

Broadband rephasing by composite sequences of π pulses

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I. INTRODUCTION

The objective of the present memo is to explore the bandwidth of a newly derived class of simple rephasing sequences. The purpose is to maximize the frequency bandwidth, i.e. the range of detunings within which rephasing is performed with very high fidelity (error less than 10^{-n} , with $n = 2, 3, 4$). For a given number of rephasing pulses this bandwidth is pushed as much as possible by using the relative phases between the rephasing π pulses rather than by usual repetition of the CPMG sequence.

We work in the rotating-wave picture in which the rapidly rotating (at the transition frequency ω_0) probability amplitudes of the two states $a_1(t)$ and $a_2(t)$ are replaced by the slowly varying (at the field-atom detuning Δ) amplitudes $c_1(t)$ and $c_2(t)$: $a_1(t) = c_1(t)e^{i\omega_0 t/2}$ and $a_2(t) = c_2(t)e^{-i\omega_0 t/2}$.

In this picture, the free evolution of a two-state system is described by the propagator

$$\mathbf{F}(t) = e^{-i\Delta\hat{\sigma}_3/2} = \begin{bmatrix} e^{-i\Delta t/2} & 0 \\ 0 & e^{i\Delta t/2} \end{bmatrix}. \quad (1)$$

The action of a rectangular rephasing pulse with Rabi frequency Ω and duration T is described by the propagator

$$\begin{aligned} \mathbf{R}(\Omega, T) &= e^{-i(\Delta\hat{\sigma}_3 + \Omega\hat{\sigma}_1)T/2} \\ &= \begin{bmatrix} \cos \frac{1}{2}\chi T - i\frac{\Delta}{\chi} \sin \frac{1}{2}\chi T & -i\frac{\Omega}{\chi} \sin \frac{1}{2}\chi T \\ -i\frac{\Omega}{\chi} \sin \frac{1}{2}\chi T & \cos \frac{1}{2}\chi T + i\frac{\Delta}{\chi} \sin \frac{1}{2}\chi T \end{bmatrix}. \end{aligned} \quad (2)$$

Here $\hat{\sigma}_k$ is the k th Pauli matrix and $\chi = \sqrt{\Omega^2 + \Delta^2}$.

It is important to note that the detuning Δ , which describes the inhomogeneous broadening and the resulting dephasing of the ensemble, is present *during* the action of the rephasing pulses. It is this fact — that the rephasing pulses are non-resonant for nearly all ions — that leads to a finite bandwidth of the rephasing sequence. Below I will compare the performance of various rephasing sequences with respect to the detuning bandwidth they can achieve.

The objective of any rephasing sequence is to produce to identity propagator,

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad (3)$$

as closely as possible, i.e. by compensating deviations in the relevant parameters to the highest possible order.

I define the rephasing error (which is the quantity I plot below) as the distance between the actual propagator \mathbf{U} and the target propagator \mathbf{I} for a sequence of $4n$ pulses (or $-\mathbf{I}$ for a sequence of $2(2n+1)$ pulses):

$$\text{rephasing error} = |U_{11} \pm 1| + |U_{12}|, \quad (4)$$

with the upper sign for a sequence of $2(2n+1)$ pulses and the lower sign for a sequence of $4n$ pulses.

II. CPMG SEQUENCES

A. A single CPMG cycle (two rephasing pulses)

Consider a sequence of two identical rectangular pulses, each of duration T , preceded by a free evolution during a time interval $\tau/2$, separated by time τ , and followed by a time interval $\tau/2$:

$$\text{CPMG : } \tau/2 - \pi - \tau - \pi - \tau/2. \quad (5)$$

The total propagator for this CPMG sequence is

$$\mathbf{U} = \mathbf{F}(\tau/2)\mathbf{R}(\Omega, T)\mathbf{F}(\tau)\mathbf{R}(\Omega, T)\mathbf{F}(\tau/2). \quad (6)$$

If the rephasing pulses have pulse area of π , i.e. $T = \pi/\Omega$, then the elements U_{11} and U_{12} have the following Taylor series expansion vs Δ :

$$U_{11} = U_{22}^* = -1 + i\frac{2\Omega\tau + \pi}{2\Omega^3}\Delta^3 + O(\Delta^4), \quad (7a)$$

$$U_{12} = -U_{21}^* = i\frac{2\Omega\tau + \pi}{2\Omega^2}\Delta^2 + O(\Delta^4). \quad (7b)$$

