Quality Analysis for Least-Squares Transformation of Unevenly Spaced Interferograms

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A least-squares method of transforming interferograms into spectra is compared with the traditional fast Fourier transform (FFT) for varying degree of point-spacing unevenness. A Gaussian distribution is assumed for the deviations from even spacing. FFT gives inferior spectra quality above a critical unevenness, which decreases as more interferograms are averaged.

Index Headings: **Spectroscopy; Fourier; Time-resolved; Interferogram.**

INTRODUCTION

Most Fourier transform spectrometers digitize the optical signal from a Michelson interferometer at even pathlength intervals determined by the zero crossings of a HeNe laser interference pattern. Deviations from an even sample spacing can seriously compromise the quality of resulting spectra. Artifacts from periodic sample position errors have been described.[1] Random position errors presumably create noise.[1]

For time-resolved Fourier transform spectroscopy (TRFTS), the problem of sample spacing accuracy is amplified. TRFTS requires simultaneous accuracy for positions and times of sampling. Depending on the time-resolved acquisition scheme, unavoidable mirror speed variations cause either timing errors or uncertain sampling positions. The well-known interleaved method[2–4] gives good position accuracy but poor timing accuracy. The new event-locked Fourier spectroscopy (ELFS)[5] assures accurate timing and hence must accept the resulting uneven sample spacing.

In this respect, ELFS is equivalent to the synchronous method,[2] where short transient events are initiated at evenly spaced positions, and the signal is sampled after an accurate delay time. Short delay times lead to small uncertainties in sampling positions. Consequences for the quality of the spectra are assumed to be negligible.

The fast Fourier transform (FFT) is the main tool in analyzing common evenly spaced interferograms. Since FFT requires even sample spacing, a new method of transformation into spectra[5] was developed as part of ELFS. This new method requires measurement of the actual sampling positions and uses least-squares fitting of harmonic functions to the unevenly spaced interferograms. This technique will be referred to as "ELFS-style analysis" hereafter. ELFS-style analysis requires more computer memory and more computation time than a regular FFT procedure for spectra with the same resolution and frequency range. Hence, regular FFT analysis would be preferable in cases where ELFS-style analysis does not result in better spectra quality. For almost equally spaced interferograms, it might be possible to ignore the unevenness and to use the more efficient FFT analysis without introducing significant noise or artifacts. This work quantitatively describes the effects of random sample-spacing unevenness on the quality of the spectra. Circumstances under which ELFS-style analysis is preferred to regular FFT are identified.

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EXPERIMENTAL

Since it is difficult to acquire interferograms with variable but known unevenness of the point spacing, numerical simulation is used. The experiment is replaced by a function $I(x)$, which gives an interferogram value for any pathlength difference x. The function used in our tests is

$$I(x) = e^{-(a_0x)^2}[\cos(a_1x + 0.3) + \cos(a_2x + 0.1) + 2\cos(a_3x - 0.5)] \quad (1)$$

with $a_0 = 158$ cm^{-1}, $a_1 = 2\pi$ 12 000 cm^{-1}, $a_2 = 2\pi$ 11 900 cm^{-1}, and $a_3 = 2\pi$ 11 000 cm^{-1}. In the spectral domain, this function describes one isolated Gaussian peak at 11 000 cm^{-1} and two partially overlapping Gaussian peaks near 12 000 cm^{-1}. The factor in front of the bracket apodizes the interferogram and gives the lines a finite width. Discrete interferograms consisting of N points (x_i, $I(x_i)$) are computed with the index i, assuming all integer values from 1 to N. For an evenly spaced interferogram the (unprimed) x_i values are found from

$$x_i = \Delta X\, i - x_0 \quad (2)$$

where ΔX is the sampling interval, and x_0 is some offset to give partially double-sided interferograms. Unevenly spaced interferograms (indicated by primed variables) have points at

$$x_i' = x_i + \Delta x_i \quad (3)$$

where the Δx_i are slight individual offsets for the points. For the simulations, the Δx_i are randomly selected according to a Gaussian distribution with a width of $\overline{\Delta x}$.[6] The width of the distribution can be varied and was used as a measure for the unevenness of the points in the interferogram.

