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Review

Theory of collective excitations in simple liquids

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Abstract. We present a parameter-free theory of the collective excitations in simple liquids such as liquid metals or rare gases. The theory is based on the mode-coupling theory (MCT), which has been previously applied successfully for explaining the liquid-to glass transition. The only input is the liquid structure factor. We achieve good agreement both for the liquid dispersion (maximum of the longitudinal current spectrum) and width (damping) with experimental findings. The time-dependent memory function predicted by MCT has a two-step exponential decay as previously found in computer simulations. Furthermore MCT predicts a scaling of the liquid dispersion with the effective hard-sphere diameter of the materials. This scaling is obeyed by the available experimental data.

1 Introduction

The description of the dynamics of simple elemental liquids (such as liquid metals or rare gases) near their triple point is hindered by the fact that the interaction between the atoms (or ion cores) cannot be treated by perturbation theory, because of the hard-sphere-like repulsion. The central quantity, which gives information about the collective dynamics of one-component liquids is the dynamical structure factor $S(q,\omega)$, which can be measured by inelastic coherent neutron or X-ray scattering [1–5][1]. It is the Fourier transform of the density-density correlation function

$$F_q(t) = \int_{-\infty}^{\infty} e^{i\omega t} S(q,\omega) = \frac{1}{N} \sum_{l,m=1}^{N} e^{i\mathbf{q}[\mathbf{r}_l(t)-\mathbf{r}_m(0)]}. \tag{1}$$

This function is also called intermediate scattering function. N is the number of particles and $\mathbf{r}_l$ are the moving positions of the atoms. The initial value $F_q(0) = S(q)$ is the static structure factor, which can be evaluated with the help of statistical mechanics

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[1] For a recent review of measurements and simulations of the dynamics of liquid metals see [6].

without knowing the dynamics. A liquid is usually referred to as “simple” if it consists of one atomic species and if it can be described with the help of a pairwise potential. The structure factor can be evaluated directly from the potential by integral equation theories derived from statistical mechanics or by Monte-Carlo techniques. It is already known for a long time that the structure factor of simple liquids, especially that of liquid metals can be quite accurately represented by that of a hard-sphere fluid. This means that the structure of a simple liquid is essentially determined by the hard-core repulsion and not by the longer-range interactions.

The most successful starting point for the dynamics as represented by the dynamic structure factor is the projector formalism of Mori and Zwanzig [7], which, applied to liquid dynamics has been called “generalised hydrodynamics”, because the relevant equations of motion reduce to those of linear hydrodynamics in the long-wavelength limit. The success of this formalism is based on the fact that the lowest frequency moments $c_q^{(n)} = \int \omega^n S(q,\omega)$ can be incorporated exactly. There are also efforts to describe the dynamics of simple liquids in terms of Ensgog’s kinetic theory of hard spheres [1,3,4,8].

In the generalised-hydrodynamics approach memory functions are introduced, which replace the damping terms in linear hydrodynamics. In early approaches [2] phenomenological expressions for these memory functions were introduced, e.g. functions decaying exponentially with characteristic relaxation times τ_q. These quantities served as adjustable parameters to fit the measured data. Of course, theories for the dynamics must provide explicit physically motivated expressions for these memory functions. Such theories are the different versions of mode-coupling theory (MCT). In the older version [9–14] both structural information ($S(q)$ or its Fourier transform $g(r)$) as well as the pair potential served as input. These theories gave a fair account of the salient features of the collective excitations of liquid argon and liquid metals. However the formalism is rather complicated and a fundamental understanding of the features of the spectra, therefore, was lacking. A simpler version of MCT [15–18] was introduced later in order to describe the liquid-to-glass transition. It turned out that this theory quite accurately describes the glassy arrest of a liquid as a function of temperature/density. The only input of this theory is the static structure factor. The theory makes non-trivial predictions about the fractal time dependence of $F_q(t)$, which have amply been verified by experiment [19]. In the following we shall show [20] that the application of this version of MCT quite accurately describes the collective dynamics of simple liquids *away from the glass transition* and allows for a very intuitive understanding of the features of the excitation spectrum.

