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Letter

Modified and generalized single-element Maxwell viscoelastic model

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In this Letter, the single-element Maxwell model is generalized with respect to the wave vector and extended with a correction function that measures the reduced viscous response. This model has only two free parameters and avoids the attenuation-frequency locking present in the original model. Through molecular simulations it is shown that the model satisfactory predicts the transverse dynamics of the binary Lennard-Jones system at different temperatures, as well as water and toluene at ambient conditions. The correction function shows that the viscous response is significantly reduced compared to the predictions of the original Maxwell model and that there exists a characteristic length scale of minimum dissipation.

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It is fascinating how well continuum hydrodynamics can describe the dynamics of fluid systems on small length scales [1–3]. The limitations of hydrodynamics depend on the specific dynamical properties, the fluid system one studies, as well as the set of constitutive models applied [4–6]. An example of the latter is that Newton's law of viscosity for the fluid stress cannot predict the viscoelastic behavior observed for even simple fluid systems on sufficiently small length scales [7,8]. A natural extension to the hydrodynamic description is to apply generalized hydrodynamics (possibly in the Zwanzig-Mori framework), where the viscosity is wave-vector and frequency dependent [9,10], or use a viscoelastic constitutive model for the stress, for example, Maxwell's model [5,11].

It is interesting to note that Boltzmann criticized the Maxwell model and proposed the generalized hydrodynamic framework, which has since been used with great success (see, e.g., Ref. [5]). Despite this criticism the Maxwell model provides a clear interpretation of the underlying processes giving valuable insight into the physics of fluids, and it is therefore still relevant.

The Maxwell model states that the total strain rate $\dot{\gamma}$ at a point is the sum of the viscous strain rate σ/η_0 and elastic strain rate $\dot{\sigma}/G$, where σ is the stress, η_0 the shear viscosity, and G the shear modulus (or modulus of rigidity). The standard dot notation is here used to denote the time derivative. Rewriting this sum, Maxwell's model can be expressed as

$$\eta_0\dot{\gamma} = (1 + \tau_M\partial_t)\sigma, \tag{1}$$

where $\tau_M = \eta_0/G$ defines the Maxwell time. The simple interpolation between a purely viscous response (dissipation) and purely elastic response (energy storage) will here be denoted the ideal mixing of viscosity and elasticity (or dissipation and storage). Note, recently, Zaccone showed [12] from non-affine molecular motion the microscopic mechanisms for the two extremes, giving a foundation for the interpolation. It is also important to mention that the fractional viscosity model (FVM) is another way of mixing the viscous and elastic responses (see Refs. [13,14]).

In a mechanical network representation, the Maxwell element is a dashpot (with viscosity η_0) serially connected to a spring (with characteristic time τ_M). The Maxwell model itself can of course also be extended in different ways, for example, one can introduce a set of Maxwell elements connected in parallel (a Maxwell-Weichert element) [15]; each element is then characterized by a viscosity and characteristic time. This leads to a larger parameter space, which is necessary in order to capture the multiple relaxation times present in many fluid systems. The Maxwell-Weichert element is sometimes referred to as a generalized viscoelastic model, however, this term will be reserved for another modeling strategy as explained in the following. The single-element Maxwell model can be generalized by allowing both η_0 and τ_M to be functions of wave vectors, that is, the viscous and elastic responses become length scale dependent. Mizuno and Yamamoto [16] introduced a combination of two parallel Maxwell elements with wave-vector-dependent viscosities and Maxwell times. They showed that by introducing the concepts of slow and fast relaxations their four-parameter model featured good agreement with molecular dynamics data for a viscous model system.