An ELFS-style analysis routine, which includes apodization and phase correction procedures, is used to extract spectra from the interferograms. ELFS-style analysis reduces to FFT analysis in the limit of even sample spacing.[5] This fact permits comparison of ELFS-style and regular FFT analysis by using the same code on two slightly different sets of simulated input data. Using the same routine for both analysis styles has the advantage of identical phase correction and apodization. For ELFS-style analysis, interferogram points (x_i', $I(x_i')$) are provided as the input data. Using (x_i, $I(x_i')$) as the input simulates regular FFT analysis by assigning the interferogram val-

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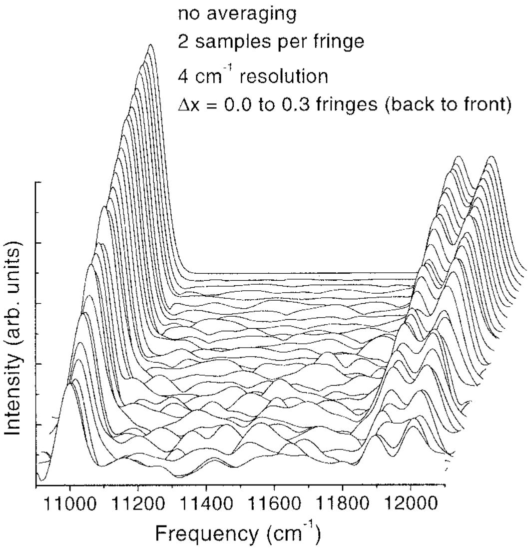

FIG. 1. Simulated spectra obtained from regular FFT analysis with increasing (back to front in steps of 0.01 fringes) unevenness $\overline{\Delta x}$ of the data point spacing.

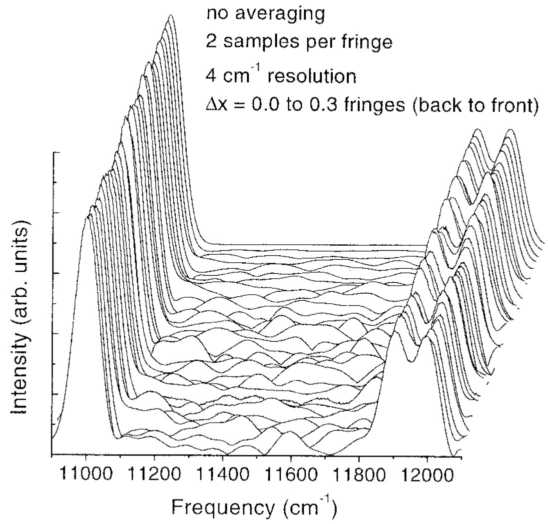

FIG. 2. Simulated spectra obtained from ELFS-style analysis with increasing (back to front in steps of 0.01 fringes) unevenness $\overline{\Delta x}$ of the data point spacing.

ues $I(x_i')$, which are found at unevenly spaced points, to the evenly spaced x_i.

RESULTS AND DISCUSSION

Interferograms with two samples per HeNe fringe ($\Delta X \approx 316$ nm) up to a maximum pathlength difference of 2.5 mm were created. The results with regular FFT analysis for varying $\overline{\Delta x}$ are shown in Fig. 1. The ideal spectrum with $\overline{\Delta x} = 0$ is plotted in the background. As the value of $\overline{\Delta x}$ increases towards the front, noise with increasing amplitude appears. In addition, the heights of the three lines deviate more and more from their original values. Apparently, the lines lose strength to the predominantly positive noise.

The results of ELFS-style analysis are shown in Fig. 2. Again, the only difference in the preparation of these spectra is the use of the primed pathlength coordinates (Eq. 3) in the interferograms. The noise appears to increase (at least initially) in a similar fashion as in Fig. 1. However, the line strengths vary only within the limits of the noise.

The differences between the spectral values $S'(v_i)$ and the ideal spectrum $S(v_i)$ may be used to quantify the spectra quality. A quality value Q is defined as the ratio of peak intensity $\hat{A}$ to the root-mean-squared (rms) value of such differences by

$$Q \equiv \hat{A}\left[\frac{1}{M}\sum_{i}^{M}(S'(v_i) - S(v_i))^2\right]^{-1/2} \tag{4}$$

