrm{L}^4\mathbb{A}]. \qquad (4)$$

Since these five operations are characterized by the bit pattern of the desired letter, it can be seen that the first register of that letter will always be zero in the five multifrequency pulses [12]. Hence the first register of the required letter will not be excited [12]. On the other hand, at least one of the aforementioned five steps will yield "1" at the first registers of the other letters, resulting in excited first registers

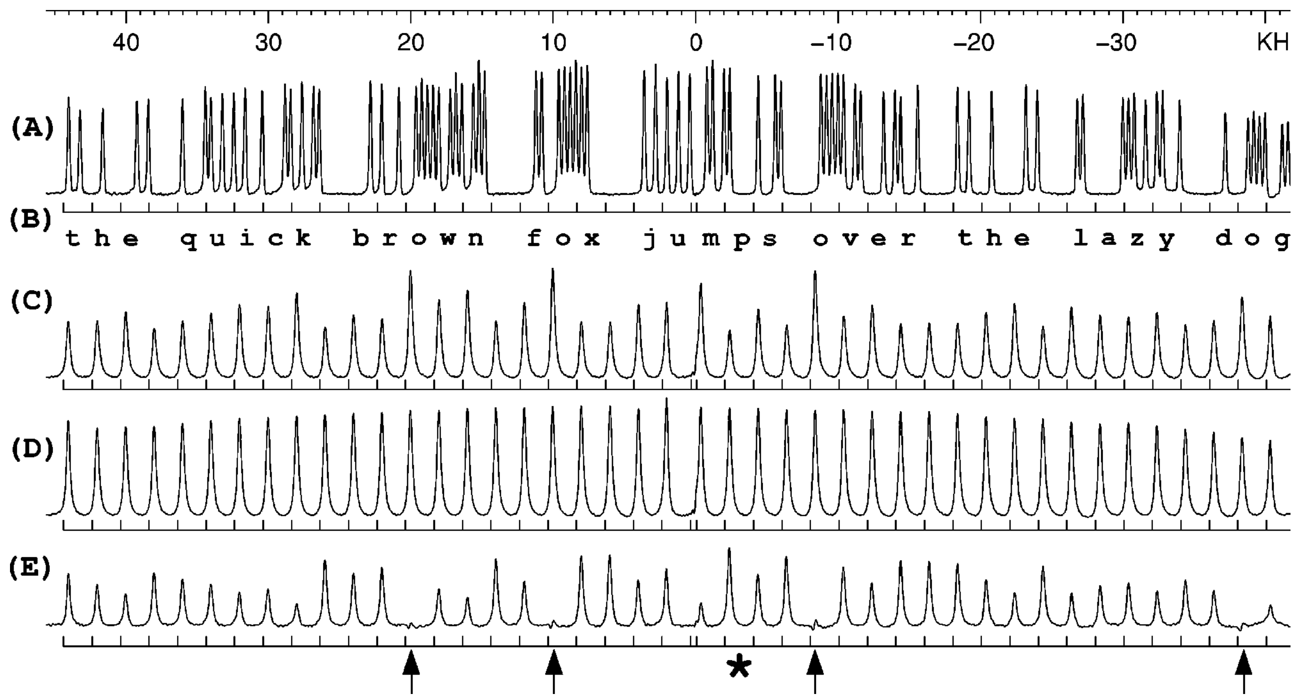

FIG. 1. (A) shows the spectrum encoding the 215 uniformly positioned bits. The spectrum corresponds to the pattern `the quick brown fox jumps over the lazy dog` (B). (C) shows the spectrum obtained by the complete experiment involving the search pulses and the read pulse. (D) shows the spectrum obtained by the application of only the read pulse. (E) shows the difference between (C) and (D). This spectrum has zero intensity at the desired letter `o` marked by the arrows. The letter `p` has highest intensity and is marked by ⋆. A total of 128 transients were recorded without any dummy scans. The flip angle for the read pulse was $\pi/2$ and for the search pulses was 18° for all the harmonics. At the bottom of each spectrum, a horizontal line with tick marks has been given, which indicates the beginning and the end of the five bits encoding each letter. All spectra shown in (A), (C), and (E) are phase sensitive.

of these letters. As illustrated in Fig. 1, these search steps were realized by the application of suitably prepared multifrequency pulses, each of which was 20 ms long and had a flip angle of 18°. All the search pulses were applied with the same phase.