In this Letter, it is shown that the generalized, i.e., wave-vector-dependent, single-element Maxwell model fails to predict the correct transverse hydrodynamics for even simple systems in the viscoelastic regime. The deviation from simulation data is quantified by simply relaxing the ideal mixing rule through a correction function. The physical interpretation of this function is that the fluid viscous property is not determined by the zero-frequency viscosity, but also by other energy storage processes than what the Maxwell time includes. This picture is in line with Boltzmann's generalized Newtonian viscosity law, but different from the Maxwell-Weichert element. The inclusion of a correction function then leads to an extended single-element generalized Maxwell model with only two free-fitting parameters at a given characteristic wave vector. The focus here is not on the dynamics of supercooled liquids or glasses (see, e.g., Refs. [17,18] for more advanced theories), but on less viscous fluid systems where application of the Maxwell model is meaningful in the first place.

The hydrodynamic function we study is the transverse velocity autocorrelation function (TVACF) defined by $C^{\perp}_{uu}(k,t) = \frac{1}{V}\langle \widetilde{u}(k_y,t)\widetilde{u}(-k_y,0)\rangle$, where V is the system volume, $\widetilde{u}$ is the Fourier coefficient of the velocity x component, and k_y the y component of the wave vector $\mathbf{k} = (0, k_y, 0)$. $\langle\cdots\rangle$ denotes the ensemble average of different uncorrelated initial conditions. Notice that to first order in the density fluctuations $C^{\perp}_{uu}$ is related to the often used transverse momentum autocorrelation function $C^{\perp}_{jj}$, by $C^{\perp}_{jj} = \rho^2 C^{\perp}_{uu}$, where ρ is the average density. In the following we omit the subscript on the wave-vector y component and set $k = k_y$.

For completeness the TVACF is derived here, and to this end we first write the momentum balance equation in Fourier space for $\mathbf{k} = (0,k,0)$, and since we investigate equilibrium relaxations we can assume zero advection, thus,

$$\rho\,\partial_t\widetilde{u} = ik\widetilde{\sigma}. \tag{2}$$

The Maxwell model introduces a characteristic elastic time and we only generalize with respect to wave vector and not frequency. Moreover, in what follows we only consider homogeneous and isotropic systems. In real space and using the Leibniz integration rule, the generalized Maxwell model reads

$$\eta_0\int_{-\infty}^{\infty} f(y-y')\partial_{y'}u\,\mathrm{d}y' \\ = \sigma(y,t) + \tau_M\partial_t\int_{-\infty}^{\infty} g(y-y')\sigma(y',t)\mathrm{d}y', \tag{3}$$

where we denote f and g the shear viscosity kernel and Maxwell time kernel, respectively. The kernels have dimensions of inverse length and must fulfill that $\int_{-\infty}^{\infty} f(y-y')\mathrm{d}y' = \int_{-\infty}^{\infty} g(y-y')\mathrm{d}y' = 1$. Newton's law of viscosity is recaptured by ignoring both the elastic component, $\tau_M = 0$, as well as the spatial correlations, that is, $f(y-y') = \delta(y-y')$, where δ is the Dirac delta. Applying the convolution theorem the generalized Maxwell model reads, in Fourier space,

$$i\eta_0 k\widetilde{f}(k)\widetilde{u}(k) = [1 + \tau_M\widetilde{g}(k)\partial_t]\widetilde{\sigma}(k,t), \tag{4}$$

with $\widetilde{f}(0) = \widetilde{g}(0) = 1$. From the momentum balance equation, Eq. (2), we get for the velocity Fourier coefficients

$$\partial_t^2\widetilde{u} + \frac{1}{\widetilde{\tau}}\partial_t\widetilde{u} + \frac{k^2\widetilde{\eta}}{\rho\widetilde{\tau}}\widetilde{u} = 0, \tag{5}$$

where we have used the shorthand notation $\widetilde{\eta} = \eta_0\widetilde{f}(k)$ and $\widetilde{\tau} = \tau_M\widetilde{g}(k)$. Introducing the shear wave speed $c_T(k)$ as $c_T^2 = \widetilde{\eta}/\rho\widetilde{\tau}$, multiplying by $\widetilde{u}(-k,0)$, and ensemble averaging, we get the dynamical equation for the TVACF,