where the summation is over the M spectral values in the range of interest. The peak intensity of the 11 000 cm^{-1} line in the ideal spectrum is used for $\hat{A}$ in all further calculations. Larger Q values indicate better agreement with the ideal spectrum. Perfect agreement gives $Q = \infty$. In Fig. 3, Q is plotted against $\overline{\Delta x}$ for ELFS-style and regular FFT analyses for cases with and without averaging of interferograms. The spectra quality tends to decrease as the unevenness of the point spacing increases. Without averaging (one scan), the qualities for ELFS and FFT analyses are similar up to an unevenness of about 20% of the sampling interval ΔX. Above this limit, ELFS spectra have a nearly constant quality, whereas FFT spectra continue to deteriorate until virtually no resemblance to the ideal spectrum remains for $\overline{\Delta x} > \Delta X$. The situation differs for averaged interferograms (64 scans). Only for very small $\overline{\Delta x}$ does FFT analysis perform better than ELFS. Above an unevenness of about 3% of the sampling interval, ELFS analysis performs better and reaches a constant level roughly three times higher than is the case without averaging. In contrast, the quality value of FFT spectra decreases at an accelerated rate until it reaches the same low level that occurs without averaging.

The quality values for ELFS analysis of averaged interferograms are nearly constant for small $\overline{\Delta x}$. Apparently, there is at least one source of noise which is independent of $\overline{\Delta x}$. The approximate evaluation of the least-squares formulae could be this source of noise as shown in Fig. 4. In

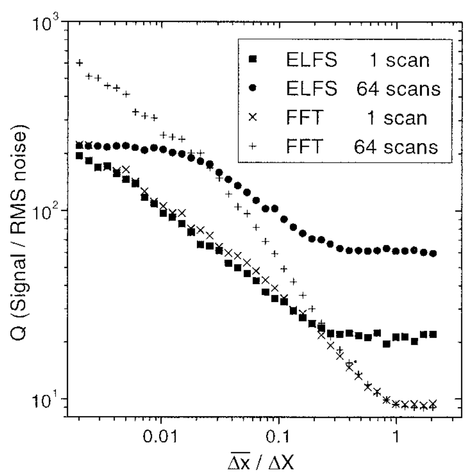

FIG. 3. Quality value of spectra for ELFS-style (solid symbols) and usual FFT (crossed symbols) analyses as function of the sampling unevenness $\overline{\Delta x}$ (in units of the average sampling interval ΔX). A larger quality value means better agreement with the ideal spectrum.

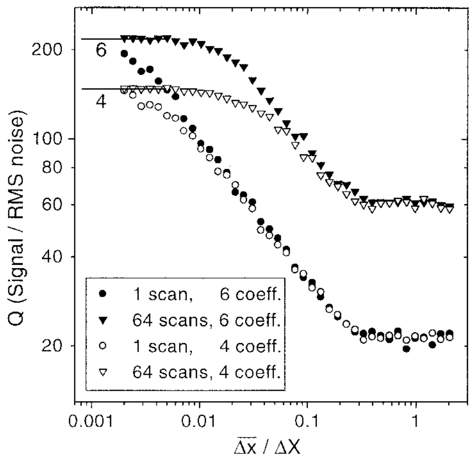

FIG. 4. Quality of spectra obtained from ELFS-style analysis using six grid points (solid symbols) and four grid points (open symbols) for the approximate evaluation of the least-squares formulae. The horizontal lines indicate apparent quality limits for four and six grid points.

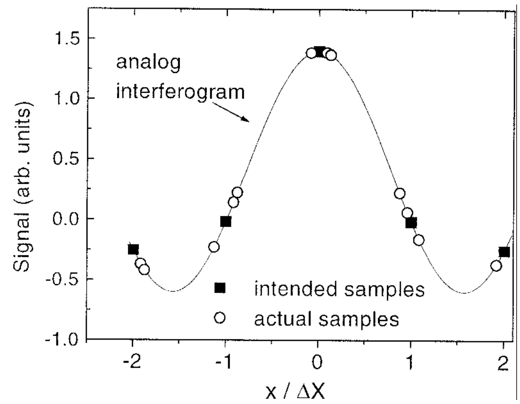

FIG. 5. Analog interferogram with intended and actual samples.