However, for better decoding purpose and enhanced graphic visualization, a reading protocol is also introduced, which is the sixth step of the algorithm. The complete experiment is performed in the following manner. A reading pulse of the form `10000 10000 10000` $\cdots$ is applied, after the search pulses, with the $(y,-y)$ phase in consecutive scans. The reading pulse is calibrated to a flip angle of $(\pi/2)$. The phase cycling for the receiver is set to $(x,-x)$, which implies that two consecutive experiments are subtracted. This phase cycling retains the direct z magnetization due to the reading pulse, and cancels all the other transverse magnetization created beforehand. Since the first register of the nondesired letters have been excited before, the remaining z magnetization detected by the reading pulse is considerably less than that of the first register of the required letter. In this work, we have searched for the 15th letter of the alphabet `o` corresponding to a binary code `01111`. The spectrum obtained by this experiment is given in Fig. 1(C). Next an experiment is performed by applying only the reading pulse in the equilibrium state [see Fig. 1(D)], without any phase cycling. Subtraction of these two experiments gives a spectrum where the first bit of every letter has a peak except the desired letters, as shown in Fig. 1(E), all other peaks being absent. These two experiments comprise the measurement protocol, which acts as an AND operation with the string of bits $\mathbb{C}$=[`10000 10000` $\cdots$], and the final result can be written as

$$\mathbb{D} = \mathbb{B} \text{ AND } \mathbb{C}. \tag{5}$$

The spectrum corresponding to $\mathbb{D}$ is given in Fig. 1(E) when the letter `o` was searched for. The first peak of the letter `o` is absent at four places of the total phrase (marked by arrows), thereby clearly identifying the desired letter.

B. Method B: XOR search algorithm

In this method, an experiment is performed to spatially encode the desired pattern on the spectrum. As a second and final step, another auxiliary experiment is performed, which spatially encodes the pattern obtained by replacing all letters of the original pattern by the desired letter. As an example, to search for the letter `o`, the second pattern needs to be a string of the letter `o`, namely,

`ooooooooooooooooooooooooooooooooooooooooooo`,

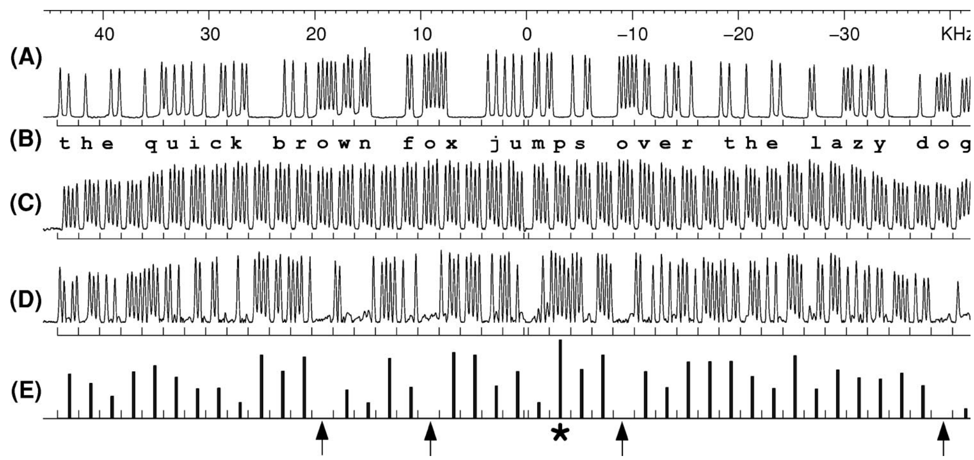

FIG. 2. (A) shows the spectrum encoding the 215 uniformly positioned bits. The spectrum corresponds to the pattern, `the quick brown fox jumps over the lazy dog` (B) shows the alpha-numeric form of encoding pattern. (C) shows the spectrum corresponding to the auxiliary pattern, that is, `ooooooooooooooooooooooooooooooooooooooooooo`. The spectra shown in Figs. 2(A) and 2(C) are phase sensitive. (D) shows the difference between (A) and (C), plotted with the absolute value of intensity. The signal for all the five bits of the required letter `o` is missing is this spectrum, clearly identifying the desired letter `o`. However, for further clarity, (E) shows the integrated absolute intensity of the peaks corresponding to each letter, including blanks. The absence of the required letter `o` is clearly evident, as marked by the arrows. The letter `p` has highest absolute intensity in (E) and is marked by ⋆. A total of 128 transients were recorded without any dummy scans. The flip angle for all the pulses were 18°. As in Fig. 1, at the bottom of each spectrum, a horizontal line with tick marks has been given, which indicates the beginning and the end of the peak pattern for a letter.

which for future reference will be named the auxiliary pattern. The absolute intensity difference spectrum between the spectra of these two experiments yields a pattern where the bits or peaks corresponding to the required letter are absent. For other letters, at least one peak is guaranteed to be present in the spectrum. This operation is essentially an XOR operation. The following example clearly illustrates the working principle of this method.