[Hereafter, all expansions vs Δ are in terms of the dimensionless ratio Δ/Ω ; for brevity I will denote the order of the neglected terms as $O(\Delta^n)$ rather than $O(\Delta^n/\Omega^n)$.] Therefore, the CPMG sequence produces the identity propagator, up to a sign,

$$U_{\text{CPMG}} = \begin{bmatrix} -1 + O(\Delta^3) & O(\Delta^2) \\ O(\Delta^2) & -1 + O(\Delta^3) \end{bmatrix}. \quad (8)$$

The bandwidth of the CPMG sequence is determined by the the first term in the element U_{12} , because it is the lowest-order deviation in U_{CPMG} . From the condition

$$\frac{2\Omega\tau + \pi}{2\Omega^2}\Delta^2 < \epsilon, \quad (9)$$

where ϵ gives the admissible error ($0 < \epsilon \ll 1$), e.g. $\epsilon = 10^{-4}$, we find

$$|\Delta_{\text{CPMG}}| < \Omega \sqrt{\epsilon \frac{2}{2\Omega\tau + \pi}}. \quad (10)$$

If the separation of the pulses τ is much larger than their width T , i.e. $\tau \gg T = \pi/\Omega$, then $\Omega\tau \gg \pi$ and we have for the bandwidth

$$|\Delta_{\text{CPMG}}| < \sqrt{\epsilon \frac{\Omega}{\tau}}. \quad (11)$$

Obviously, the bandwidth is inversely proportional to $\sqrt{\tau}$, i.e. the larger the separation, the smaller the bandwidth. Also, the bandwidth increases with $\sqrt{\Omega}$ — a sign of power broadening — which implies that shorter (and hence stronger) rephasing pulses are beneficial for larger rephasing bandwidth.

A quick estimate for $\Omega = 2\pi \times 150$ kHz and $\tau = 300$ μ s gives

$$|\Delta_{\text{CPMG}}| < \sqrt{\epsilon} \times 2\pi \times 8.9 \text{ kHz} \quad (12)$$

If $\epsilon = 0.01$ then $|\Delta_{\text{CPMG}}| < 2\pi \times 1$ kHz!

B. Two CPMG cycles (four rephasing pulses)

Consider now a sequence of two CPMGs,

$$\text{CPMG}^2: \quad \tau/2 - \pi - \tau - \pi - \tau - \pi - \tau - \pi - \tau/2. \quad (13)$$

In a similar fashion as for a single CPMG cycle, for rephasing π pulses we find

$$U_{11} = 1 - i \frac{2\Omega\tau + \pi}{\Omega^3} \Delta^3 + O(\Delta^4), \quad (14a)$$

$$U_{12} = -i \frac{2\Omega\tau + \pi}{\Omega^2} \Delta^2 + O(\Delta^4). \quad (14b)$$

It is important to note that the rephasing order for CPMG^2 is the same as for CMPG : $O(\Delta^2)$. In the long-separation limit $\tau \gg T = \pi/\Omega$ we find

$$|\Delta_{\text{CPMG}^2}| < \sqrt{\epsilon \frac{\Omega}{2\tau}}, \quad (15)$$

i.e. the bandwidth *decreases* by a factor $\sqrt{2}$.

C. n CPMG cycles ($2n$ rephasing pulses)

For a rephasing sequence of n CPMG cycles (comprising $2n$ rephasing π pulses)

$$\text{CPMG}^n: \quad (\tau/2 - \pi - \tau - \pi - \tau/2)^n, \quad (16)$$

we find

$$U_{11} = (-1)^n - i \frac{n(2\Omega\tau + \pi)}{2\Omega^3} \Delta^3 + O(\Delta^4), \quad (17a)$$

$$U_{12} = -i \frac{n(2\Omega\tau + \pi)}{2\Omega^2} \Delta^2 + O(\Delta^4). \quad (17b)$$

The bandwidth is

$$|\Delta_{\text{CPMG}^n}| < \sqrt{\epsilon \frac{\Omega}{n\tau}}, \quad (18)$$

i.e. the rephasing bandwidth decreases as \sqrt{n} .

Note that $2n\tau = \mathcal{T}$ is essentially the total duration of the rephasing sequence. For a given total duration \mathcal{T} , the bandwidth (18) depends on \mathcal{T} only but not on the pulse separation τ itself.

