# Application of forward linear prediction method to high-resolution NMR spectra in inhomogeneous fields

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## Introduction

Intermolecular multiple quantum coherence (iMQC) is caused by intermolecular dipolar interactions and can be used to obtain high-resolution NMR spectra from inhomogeneous fields [1,2]. However, when 2D iMQC spectra are acquired with insufficient increments, wiggles around strong peaks and bad resolution will occur due to the truncation or interferogram. Weighting or apodization functions can remove this distortion, but at the expense of undesired line broadening. A better way to improve resolution may be extending the data set by linear prediction (LP) [3,4]. Here we reported our results on the application of forward LP on the indirect dimension of 2D intermolecular double quantum coherence (iDQC) spectral data sets acquired in inhomogeneous fields with small increments. The results show that compared to normal discrete Fourier transform, the use of forward LP can shorten sampling time by a factor of eight or more at the same level of sensitivity and resolution.

## Methods

To demonstrate the efficiency of forward LP, we use the pulse sequence shown in Fig. 1 which can efficiently suppress solvent signal. In order to select the coherence transfer pathway $0\rightarrow+2\rightarrow0\rightarrow+1\rightarrow-1$, the areas of the first and third gradients must have a ratio of 1:(−2). The second gradient dephases all coherences except intermolecular zero quantum coherence (iZQC). The third gradient refocus the desired coherence terms. The second and third RF pulses are selective for solvent. A two-step phase cycling scheme ($\varphi = (x, y)$ with receiver phase $\varphi_{rec} = (x,-x)$) is designed to obtain the signal originating from iDQC created in the $t_1$ period. The LP extrapolation is based on two assumptions. The first assumption is that the sampled time-domain NMR signal (FID) is a sum of many exponentially damped sinusoids. The second assumption is that the $n$th data point of FID can be expressed as a linear combination of past or latter data values. We used the standard Varian linear prediction software package which is based on the algorithm of Barkhuijsen. The sample was a mixture of methyl ethylic ketone (solute) and cyclohexane (solvent).

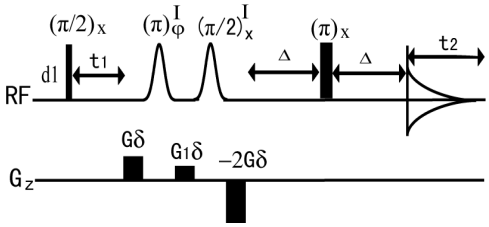


Fig.1. 2D iDQC pulse sequence

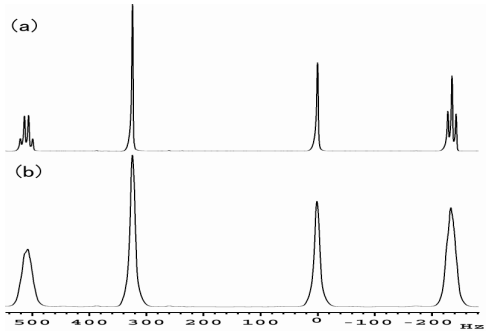


Fig. 2. Conventional 1D $^1$H NMR spectra of the mixture of methyl ethylic ketone and cyclohexane acquired in a well-shimmed field (a) and in an inhomogeneous field of about 60 Hz line-width (b).

## Results and Discussion

Fig. 2a shows the conventional 1D $^1$H NMR spectrum in a well-shimmed field. It is clear that the signal of $CH_2$ from ethyl split into a quartet and the signal of $CH_3$ from ethyl split into a triplet. These splitting cannot be observed in the spectrum acquired in an inhomogeneous field of about 60 Hz line-width (Fig.2b).

Fig. 3 shows the accumulated projections of the sheared 2D iDQC spectra obtained with the pulse sequence shown in Fig. 1 in the same inhomogeneous field as Fig. 2b. All 2D spectra were zero filling to a 4096×4096 data matrix before DFT except Fig. 3d. Figs. 3a and 3c show big wiggles around strong peaks and bad resolution due to insufficient increments in F1 dimension. To get a better spectrum experimentally, 1024 increments in F1 dimension were required, which cost about 4 hours. Similar effect can be achieved by extending the data set of Fig. 3c with forward LP to 1024 and zero filling to 4096 (Fig. 3d). Fig. 3d and 3b have the same level of sensitivity and resolution, and clearly show the multiplet patterns. Although forward LP results in slight spectral distortion, it can effectively extend the data sets acquired from inhomogeneous fields even for shorter data records and lower signal-to-noise ratio.

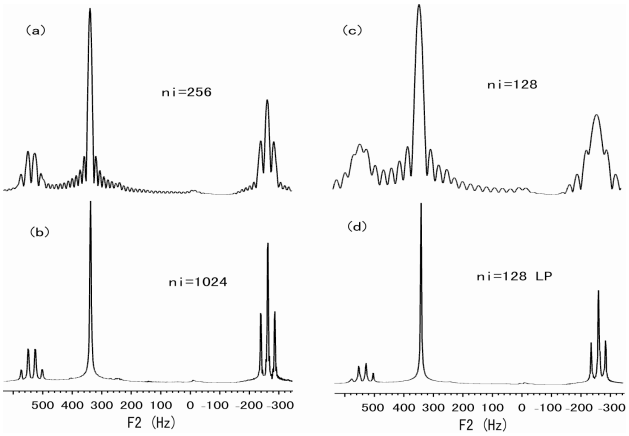


Fig. 3. Accumulated projections of the sheared 2D iDQC spectra: (a) 256 increments in F1 dimension, (b) 1024 increments in F1 dimension, (c) 128 increments in F1 dimension, (d) same as (c) with F1 dimension linear prediction to 1024.

## Acknowledgments

This work was supported by the NNSF of China under Grants (Nos 20573084 and 10774125), and NCET of Ministry of Education of China.

## References

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