Search string: `t` `h` ⋯ `o` ⋯

Encoded pattern: `10100 01000` ⋯`01111`⋯

Auxiliary pattern: `01111 01111` ⋯`01111`⋯

Difference(XOR): `11011 00111` ⋯`00000`⋯ (6)

It is evident that the bits corresponding to the desired letter are guaranteed to be zero, whereas every other letter will have at least one nonzero bit.

For both of these experiments the flip angle is identical (18°). Under this condition, the difference spectrum does not have bits or peaks corresponding to the desired letter. The experimental demonstration of this method is shown in Fig. 2, where Fig. 2(A) shows the original pattern, Fig. 2(B) the string of letters, and Fig. 2(C) the auxiliary pattern of all letters being the letter `o`. The difference spectrum plotted with the absolute values of intensities [Fig. 2(D)] contains the result of the search and absence of the letter `o`. However, to clearly indicate the absence of the desired letter, the sums of absolute intensities of the peaks corresponding to each letter have been plotted in Fig. 2(E). This clearly shows the absence of the required letter `o`, also marked with arrows.

In Fig. 2(E) the intensities of the peaks corresponding to the letters `g`, `k`, `m`, and `n`, are small compared to all other non-searched letters. This is due to the fact that the binary codes for these letters (`g`=7=`00111`, `k`=11=`01011`, `m` =13=`01101`, `n`=14=`01110`) differ from the binary code of the required letter `o` (`01111`) only in one of the bits; hence the XOR operation yields the lowest nonzero absolute intensities of one unit for these letters. This sets the lowest limit for discrimination in these experiments. Similarly the binary code for the letter `p` (`10000`) is complementary to the searched letter `o` (`01111`) and hence this letter has the highest absolute intensity of five units. Thus, by this method, the complementary letter `p` is also searched for simultaneously without any additional effort [marked by ⋆ in Fig. 2(E)]. Also in method A, the letter `p` has highest intensity [also marked by ⋆ in Fig. 1(E)] and the letters `g`, `k`, and `m` have lowest nonzero intensity. However, the letter `n` should have also yielded low intensity, but this seems to be an experimental artifact. Both these methods can also discriminate groups of other letters which have theoretical intensities of 2 (`c`, `e`, `f`, `i`, `j`, `l`, w), 3 (`a`, `b`, `d`, `h`, `s`, `u`, `v`, `y`, `z`), and 4 (`q`, `r`, `t`, `x`) (see Fig. 3). The equivalence of intensity for each letter under both the methods is due to the fact that the bits at the first register of a letter in the steps of method A are identical to the bits of the same letter obtained after the XOR operation in method B.

To compare methods A and B, we have calculated the *average absolute deviation* (Δx), from the experimental intensities $\{x_i^E\}$ and the theoretical intensities $\{x_i^T\}$, defined by [18],