For a given total duration \mathcal{T} , the dependence of the bandwidth on the number of rephasing cycles is derived by taking into account the next $O(\Delta^4)$ term in U_{12} , which in the limit $\tau \gg T = \pi/\Omega$ reads

$$U_{12} = -i \frac{n\tau}{\Omega} \Delta^2 - i n \frac{\tau^3}{24\Omega} \Delta^4 + O(\Delta^6) \quad (19)$$

The condition $|U_{12}| < \epsilon$ leads to the bandwidth

$$|\Delta_{\text{CPMG}^n}| < \left(\frac{24\Omega}{n\tau^3} \right)^{1/4} = \left(\frac{48\Omega}{\mathcal{T}\tau^2} \right)^{1/4}, \quad (20)$$

which shows that the bandwidth decreases as $\tau^{-1/2}$. This explains the deterioration of the rephasing efficiency for longer separation between the rephasing pulses observed in Georg's experiment (Fig. 4 of PRL2013).

III. PHASED REPHASING SEQUENCES

Far better frequency bandwidths of the rephasing sequences can be obtained by using phased pulses, i.e. composite rephasing sequences.

A. Two pulses

For just two pulses, a phase relation ϕ between them does not improve the bandwidth. We have

$$U_{11} = -e^{-i\phi} - \frac{1 - e^{-i\phi}}{\Omega^2} \Delta^2 + O(\Delta^3), \quad (21a)$$

$$U_{12} = \frac{1 - e^{-i\phi}}{\Omega^2} \Delta + O(\Delta^2). \quad (21b)$$

Obviously, the optimal phase is $\phi = 0$, i.e. the CPMG sequence.

B. Four pulses

For four pulses, the availability of relative phases makes it possible to construct more efficient rephasing sequences. I have found two rephasing sequences, which are more efficient than CPMG^2 .

1. R4a sequence

The first sequence is

$$\text{R4a: } \tau/2 - \pi_0 - \tau - \pi_\pi - \tau - \pi_\pi - \tau - \pi_0 - \tau/2, \quad (22)$$

where the notation π_ϕ means a pulse with area π and phase ϕ . Because all rephasing sequences below have the same structure as (22), with π pulses separated by repetition time τ , I shall use the short notation in which only the phases are listed:

$$\text{R4a: } (0, \pi, \pi, 0). \quad (23)$$

The propagator elements read

$$U_{11} = 1 + i \frac{2\Omega\tau + \pi}{\Omega^3} \Delta^3 + O(\Delta^4), \quad (24a)$$

$$U_{12} = -i \frac{2(2\Omega\tau + \pi)}{\Omega^4} \Delta^4 + O(\Delta^5). \quad (24b)$$

Obviously, this sequence has the same accuracy as CPMG² regarding U_{11} , but it improves by two orders regarding U_{12} . Hence overall it is accurate up to order $O(\Delta^3)$, one better than CPMG. In the long-separation limit $\tau \gg T = \pi/\Omega$ we find

$$|\Delta_{\text{R4a}}| < \left(\epsilon \frac{\Omega^2}{2\tau} \right)^{1/3}, \quad (25)$$

where this estimate is derived by requiring that the lowest-order error in \mathbf{U} , i.e. the $O(\Delta^3)$ term in U_{11} , is less than ϵ .

2. R4b sequence

The second four-pulse sequence is

$$\text{R4b: } (0, 0, \pi, \pi). \quad (26)$$

The propagator elements read

$$U_{11} = 1 - i \frac{2\Omega\tau + \pi}{\Omega^3} \Delta^3 + O(\Delta^4), \quad (27a)$$

$$U_{12} = \frac{(2\Omega\tau + \pi)^2}{2\Omega^5} \Delta^5 + O(\Delta^6). \quad (27b)$$

This sequence gains an additional order in U_{12} compared to R4a. It has the same bandwidth (25) as the sequence R4a.

Because the leading orders of the errors in R4a and R4b are the same, $O(\Delta^3)$, the two sequences perform similarly. Their bandwidth is compared with the CPMG sequences in Fig. 1. Clearly, the bandwidth of the R4 sequence is much larger than those of CPMG and CPMG². For the error level $\epsilon = 0.01$ both CPMG and CPMG² have bandwidth of less than 2 kHz, whereas the R4 sequence has a bandwidth of about 28 kHz. The logarithmic scale in the lower frame reveals the slight shrinking of the CPMG² profile compared to the one for CPMG.