$$\partial_t^2 C^{\perp}_{uu} + \frac{1}{\widetilde{\tau}}\partial_t C^{\perp}_{uu} + c_T^2k^2C^{\perp}_{uu} = 0, \tag{6}$$

for any wave vector k. The eigenvalues (or modes) to this problem are

$$\omega_{1,2} = -1/(2\widetilde{\tau}) \pm \sqrt{1/(2\widetilde{\tau})^2 - (c_Tk)^2}. \tag{7}$$

In the viscoelastic regime $1/\widetilde{\tau}^2 < 4(c_Tk)^2$, or equivalently $1/\widetilde{\tau} < 4\widetilde{\eta}k^2/\rho$, the solution reads

$$C^{\perp}_{uu}(k,t) = \frac{k_BT}{\rho}e^{-\Gamma t}\cos(\omega_0 t) \tag{8}$$

by application of the equipartition theorem, and where we define the attenuation coefficient $\Gamma = 1/(2\widetilde{\tau})$ and frequency $\omega_0^2 = |1/(2\widetilde{\tau})^2 - (c_Tk)^2|$. It is clear that the frequency can be written as functions of $\widetilde{\tau}$, or equivalently, via the attenuation coefficient

$$\omega_0^2 = 4\Gamma|\Gamma - 2\widetilde{\eta}k^2/\rho|. \tag{9}$$

If $\widetilde{\eta} = \eta_0\widetilde{f}$ is known, we obtain a single-parameter model, and in this case the attenuation determines the frequency, thus, the Maxwell model exhibits attenuation-frequency locking.

There is an important point worth highlighting: In the viscous regime $1/\widetilde{\tau} > 4\widetilde{\eta}k^2/\rho$, the solution to Eq. (6) is topologically different from Eq. (8) [19]. In particular, we have the general solution $C^{\perp}_{uu}(k,t) = C_1e^{\omega_1 t} + C_2e^{\omega_2 t}$, where C_1 and C_2 are integration constants, and $\omega_1 \approx -1/\tau_M + \eta_0k^2/\rho$ and $\omega_2 \approx -\eta_0k^2/\rho$. Now, since $\lim_{k\to 0} C^{\perp}_{uu} = k_BT/\rho$ for all t we must have that $C_1 = 0$ and $C_2 = k_BT/\rho$. This means that we recapture the Newtonian model as $k \to 0$ [3], which is identical to a nonfractional viscosity model. In the following we focus on the viscoelastic regime alone.

The locking phenomenon is not in agreement with observations. This can clearly be illustrated through a set of standard molecular dynamics simulations of a simple binary fluid. The cubic periodic three-dimensional system is composed of 8000 A and B particles with a mixing ratio 80:20, respectively. The A and B particles have different interaction parameters which avoid crystallization—see Refs. [20,21] and Ref. [22], respectively, for details. The simulation is carried out using the simulation package MOLSIM [23] in the canonical ensemble in the temperature range 0.45–1.0ϵ/k_B, where k_B is Boltzmann's constant and ϵ the simulation energy scale. The mass density is the standard $1.2m/\sigma^3$, where m and σ are the simulation mass and length scales. From hereon all quantities are given in terms of ϵ, m, and σ; as usual, we omit writing these dimensions explicitly. The viscosity ranges from 15.3 at $T = 1$ to approximately 3571 at $T = 0.45$. The TVACF is calculated directly from the microscopic definition of the streaming velocity, which to first order in density fluctuations reads $\widetilde{u}(k,t) = m/\rho\sum_i v_i(t)e^{-iky_i(t)}$, where v_i is the particle velocity x component and y_i the particle y position [3]. It is important to state that the TVACF has been compared to the results from the momentum current autocorrelation function, justifying the first-order fluctuation approximation (at least away from the critical point in the thermodynamic phase space). We only use $\widetilde{\tau}$ as the fitting parameter (see below), and note that the viscosity kernel $\widetilde{\eta} = \eta_0\widetilde{f}(k)$ can be calculated from the wave-vector-dependent stress or the TVACF itself (see Ref. [24]). Here, the latter method is used, and to highlight that it is the TVACF from the simulation, we use the subscript MD rather than uu, i.e.,