ELFS-style analysis, the exact evaluation of harmonic functions at uneven intervals is replaced by an approximation with the use of a certain number of neighboring points on an even grid and an interpolation technique.[5] Six grid points/coefficients are used for the data in Fig. 3. Figure 4 shows the effect of decreasing the number of grid points on the quality of the spectra. Apparently, using fewer coefficients raises the noise floor (lower quality limit), as indicated by the numbered horizontal lines. For the values of $\overline{\Delta x}$ in Fig. 4, the spectra quality does not exceed these limits even with averaging. For medium and large values of $\overline{\Delta x}$, the noise contribution from the approximate evaluation becomes less important and the spectra quality for four and six coefficients is approximately equal. The exact evaluation of the ELFS formulae takes several orders of magnitude more time than the approximate method, making it currently impractical. However, test runs seem to indicate an equal or better quality of the spectra than either FFT and ELFS analyses for all $\overline{\Delta x}$.

The quality dependence on $\overline{\Delta x}$ differs, depending on the spectral content of the interferogram. High optical frequencies lead to steep slopes in the interferogram and to large changes of $I(x_i')$ with variations of Δx_i. This situation is shown in Fig. 5. The sampling positions at $\pm\Delta X$ lie on steep slopes, which leads to a large range of possible interferogram values and potentially to noise. By plotting the spectra quality vs. $\overline{\Delta x}/\Delta X$ in Figs. 3 and 4, where ΔX is approximately half the inverse maximum optical frequency, the dependence of the curves on the spectral content of the spectra has been reduced.

Figure 5 also explains why line strengths decrease with $\overline{\Delta x}$ when FFT analysis was used. The interferogram value assigned to zero pathlength difference determines the integrated strength of all lines. Sampling positions different from $x = 0$ give smaller interferogram values and hence lower line strengths. Averaging improves the situation only if actual samples are quite close to their intended position. ELFS analysis does not exhibit this problem, since the actual sampling positions are used for calculations.

Practical conclusions may now be drawn. Depending on the number of averaged interferograms, one can extract from Fig. 3 a critical ratio $\overline{\Delta x}/\Delta X$, which defines a threshold above which one should use ELFS-style analysis. If the unevenness of the sampling positions is unknown, an approximate value may be found from the magnitude of mirror speed variations. For continuously scanning interferometers, an estimate may be obtained by observing the HeNe reference signal or the interferogram of another single-line source on an oscilloscope. Variations in the fringe period indicate speed changes. If the time delay between accurate knowledge of position and the actual sampling is t_d, and mirror speed variations are of size $\overline{\Delta v}$, the sampling position error is $\overline{\Delta x} = 2\overline{\Delta v}t_d$. The factor "2" is for instruments where the actual changes in pathlength difference are twice as fast as the mirror speed. For a single interferogram (no averaging), the quality numbers for both analysis types are comparable for $\overline{\Delta x}/\Delta X \leq 0.2$. For 64 averaged interferograms, they are comparable for $\overline{\Delta x}/\Delta X \leq 0.03$. At a typical mirror speed of 0.5 cm/s with variations of 3% and sampling twice per fringe, it takes about 200 μs to reach the critical unevenness without averaging (30 μs for 64 averages). In other words, ELFS-style analysis will give better spectra for observation times (difference between the moment of accurate time and position knowledge and the sampling time) longer than 200 μs in TRFTS without coaddition.

The foregoing simulations assumed random Δx_i with a Gaussian distribution. Periodic mirror speed variations would cause periodic changes in the sampled interferogram intensity, giving artifacts when regular FFT analysis is being used.[1] Speed spikes may cause large-amplitude Δx_i outside the Gaussian distribution considered here. The effect of such nonrandom sampling errors is difficult to characterize. In practice, the best plan may be to apply both analysis techniques to an actual data set to decide which technique to use for other spectra with similar spectral content.

To compare FFT and ELFS analyses for actual data, we acquired time-resolved interferograms in steps of 1.5 μs from Nd^{3+}:$CsGd_2F_7$ photoluminescence at 80 K after short-pulse excitation at 532 nm. A spectral resolution of 2 cm^{-1} was chosen. No averaging was performed. The scan speed of our interferometer exhibits the expected random noise but also position-dependent shifts and spikes.[4] The random speed noise is only 3% of the average speed (0.15 cm/s). Within the 300 μs observation time, sampling position errors of about 30 nm (2 × 0.15