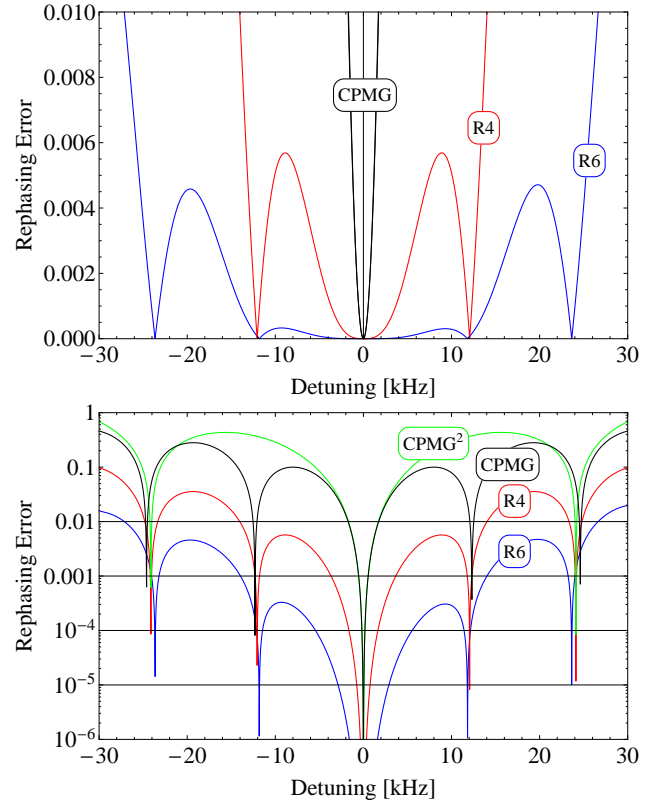


FIG. 1: Comparison of the rephasing efficiency of the CPMG, CPMG², R4 and R6 rephasing sequences. In the upper frame CPMG and CPMG² produce indiscernible curves. The total rephasing time is 1000 μs . The Rabi frequency is $\Omega = 2\pi \times 150$ kHz, the pulse duration is 3.3 μs (meaning pulse area π of each individual pulse), and the pulse shape is rectangular.

C. Six, eight and ten pulses

1. R6 sequence

For six pulses, the highest-order rephasing sequences are

$$\text{R6a: } (0, \frac{2}{3}\pi, 0, 0, \frac{2}{3}\pi, 0), \quad (28a)$$

$$\text{R6b: } (0, \frac{2}{3}\pi, \frac{2}{3}\pi, 0, \frac{2}{3}\pi, \frac{2}{3}\pi). \quad (28b)$$

The propagator elements have orders $U_{11} = 1 + O(\Delta^5)$ and $U_{12} = O(\Delta^4)$. These sequences gain two orders in Δ in U_{11} compared to R4a and R4b, and one order overall. In the long-separation limit $\tau \gg T = \pi/\Omega$ we find

$$|\Delta_{\text{R6}}| < \left(\epsilon \frac{\Omega^3}{3\tau} \right)^{1/4}. \quad (29)$$

The rephasing by the R6b sequence is illustrated in Fig. 1 where it is seen that it outperforms all lower-order sequences.

Note that the R6 sequence has the structure R3R3, where $\text{R3} = (0, \frac{2}{3}\pi, \frac{2}{3}\pi)$ or $(0, \frac{2}{3}\pi, 0)$. All rephasing sequences of $2(2n+1)$ pulses have the same structure, and all of them produce the propagator $-\mathbf{I}$, rather than \mathbf{I} .

2. R8 sequences

For eight pulses, there are four different rephasing sequences,

$$\text{R8a} : \left(0, 0, \frac{3}{2}\pi, \frac{1}{2}\pi, \pi, \pi, \frac{1}{2}\pi, \frac{3}{2}\pi\right), \quad (30a)$$

$$\text{R8b} : \left(0, \frac{1}{2}\pi, \frac{3}{2}\pi, \pi, \pi, \frac{3}{2}\pi, \frac{1}{2}\pi, 0\right), \quad (30b)$$

$$\text{R8c} : \left(0, \pi, \frac{3}{2}\pi, \frac{3}{2}\pi, \pi, 0, \frac{1}{2}\pi, \frac{1}{2}\pi, 0\right), \quad (30c)$$

$$\text{R8d} : \left(0, \frac{1}{2}\pi, \frac{1}{2}\pi, 0, \pi, \frac{3}{2}\pi, \frac{3}{2}\pi, \pi\right). \quad (30d)$$

