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Why the observed mean square motional displacement depends on wave vector Q DERYA VURAL, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716-2593, USA — The motional mean square displacement (MSD) of hydrogen (H) in proteins is extensively measured using neutron scattering techniques. The MSD increases rapidly with temperature near room temperatures and a large MSD is often associated with protein function. One shortcoming of these measurements is that the observed MSD depends on the wave vector (Q) of the neutron data used to obtain the MSD. This dependence is often attributed to use of the Gaussian approximation made to the scattering function in the analysis of the data. To test this we have simulated the protein lysozyme and calculated the intermediate scattering function (ISF), both the full ISF and the ISF in the Gaussian approximation. We find that the MSD extracted in the usual way was the same and still Q dependent in both cases. Also, direct calculation of the terms beyond the Gaussian approximation shows these terms are small. Rather, we find that the apparent Q dependence of the MSD arises from the “dynamical diversity” of the H in lysozyme. Specifically, if the ISF of an individual H in the protein is calculated and the MSD extracted in the usual way, then the MSD is independent of Q . This Q dependence arises from ignoring the dynamical diversity in the data analysis.

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