2 Formalism

Within the Mori-Zwanzig formalism the dynamical structure factor $S(q,\omega)$, which is proportional to the inelastic coherent neutron or inelastic ionic X-ray scattering cross-section can be expressed in terms of the memory function $M_q(t)$, or its Fourier-Laplace transform

$$M_q(\omega) = \int_0^\infty \mathrm{d}t e^{-i\omega t} M_q(t) \tag{2}$$

as

$$\begin{aligned} S(q,\omega) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t F_q(t) e^{-i\omega t} \\ &= \frac{1}{\pi}\mathrm{Re}\left\{ \frac{S(q)}{i\omega + \dfrac{\Omega_0^2(q)}{i\omega + M_q(\omega)}} \right\}. \end{aligned} \tag{3}$$

As stated above, this formulation guarantees that the first two sum-rule requirements, namely those of the 0-th and second moment $c_q^{(0)}$ and $c_q^{(2)}$ are fulfilled. $\Omega_0(q)$ is the unrenormalised sound dispersion

$$\Omega_0^2(q) = v_{th}^2 q^2 / S(q) = c_q^{(2)} / c_q^{(0)} \,, \tag{4}$$

where v_{th} is the thermal velocity defined by $v_{th}^2 = k_B T/m$. Expression (3) can be cast into a generalised harmonic oscillator equation ("generalised Langevin equation" [3,4,7]) by transforming it into the time representation

$$\ddot{F}_q(t) + \int_0^t \mathrm{d}\tau M_q(t-\tau)\dot{F}_q(\tau) + \Omega_0^2(q) F_q(t) = 0. \tag{5}$$

In the version of mode-coupling theory, which is the basis of the theory of the glass transition [15,18] the memory function $M_q(t)$ is represented self-consistently by linear combinations of products of $F_q(t)$ in the following way:

$$M_q(t) = \Omega_0^2(q) \frac{1}{2V} \sum_{\mathbf{q}_1,\mathbf{q}_2}^{\mathbf{q}_1+\mathbf{q}_2=\mathbf{q}} V_{\mathbf{q}\mathbf{q}_1\mathbf{q}_2} F_{q_1}(t) F_{q_2}(t). \tag{6}$$

Here V is the total volume. The vertex (in a version where the three-body static correlation functions are simplified by the convolution approximation, see [15,17,18]) is given by

$$V_{\mathbf{q}\mathbf{q}_1\mathbf{q}_2} = \frac{1}{n} S(q) W_{\mathbf{q}\mathbf{q}_1\mathbf{q}_2}^2 \tag{7}$$

where $n = N/V$ is the particle density,

$$W_{\mathbf{q}\mathbf{q}_1\mathbf{q}_2} = \frac{1}{q^2} \mathbf{q} \cdot [\mathbf{q}_1 n c(q_1) + \mathbf{q}_2 n c(q_2)] \tag{8}$$

where

$$c(q) = \frac{1}{n} \left(1 - \frac{1}{S(q)} \right) \tag{9}$$

is the direct correlation function.

Equations (4) to (9) are a closed set of equations for $F_q(t)$ which can be solved self-consistently on a computer with the initial conditions $F_q(0) = S(q)$ and $\dot{F}_q(0) = 0$.

3 Results

3.1 Liquid metals

The only input for the self-consistent MCT equations (4) to (9) is the static structure factor $S(q)$. As noticed above this function for liquid metals and rare gases resembles closely that of hard spheres.[2] At wavenumbers larger than that of the principal peak of $S(q)$, there is a significant deviation as the HS-PY structure factor does not decay as rapidly towards the uncorrelated value $S(q) = 1$ as the experimental data. This can be explained by the fact that the radial pair distribution function

$$g(r) = 1 + n \int \frac{\mathrm{d}^3\mathbf{q}}{(2\pi)^3} e^{i\mathbf{q}\mathbf{r}} [S(q) - 1] \tag{10}$$

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[2] For hard spheres the Perkus-Yevick integral equations (HS-PY) can be solved analytically [21,22].

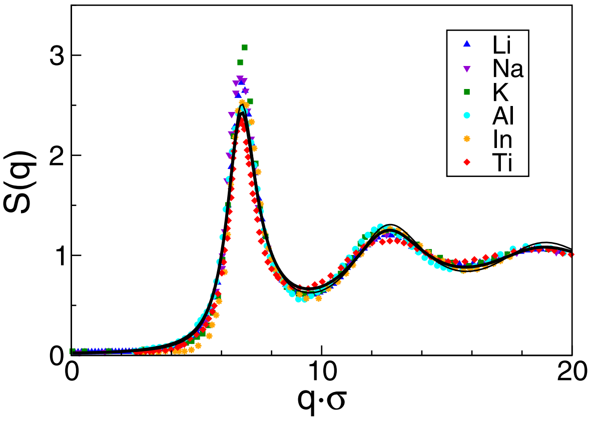

Fig. 1. Static structure factors of several liquid metals. Thin black line: Hard-Sphere PY structure factor, thick black line: Eq. (11), both calculated with packing fraction $\varphi = 0.45$. References for the experimental data can be found in [6].