The first three of these sequences have orders $U_{11} = 1 + O(\Delta^5)$ and $U_{12} = O(\Delta^6)$, and gain two orders in U_{12} compared to R6. The last one has $U_{11} = 1 + O(\Delta^5)$ and $U_{12} = O(\Delta^7)$. All these sequences have an overall order $O(\Delta^5)$, one better than R6. In the long-separation limit $\tau \gg T$ we find for all sequences

$$|\Delta_{\text{R8}}| < \left(\epsilon \frac{\Omega^4}{4\tau}\right)^{1/5}. \quad (31)$$

The performance of all R8 sequences is similar.

3. R10 pulses

There are two symmetric ten-pulse sequences, of the form R5^2 ,

$$\text{R10a} : \left(0, \frac{2}{5}\pi, \frac{6}{5}\pi, \frac{2}{5}\pi, 0, 0, \frac{2}{5}\pi, \frac{6}{5}\pi, \frac{2}{5}\pi, 0\right), \quad (32a)$$

$$\text{R10b} : \left(0, \frac{4}{5}\pi, \frac{2}{5}\pi, \frac{4}{5}\pi, 0, 0, \frac{4}{5}\pi, \frac{2}{5}\pi, \frac{4}{5}\pi, 0\right). \quad (32b)$$

There are several other sequences with asymmetric phases, which deliver similar performance.

IV. HIGHER-ORDER REPHASING SEQUENCES

It turns out that for $2(2n+1)$ pulses, the rephasing sequences have the symmetric form R^2 , where R is a sequence of $2n+1$ pulses. For $4n$ pulses, the rephasing sequences have the form RR_π , where R is itself a symmetric sequence of $2n$ pulses. It turns out that for sequences of $4n$ and $2(2n+1)$ pulses there are very simple analytic formulas for the phases.

A. General formula for sequences of $2(2n+1)$ pulses

For rephasing sequences of $2m$ pulses, with $m = 2n+1$ and $n = 0, 1, 2, \dots$, the phases are given by

$$\text{R2m} : \phi_k = \frac{k(k-1)}{n}\pi, \quad (k = 1, 2, \dots, n). \quad (33)$$

The first few of these sequences are listed in Table I. Note that the CPMG sequence is the lowest order ($n = 0$) sequence of this family. These sequences consist of two

R2m	phases of R2m
R2	$(0, 0)\pi$
R6	$(0, \frac{2}{3}, 0, 0, \frac{2}{3}, 0)\pi$
R10	$(0, \frac{2}{5}, \frac{6}{5}, \frac{2}{5}, 0, 0, \frac{2}{5}, \frac{6}{5}, \frac{2}{5}, 0)\pi$
R14	$(0, \frac{2}{7}, \frac{6}{7}, \frac{12}{7}, \frac{6}{7}, \frac{2}{7}, 0, 0, \frac{2}{7}, \frac{6}{7}, \frac{12}{7}, \frac{6}{7}, \frac{2}{7}, 0)\pi$
R18	$(0, \frac{2}{9}, \frac{2}{3}, \frac{4}{9}, \frac{2}{3}, \frac{4}{9}, \frac{2}{3}, \frac{2}{9}, 0, 0, \frac{2}{9}, \frac{2}{3}, \frac{4}{9}, \frac{2}{3}, \frac{4}{9}, \frac{2}{3}, \frac{2}{9}, 0)\pi$

TABLE I: Phase of several high-order rephasing sequences R2m , with $m = 2n+1$ and $n = 0, 1, 2, \dots$

