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ABSTRACT

In magic-angle spinning (MAS), the Hamiltonian of the system changes periodically with time, so the spectrum shows sidebands at multiples of the rotor frequency. This changing Hamiltonian (and hence, the changing Liouvillian) complicates the simulation of the lineshape considerably. A simple case is that of a spin-1/2 with an anisotropic chemical shift, spinning at the magic angle. Perhaps the most famous solutions to this problem of calculating spinning sideband intensities are those of Herzfeld and Berger, and Maricq and Waugh; but there are many alternatives. Floquet theory is a very powerful approach, which we describe here. We illustrate the theory by explicit calculation of the sideband patterns.

Floquet theory works by expanding the periodic (due to sample spinning) Hamiltonian into a Fourier series. The *time-independent* Fourier components become the blocks in a much larger, time-independent, effective Hamiltonian. The same can be done with the Liouvillian superoperator. The effective Hamiltonian (or Liouvillian) can then be treated using familiar methods used for time-independent problems.

The considerable increase in size of the problem is normally anathema, and it offers no particular benefit in the specific case treated here. The power of the method is its generality. Regardless of the complexity of the time dependence of the Hamiltonian, the Floquet approach is the same. Therefore, learning how to calculate sideband intensities in this way gives us the tools to solve much more difficult problems.