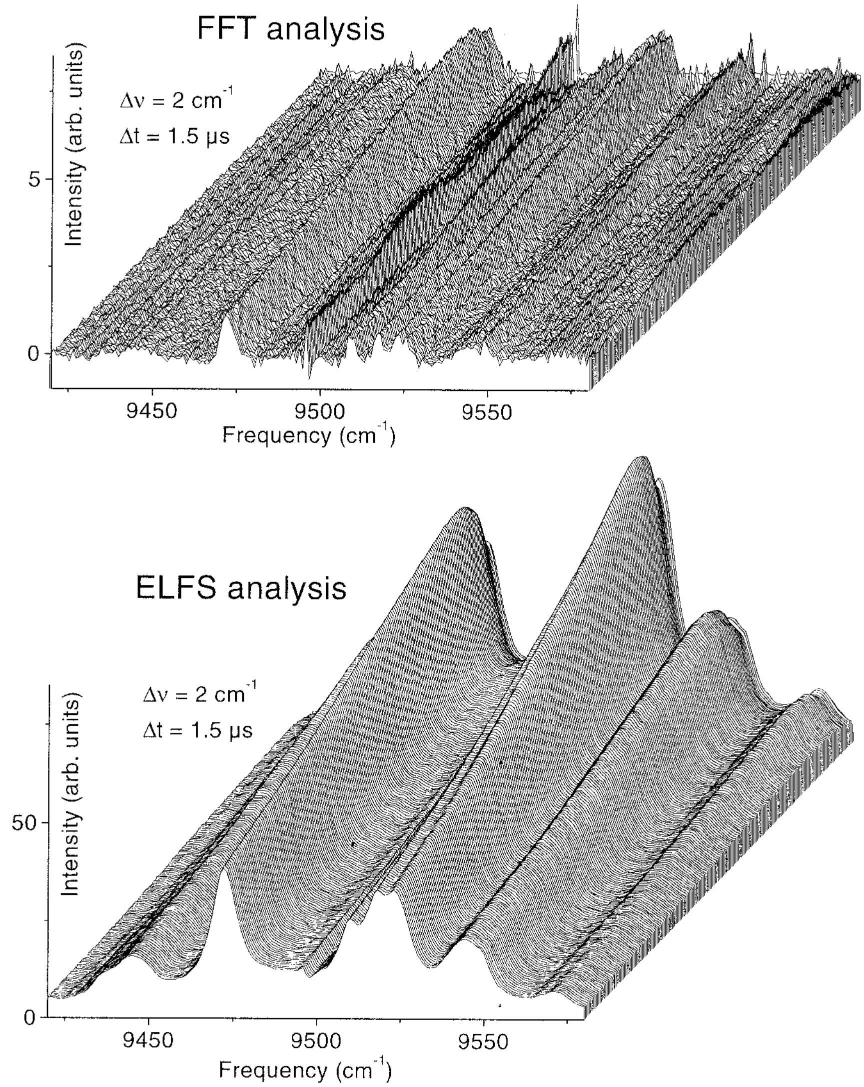

FIG. 6. Spectra calculated from an actual (not simulated) data set with FFT analysis (top) and ELFS analysis (bottom). The difference is much larger than expected from only random mirror speed variations. The signal is 80 K Nd:$CsGd_2F_7$ photoluminescence excited by a Q-switched YAG laser at 532 nm. Time increases forward in 1.5 μs steps. The intensity oscillation at early times is detector response.

cm/s × 0.03 × 300 μs) can accumulate from the random speed noise component. This is approximately 10% of the sampling interval. Hence, according to the simulation results, one expects similar performance from both FFT and ELFS analysis techniques without averaging. Figure 6 shows the spectra obtained with FFT analysis (top) and ELFS analysis (bottom). The superiority of the spectra quality for ELFS analysis is obvious. Apparently, the nonrandom contributions to the speed variations cause a strong degradation of spectra quality for FFT analysis, whereas ELFS analysis gives acceptable spectra with high signal-to-noise ratio. This example emphasizes the utility of ELFS-style data acquisition and analysis and shows that the $\overline{\Delta x}$ limits derived in this paper for the usefulness of FFT are upper bounds. In practice, ELFS will be superior for much smaller $\overline{\Delta x}$ values because of the nonrandom deviations that generally can occur.

The constant quality level for ELFS-style analysis at large values of $\overline{\Delta x}$ (Figs. 3 and 4) has an interesting implication. If $\overline{\Delta x}$ cannot be kept below 20% of the sampling interval, there is no longer an advantage in attempting to evenly distribute the interferogram samples. A random distribution of samples becomes acceptable (although accurate knowledge of the sampling positions x_i' is still required).

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