$$\eta_0\widehat{f}(k,\omega) = \frac{\rho}{k^2}\frac{C^{\perp}_{\mathrm{MD}}(k,t=0) - i\omega\widehat{C}^{\perp}_{\mathrm{MD}}(k,\omega)}{\widehat{C}^{\perp}_{\mathrm{MD}}(k,\omega)}, \tag{10}$$

where $\widehat{C}^{\perp}_{\mathrm{MD}} = \int_0^{\infty} C^{\perp}_{\mathrm{MD}}(k,t)e^{-i\omega t}\,\mathrm{d}t$; we have $\widetilde{f}(k) = \lim_{\omega\to 0}\widehat{f}(k,\omega)$. At each temperature the system is initially equilibrated for 10^8 time steps; after the equilibration the system is simulated further using 5×10^8 integrator time

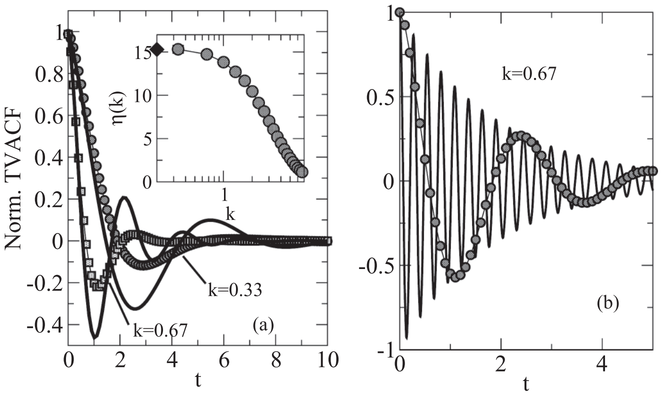

FIG. 1. (a) The TVACF for the binary Lennard-Jones system at $T = 1.0$. Circles connected with lines represent simulation data and solid lines the least-squares fit of Eq. (8) using $\widetilde{\tau}$ as the fitting parameter. The inset shows the system viscosity kernel $\eta(k) = \eta_0 \widetilde{f}(k)$, and the black diamond at $k = 0$ represents the Green-Kubo shear viscosity value. (b) Same as in (a), but for $T = 0.45$ and only $k = 0.67$.

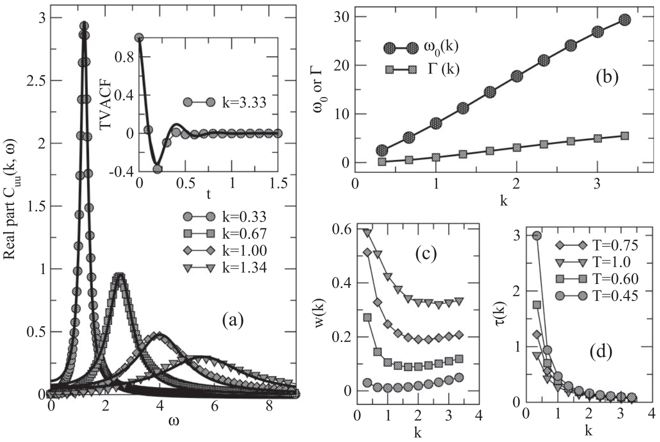

FIG. 2. (a) Real part of the TVACF spectrum for the binary Lennard-Jones system at $T = 0.45$. Symbols connected with lines represent simulation data (Fourier-Laplace transformed) and solid lines the least-squares fit of Eq. (12). (b) Dispersion plot for Γ and ω_0. (c) and (d) The correction function and Maxwell relaxation time as functions of wave vector and at different temperatures.

steps divided into five blocks of 108 time steps in order to perform simple statistics and check the system equilibration.

