CAUSAL CORRELATION FUNCTIONS AND FOURIER TRANSFORMS: APPLICATION IN CALCULATING PRESSURE INDUCED SHIFTS

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By adopting a concept from signal processing, instead of starting from the correlation functions which are even, one considers the causal correlation functions whose Fourier transforms become complex. Their real and imaginary parts multiplied by 2 are the Fourier transforms of the original correlations and the subsequent Hilbert transforms, respectively. Thus, by taking this step one can complete the two previously needed transforms. However, to obviate performing the Cauchy principal integrations required in the Hilbert transforms is the greatest advantage. Meanwhile, because the causal correlations are well-bounded within the time domain and band limited in the frequency domain, one can replace their Fourier transforms by the discrete Fourier transforms and the latter can be carried out with the FFT algorithm. This replacement is justified by sampling theory because the Fourier transforms can be derived from the discrete Fourier transforms with the Nyquis rate without any distortions. We apply this method in calculating pressure induced shifts of H_2O lines and obtain more reliable values[a]. By comparing the calculated shifts with those in HITRAN 2008 and by screening both of them with the pair identity and the smooth variation rules, one can conclude many of shift values in HITRAN are not correct.

[a] Q. Ma, R. H. Tipping, and N. N. Lavrentieva, JQSRT dio:10.1016/j.jqsrt.2012.02.012 (2012).