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Comparison of two simple models for high frequency friction: Exponential vs. Gaussian wings STEVEN ADELMAN, Purdue University — We describe new methods for ruling out unphysical forms for the high frequency friction $\lim_{\omega\to\infty} \beta(\omega)$ needed to compute vibrational energy relaxation times. These are based on the fluctuating force autocorrelation function(faf) $C(t) = \langle\tilde{\Im}^2\rangle_0^{-1}\langle\tilde{\Im}(t)\tilde{\Im}\rangle_0$,which is proportional to the Fourier transform of $\beta(\omega)$. Here we compare two model faf's $C_{se}(t)$ = sech (t/τ) and $C_{ga}(t) = \exp\left[-\frac{1}{2}\left(\frac{t}{\tau}\right)^2\right]$. These give respective high frequency frictions which have incompatible exponential and Gaussian forms. We apply our procedures to eliminate $C_{se}(t)$. We do this by showing from $\beta_{se}(\omega) \equiv \frac{\langle\Im^2\rangle_0}{k_BT}\int_0^\infty \cos\omega t C_{se}(t)dt$ that $\lim_{\omega\to\infty}\beta_{se}(\omega)$ derives from the long time "tail" of $C_{se}(t)$. We then note that $C_{se}(t)$ is built only from short time quantities, rendering the form of this "tail" artifactual. Thus the exponential form of $\lim_{\omega\to\infty}\beta(\omega)$, is also artifactual.

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