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## ABSTRACT

This paper presents a general method for simulating the effect of chemical exchange on MAS NMR spectra of solid samples. The complication in MAS spectra is that the Hamiltonian itself is time-dependent, due to the spinning of the sample. The approach taken in this work is to use Floquet theory to convert the problem into a time-independent form, and then use established methods (used in liquid NMR simulations) to calculate the lineshape. Floquet theory has been admired for its elegance, but criticised for its computational inefficiencies. This is because it removes the time dependence of the system by expanding the problem in a Fourier-like series. This makes a relatively small, time-dependent calculation into a much larger time-independent one. Typically, we use twice as many Floquet blocks as there are spinning sidebands, so the increase in size is substantial. The problem that this creates stems from the fact that the usual Householder methods for diagonalizing a matrix scale as the cube of the size of the matrix. This would make a Floquet calculation prohibitively long. However, the Floquet matrix is inherently sparse, so sparse matrix methods can produce substantial computational savings. Also, fully diagonalizing a matrix is expensive, but converting the matrix to a tridiagonal form (using iterative Lanczos methods) is much cheaper. The use of the Lanczos methods makes the Floquet calculations feasible as a general method for systems of more than one spin. We show how to set up the full matrix describing chemical exchange in a spinning sample, but the details of how the Lanczos methods work are not included - they are described elsewhere. We then validate the theory by simulating the MAS spectra of dimethylsulfone with both natural abundance of $^{13}C$, and

with both methyl groups labelled with $^{13}C$. The latter system has both dipolar and chemical shielding anisotropy terms contributing to the spectrum.