Figure 1(a) shows the least-squares fit of Eq. (8) to the averaged simulation data at $T = 1.0$. The viscosity kernel used as the input is shown in the figure inset; the kernel result is checked against the standard Green-Kubo integral of the stress autocorrelation function $\eta_0 = \frac{V}{k_B T} \int_0^\infty \langle \sigma(t) \sigma(0) \rangle \, dt$. It is clear that the wave-vector-dependent Maxwell model cannot capture the correct relaxation dynamics, partly due to the locking. The effect of the locking becomes even more extreme as we approach the supercooled regime as shown in Fig. 1(b).

Recall the definition of the Maxwell time $\tau_M = \eta_0/G$. Since the viscosity kernel has reached the Green-Kubo limit at around $k = 0.33$, one can expect the system to be wave-vector independent for $k \leqslant 0.33$. The fit in Fig. 1(a) to the TVACF data yields a Maxwell relaxation time $\tau_M \approx \tau_M g(k = 0.33) = 0.85$, whereas estimating this value from the stress autocorrelation function $\tau_M = \eta_0/G$ with $G = V/k_B T \langle P_{xy}(0) P_{xy}(0) \rangle$ (see Refs. [25,26]) gives 0.24 [27]. This further highlights the failure of the Maxwell model and why the Maxwell time is here found from fitting rather than from independent methods. Despite the large quantitative discrepancy between the model and the simulation data, the relaxation is dominated by a damped harmonic oscillation, and this motivates an extension of the generalized one-element Maxwell model.

As stated above, we introduce a correction function w, which is a measure of the deviation from the ideal mixing; specifically, it will measure the system's reduced viscous response. In the general case, we must expect that the deviation is length-scale dependent, i.e., w is wave-vector dependent, and we get $\widetilde{\eta} = \eta_0 w(k) \widetilde{f}(k)$. Notice that in real space w is a kernel itself. The TVACF has the same form as Eq. (8), but now with frequency

$$\omega_0^2 = 4\Gamma|\Gamma - 2w\widetilde{\eta}k^2/\rho|. \tag{11}$$

For a given wave vector this results in a two-parameter model if we know the viscosity kernel. Only the real-valued correction is considered, and since we expect additional energy storage processes we also expect the bounds $0 < w < 1$. In particular, as we approach the highly elastic regime, $w \approx 0$.

Following the literature [9,10,16], we fit the corrected model to the real part of the corresponding TVACF spectrum; this enhances the deviation between theory and data. The spectrum is in terms of attenuation and frequency,

$$\widehat{C}_{uu}^{\perp}(k, \omega) = \frac{k_B T}{\rho} \frac{i\omega + \Gamma(k)}{[i\omega + \Gamma(k)]^2 + \omega_0^2(k)}. \tag{12}$$

Figure 2(a) shows the least-squares fit of the real part of Eq. (12) to simulation data for the binary Lennard-Jones system at $T = 0.45$. The fitting parameters used are $\widetilde{\tau}$ and w. Again, $\widetilde{\eta}$ is found independently from Eq. (10). As one expects, the agreement is not perfect, however, the corrected model does capture the main relaxation dynamics. The inset shows the TVACF for the largest wave vector studied, namely $k = 3.33$; this corresponds to a characteristic length scale of just 1.89 or below two particle diameters. In Fig. 2(b) the dispersion plots for the frequency and attenuation coefficients are shown. The linear dispersion for ω_0 follows the results from Mizuno and Yamamoto [16]. The squared wave-vector dependency reported for Γ is less clear with the wave vectors studied here. This indicates that this two-parameter model also captures the correct multiscale dynamics. Figure 2(c) shows that w decreases as the temperature decreases; this is in agreement with the expectation above, namely, that the viscous response is reduced compared to the ideal mixing case. Interestingly, the correction function features a minimum which shifts towards lower k values as the temperature decreases. For $T = 0.45$ the minimum is located at approximately $k = 1$, corresponding to a length scale of around six particle diameters. This indicates the existence of a characteristic length scale of minimum energy dissipation, taking the usual wave-vector-dependent viscosity into account. For completeness, the wave-vector-dependent Maxwell time $\widetilde{\tau}$ is also

