

Abstract Submitted
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Protein dynamics, solvation, and quasielastic scattering PAUL FENIMORE, Theoretical Division, Los Alamos National Laboratory — Quasielastic Mössbauer and neutron scattering (QES) have been used to measure protein dynamics for about 50 years. These low energy transfer spectra show two prominent features: a sharp elastic line and a broad quasielastic band. Current theory assumes that the elastic line and the quasielastic band are independent features of the spectrum, caused by motions in the sample. Current practice extracts information about dynamics from the spectra by assuming specific models with a few parameters that are determined by data fitting. We claim that this approach is flawed; it is based on questionable assumptions and has no predictive power. We propose a model where the elastic line and the broad band are one inhomogeneous spectrum of shifted, sharp natural-width lines. The model makes predictions of QES lineshapes and elastic fractions for Mössbauer and neutron scattering. Essential features of this description include: (i) QES lineshape and elastic fraction are sensitive to protein vibrations, and fluctuations slaved to the hydration shell and bulk solvent. (ii) Independently measured dielectric fluctuation spectra predict the QES lineshape.

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