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Exploring the nonlocal dielectric susceptibility of liquid water in the terahertz regime - propagating modes, Debye relaxation and overscreening[1] DANIEL ELTON, MARIVI FERNANDEZ-SERRA, Stony Brook University — There is great interest in the dielectric and infrared spectra of water between 1-1000 cm^{-1} (.03-30 THz). To gain insight into this region we study the nonlocal (wavelength dependent) dielectric susceptibility. A curious feature of water is the presence of a propagating mode in the librational region. For the first time we study the temperature dependence of this mode and its range of propagation. We show that the librational band has two components - non-dispersive and dispersive. Previously this mode was suggested to be analogous to an optical phonon propagating along the H-bond network. We suggest a possible alternative - that it is the dipolaron mode predicted for dipolar systems.[2] Next we study the region of .1-10 THz which is relevant to understanding the coupling between proteins and water. We show that in addition to H-bond vibrations, intramolecular inertial relaxations also contribute. We find that the Debye peak is dispersive, confirming its long range cooperativity. We report the first temperature dependent study of the static nonlocal susceptibility, which exhibits a negative region, a phenomena called overscreening. We compare a rigid model (TIP4P/ε), a flexible model (TIP4P/2005f) and a polarizable model (TTM3-F).

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[2]PRL **46**, 950 (1981).

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