Abstract Submitted
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Analytical modeling of line shapes in multidimensional spectroscopy REBECCA CONRAD, MARK SIEMENS, University of Denver — Two-dimensional coherent spectroscopy (2DCS) is a powerful tool that has provided new insight into decoherence dynamics and coherent energy transport in biological and nanostructured materials. In order to determine physical properties from experimental 2D spectra, comparisons must be made to calculations based on the Optical Bloch Equations (OBEs). In this work, analytical and graphical models were produced to discover more about the connection between fundamental physical properties of materials and spectroscopic line shapes. We used the Projection-Slice theorem of Fourier transforms to simplify the calculation by rotating the solution to the OBEs to a diagonal/cross-diagonal space, which enabled an analytical solution. In contrast to numerical computational models used in the past to simulate solutions to the OBEs, our analytical representation is much more efficient, and therefore provides a faster and more direct way to analyze experimental data.

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