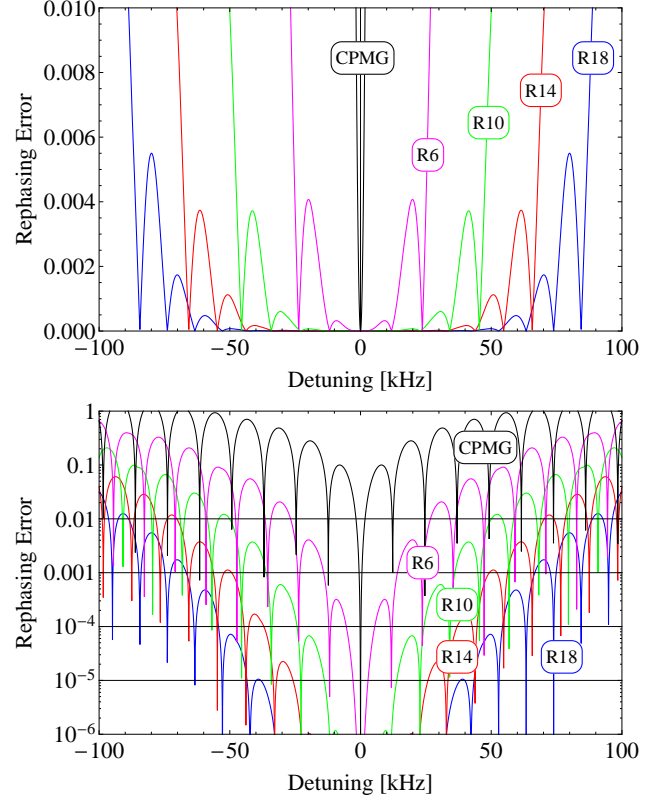


FIG. 2: Rephasing error for several rephasing sequences with $2(2n+1)$ pulses for total rephasing time of $1000 \mu\text{s}$. The Rabi frequency is $\Omega = 2\pi \times 150 \text{ kHz}$, the pulse duration is $3.3 \mu\text{s}$ (meaning pulse area π of each individual pulse), and the pulse shape is rectangular.

identical sequences of $2n+1$ pulses, each of which is exactly one of the Bm pulses of Torosov and Vitanov, PRA **83**, 053420 (2011), with $m = 2n+1$! Hence these sequences can be represented as $(\text{Bm})^2$. Because the Bm pulses are designed to compensate variations in the pulse area one can view the rephasing sequences R2m as a CPMG sequence in which the two π pulses are replaced by composite Bm pulses. The naive expectation is that the R2m sequences will have high compensation of pulse area errors and low compensation of detuning. However, it turns out that they have very high compensation of detuning — of order $O(\Delta^{2n+2})$ — too!

The rephasing efficiency of these sequences is demonstrated in Fig. 2. Clearly, the rephasing bandwidth in-

R4n	phases of R4n
R4	$(0, 0, 1, 1)\pi$
R8	$(0, \frac{1}{2}, \frac{1}{2}, 0, 1, \frac{3}{2}, \frac{3}{2}, 1)\pi$
R12	$(0, \frac{2}{3}, 1, 1, \frac{2}{3}, 0, 1, \frac{5}{3}, 0, 0, \frac{5}{3}, 1)\pi$
R16	$(0, \frac{3}{4}, \frac{5}{4}, \frac{3}{2}, \frac{3}{2}, \frac{5}{4}, \frac{3}{4}, 0, 1, \frac{7}{4}, \frac{1}{2}, \frac{1}{2}, \frac{1}{4}, \frac{7}{4}, 1)\pi$
R20	$(0, \frac{4}{5}, \frac{7}{5}, \frac{9}{5}, 0, 0, \frac{9}{5}, \frac{7}{5}, \frac{4}{5}, 0, 1, \frac{9}{5}, \frac{2}{5}, \frac{4}{5}, 1, 1, \frac{4}{5}, \frac{2}{5}, \frac{9}{5}, 1)\pi$
R24	$(0, \frac{5}{6}, \frac{3}{2}, 0, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{3}, 0, \frac{3}{2}, \frac{5}{6}, 0, 1, \frac{11}{6}, \frac{1}{2}, 1, \frac{4}{3}, \frac{3}{2}, \frac{4}{3}, \frac{1}{2}, \frac{1}{2}, \frac{11}{6}, 1)\pi$

TABLE II: Phase of several high-order rephasing sequences R4n.

creases rapidly with the order of the rephasing sequence.

We note that all rephasing sequences R2m, like the CPMG and R6 discussed above, produce the propagator $-\mathbf{I}$, rather than \mathbf{I} .

Finally, it is interesting to verify the performance of similar rephasing sequences, which are constructed as a pair of two identical universal CPs: UU.