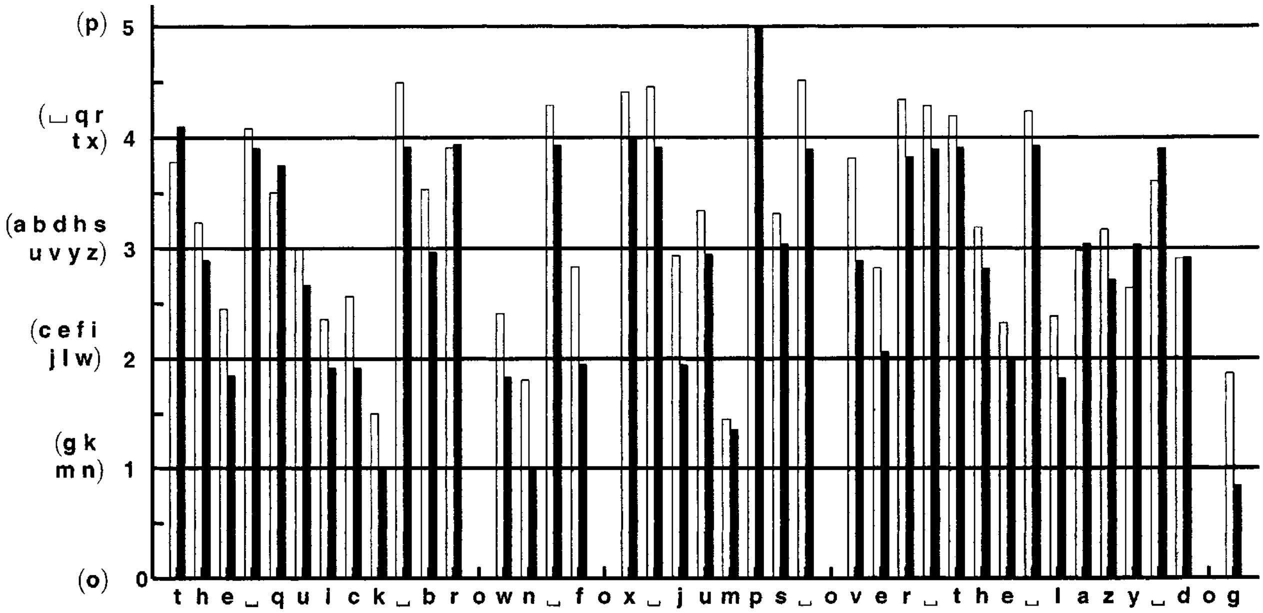

FIG. 3. The intensities of the peaks of the spectra in Figs. 1(E) and 2(E) are plotted in a single graph for comparison. The empty rectangular bars correspond to the peak intensities obtained by method A [Fig. 1(E)], and the solid rectangular bars correspond to the integrated absolute peak intensities obtained by method B [Fig. 2(E)]. The horizontal lines give theoretically expected peak intensities for various letters, which are identified on the vertical scale (along the y axis). The ⊔ sign indicates a blank space. Since the experimental excitation profiles show unequal excitation over the entire spectral range [lower intensities near the ends in Figs. 1(D) and 2(C)], the intensity values of Figs. 1(E) and 2(E), plotted here, have been normalized with respect to the intensities of Figs. 1(D) and 2(C), respectively.

$$\Delta x = \frac{1}{N}\sum_{i=1}^{N} |x_i^E - x_i^T|, \quad (7)$$

where Δx is an indicator of the variance of the experimental data from the theoretical values. Our experimental results of Fig. 3 yielded

$$\Delta x_A = 0.355 \quad \text{and } \Delta x_B = 0.096. \quad (8)$$

This indicates that the variance is less by a factor of almost 4 for method B, compared to method A.

Method B proves to be easier than the method A. Method A needs six bit-shifted multifrequency pulses, whereas method B uses a single multifrequency pulse. This also results in better reproduction of the intensities of various letters as seen by the above analysis.

IV. EXPERIMENTAL DETAILS

The experiments were carried out on the protons of water (90 vol % H_2O with 10 vol % D_2O) at 300 K with a Bruker DRX-500 spectrometer with operating proton Larmor frequency at 500 MHz. The gradient strength was ~18 G/cm for all the experiments. All the multifrequency pulses used in the search algorithm were calibrated for a flip angle of 18° for each harmonics, for all experiments, corresponding to the letter o. In realizing the method A, the reading pulse was calibrated to a flip angle of $\pi/2$ for all harmonics. All multifrequency pulses including the reading pulse were of duration 20 ms. While recording the spectra in Figs. 2(A) and 2(C), the flip angle for all the multifrequency pulses has been kept to 18° for each harmonic. A total of 128 transients were recorded for the spectra in Figs. 1 and 2, along with eight dummy scans. The recycle delays for all experiments were set to 5 s.

The use of spatial encoding provides several advantages over the liquid-crystal method [12]. The principal advantage lies in the uniformity of the intensity and the relaxation of the bits. Since the bits or slices are spatially separated, the mixing of magnetization between the slices is prevented. Also, spatial encoding gives a large signal-to-noise ratio, and thus requires the acquisition of a small number of transients. While this method (as used in this paper) has lower resolution compared to the liquid-crystal method [12], it can be improved by higher-selectivity pulses and larger gradients. However, it should be noted that the main emphasis of this paper is to demonstrate the use of spatial encoding in the field of NMR information processing. Diffusion of molecules between different slices may cause some errors in the computation by decreasing the resolution of the slices (see [17]); however, for the computations performed in this work, the effect of diffusion was found to be negligible.

V. CONCLUSION

In this paper, the use of spatial encoding to implement two parallel search algorithms has been demonstrated. In the presence of a magnetic field gradient, spatial information is mapped onto the spectrum. The spectrum is excited with a properly prepared multifrequency rf pulse, to store an input pattern on the slices of the sample. This encoded pattern has been used as an unsorted database to implement parallel search algorithms. In this work, the letter o has been searched for (using two parallel search algorithms) from a 215-bit input pattern of `the quick brown fox jumps over the lazy dog`. Our proposed search algorithm is faster and easier to implement compared to an earlier search algorithm.

The proposed technique of spatial encoding has several advantages. In principle, the spectral width can be increased conveniently by increasing the strength of the applied gradient. This would allow computation on a much larger number of registers. Moreover, suitable molecules with small relaxation rates can be chosen. This would ensure minimized loss of information during more complex computations with a higher number of pulses. More advanced computations can be contemplated using spatial encoding.

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