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Motional displacements in proteins incorporating dynamical diversity[1] DERYA VURAL, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, P.O. Box 2008, Tennessee 37831 , USA, JEREMY SMITH, UT/ORNL Center for Molecular Biophysics, Oak Ridge National Laboratory, P.O. Box 2008, Tennessee 37831, USA, HENRY GLYDE, Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716-2570, USA
— The average mean square displacement (MSD), $\langle r^2 \rangle$, of hydrogen H in proteins is measured using incoherent neutron scattering methods. The observed MSD shows a marked increase in magnitude at a temperature $T_D \simeq 240$ K. This is widely interpreted as a dynamical transition to large MSDs which make function possible in proteins. However, when the data is interpreted in terms of a single averaged MSD, the extracted $\langle r^2 \rangle$ depends on the neutron momentum transfer, $\hbar Q$, used in the measurement. We have shown recently that this apparent dependence on Q arises because the dynamical diversity of the H in the protein is neglected[2]. We present models of the dynamical diversity of H in Lysosyme that when used in the analysis of simulated neutron data lead to consistent, Q independent values for the average MSD and for the diversity model.
2. D. Vural and L. Hong, J. C. Smith and H. R. Glyde. *Phys. Rev. E* **91**, 052705 (2015).

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