B. General formula for sequences of 4n pulses

The rephasing sequence R4n of 4n pulses has the structure

$$R4n = (r_n)_0 (r_n^{-1})_0 (r_n)_\pi (r_n^{-1})_\pi, \quad (34)$$

where

$$(r_n)_0 = (\phi_1, \phi_2, \dots, \phi_{n-1}, \phi_n) \quad (35a)$$

$$(r_n^{-1})_0 = (\phi_n, \phi_{n-1}, \dots, \phi_2, \phi_1), \quad (35b)$$

$$(r_n)_\pi = (\phi_1 + \pi, \phi_2 + \pi, \dots, \phi_{n-1} + \pi, \phi_n + \pi) \quad (35c)$$

$$(r_n^{-1})_\pi = (\phi_n + \pi, \phi_{n-1} + \pi, \dots, \phi_2 + \pi, \phi_1 + \pi). \quad (35d)$$

Its phases are

$$\phi_k = \frac{(k-1)(k-n)}{2n}\pi. \quad (36)$$

with $k = 1, 2, \dots, 4n$. The phases of the a few rephasing sequences of this class are listed in Table II. Figure 3 compares several high-order rephasing sequences using the same total cycle duration of 1 ms and the same Rabi frequency. As the order of the sequences increases, the rephasing error is rapidly damped and the detuning bandwidth increases considerably.

C. Comments

All of these demonstrate that longer phased sequences provide much larger detuning bandwidth than the repetition of simple CPMG sequences. In each rephasing sequence, I have assumed that each rephasing pulse has a pulse area π , which is clearly an approximation in a real

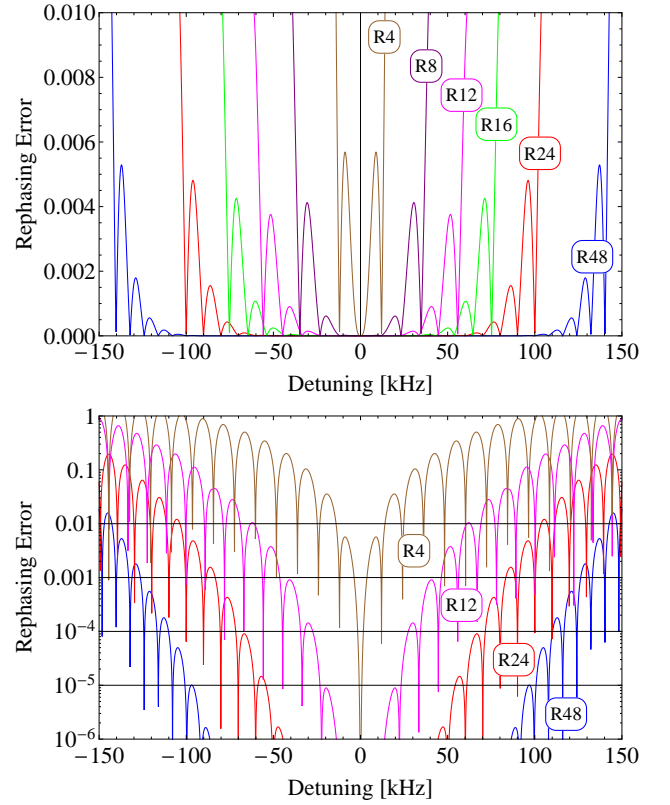


FIG. 3: Rephasing error for several rephasing sequences with 4n pulses for total rephasing time of 1000 μ s. The Rabi frequency is $\Omega = 2\pi \times 150$ kHz, the pulse duration is 3.3 μ s (meaning pulse area π of each individual pulse), and the pulse shape is rectangular.

experiment. This assumption was made in order to single out the affect of the pulse phases and to demonstrate that the bandwidth can be increased by merely selecting a set of phases. These rephasing sequences can be made robust to parameter variations by replacing the rephasing pulses by composite pulses. Because the sequences presented here are already robust against variations in the detuning, one can use simple composite pulses, which stabilize against the pulse area errors only, e.g.

$$B3 : (0, \frac{2}{3}\pi, 0), \quad (37a)$$

$$B5 : (0, \frac{2}{5}\pi, \frac{6}{5}\pi, \frac{2}{5}\pi, 0), \quad (37b)$$

as in Torosov and Vitanov, PRA **83**, 053420 (2011). These pulses have already been tested by Daniel (unpublished but I have seen them and showed them in a few talks)!

It is curious to note that Bm CPs of Torosov emerge naturally in the R2m rephasing sequences, with $m = 2n + 1$. I have not checked, but it is probably true that these rephasing sequences compensate both the detuning and the pulse area.