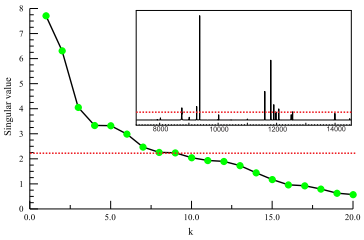
SINGULAR VALUE DECOMPOSITION-BASED MODELING OF TIME DOMAIN SIGNALS IN BROADBAND MICROWAVE SPECTROSCOPY

A. J. MINEI, *Department of Chemistry and Biochemistry, Division of Natural Sciences, College of Mount Saint Vincent, 6301 Riverdale Avenue, Riverdale, New York, 10471*; S. A. COOKE, *School of Natural and Social Sciences, Purchase College SUNY, 735 Anderson Hill Road, Purchase, NY 10577, USA.*



A singular value decomposition (SVD) signal processing method is newly applied to molecular free induction decays (FIDs) obtained using a time domain, broadband rotational spectrometer. It is demonstrated that for the strongest spectral transitions the SVD method can determine transition frequencies with a precision matching that of the fast Fourier transform method. Furthermore, the SVD-based analysis produces information concerning transition phase, amplitude, damping, and frequency for the strongest molecular signals. These parameters are shown as useful in regards to time-domain signal filtering. The computational expense of the SVD method is high and therefore this approach has the disadvantage that with our present computers the full molecular FID must be considerably truncated. The effects of FID truncation on the determined transition frequencies have been examined. Conversely, this truncation method illustrates that broadband spectra may be recovered from fragments as small as 1 % of the complete FID. The success of the SVD-based method is further examined in regards to weak signal detection, and frequency dependent detection. The pure rotational spectrum of 1H,1H,2H-perfluorocyclobutane is used for illustrative purposes in this study.