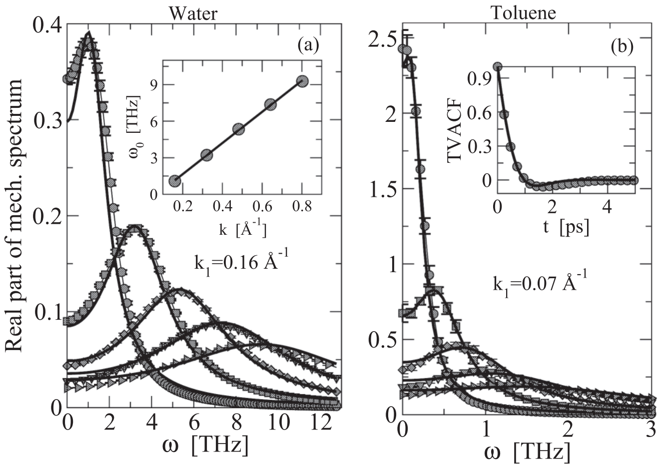

FIG. 3. (a) Real part of the TVACF spectrum for water. The inset shows the dispersion relation for ω_0. (b) As in (a), but for liquid toluene. The inset shows the TVACF (time domain) for $k = 0.28$ Å. In both (a) and (b) circles with lines represent data and the solid line fits to Eq. (12). k_1 is the fundamental wave vector (black) and the data/fits the subsequent modes.

plotted [Fig. 2(d)]. This shows the well-known "anomaly": The attenuation is very small (the Maxwell time is large) on large length scales, but decreases abruptly on the microscopic scale.

The corrected model is tested for water [Fig. 3(a)] and liquid toluene [Fig. 3(b)] at ambient conditions. The water model, the SPC/Fw model, is a flexible version of the simple point charge model (see Ref. [28]) where the Coulomb interactions are evaluated with the cut and shifted method [29], and the toluene model is a united-atomic-unit model [6]. Again the reader is referred to the Supplemental Material [22] for more details. Clearly, the corrected model also performs well for these fluid systems, in particular, the linear dispersion relation for ω_0 is present (shown for water). For water the viscous corrections vary from 0.54 to 0.34 in the wave-vector range $k = 0.16$–0.8 Å^{-1}, indicating that the viscous response is significantly reduced for these more realistic model systems as well.

In conclusion, the single-element Maxwell model was extended using a correction function that, phenomenologically, includes the reduced viscous response not captured by the original model. It was shown that with only two fitting parameters, namely, the Maxwell relaxation time and the correction function, the model predictions agreed very well with data for the TVACF of different fluid systems. The dispersion curve of the frequency followed previous results by Mizuno and Yamamoto [16]. From the correction function it is concluded that the system viscous response is significantly reduced when comparing to the predictions from the original model. This reduction increases with decreasing temperature as expected and the reduction features a minimum for low temperatures defining a length scale of minimum dissipation. It can be concluded that the damped oscillations observed in the TVACF for the model systems studied here (binary fluid, water, and toluene) follow to a good approximation the functional form predicted by the single-element Maxwell model [Eqs. (8) and (12)], and a better quantitative agreement is achieved by simply relaxing ideal mixing. Naturally, this cannot be concluded for complex and viscous liquids where the mechanical spectra differ qualitatively from the single-element Maxwell predictions (see, e.g., Ref. [30]).

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