in PY approximation abruptly jumps from 0 to its maximum value at $r = \sigma$, where σ is the hard-sphere diameter. This is, of course, not the case for real liquids with a continuous pair potential, in which $g(r)$ rises continuously in a smooth way towards its maximum at a value of r, which is slightly larger than σ. We found that the experimentally measured $S(q)$ data of several liquid metals can be quite satisfactorily approximated in the total q range by the formula

$$S(q) = 1 + [S_{HS}(q) - 1]e^{-\frac{1}{2}(\lambda q\sigma)^2} \tag{11}$$

with $\lambda \approx 0.05$, where $S_{HS}(q)$ is the HS-PY structure factor. This corresponds to a convolution of $g_{HS}(r) - 1$ with a Gaussian of width $\sigma\lambda$. In Fig. 1 we have plotted the static structure factors of the six liquid metals, for which $S(q, \omega)$ data are available in the literature, against the scaled wavenumber. We observe that the data collapse to a single curve and can be nicely represented by expression (11).

In what follows we use the hard-sphere diameter σ as length scale. As frequency scale we use a quantity ω_0, which is the isothermal velocity v_T, divided by σ:

$$\omega_0 = \frac{v_T}{\sigma} = \frac{v_{th}}{\sigma\sqrt{S(q=0)}} = \frac{1}{\sigma}\sqrt{\frac{k_B T}{mS(q=0)}} \tag{12}$$

v_T can be obtained either from the measured ultrasonic sound velocity $v_S = v_T/\kappa$ (where κ is the ratio of the specific heats at constant pressure and volume) or from $S(q = 0)$. κ is approximately unity in the ps^{-1} frequency regime (see, however, the table given in [6]). It should be noted that in these units the scaled isothermal sound velocity is fixed to unity. Using these units and expression (11) for $S(q)$ the theory depends only on two parameters, namely the packing fraction

$$\varphi = \frac{\pi}{6} n\sigma^3 \tag{13}$$

which controls the density dependence, and the decay constant λ, which we set equal to 0.05 throughout.

As demonstrated in the MCT literature [15–18] there exists a critical value of the packing fraction $\varphi_c \approx 0.55$, beyond which the function $F_q(t)$ does not decay towards zero, but remains at a finite value $F_q(\infty) = S(q)f_q$. This means, according

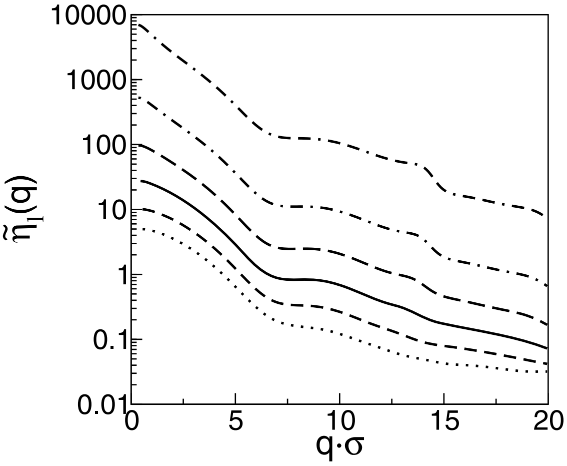

Fig. 2. Viscosity $\tilde{\eta}_\ell(q)$ as defined in the text for $\varphi = 0.35$ (dots), 0.4 (short dashes), 0.45 (straight line), 0.49 (long dashes), 0.54 (dash-dots).

to a fundamental principle of statistical mechanics, that the dynamics of the density fluctuation is no more ergodic: the glassy state is a non-ergodic state.[3] This transition towards a non-ergodic state is accompanied by a divergence of the shear viscosity according to a power law $\eta_S \propto |\varphi - \varphi_c|^{-\gamma}$.

The behavior of the viscosity can be related to the time integral over $F_q(t)$, as well as that over $M_q(t)$ in the $q \to 0$ limit, i.e. to $S(q, \omega = 0)$ and $M_q(\omega = 0)$:

$$\begin{aligned} \lim_{q\to 0} S(q, \omega{=}0) &= \lim_{q\to 0} \frac{1}{\pi} \frac{S^2(q)}{v_{th} q^2} M_q(\omega{=}0) \\ &= \frac{1}{\pi} \frac{S^2(0)}{v_{th} m n} \underbrace{(\eta_B + (4/3)\eta_S)}_{\eta_\ell} . \end{aligned} \tag{14}$$

Here m is the atomic mass, i.e. mn is the mass density. η_B is the bulk viscosity and η_ℓ the longitudinal viscosity. We can define a q dependent scaled longitudinal viscosity as

$$\tilde{\eta}_\ell(q) = \frac{1}{\pi \rho k_B T} \eta_\ell(q) \cdot \omega_0 = S(q, \omega = 0)/S(q)^2 \cdot \omega_0 . \tag{15}$$

As can be seen from Fig. 2 this quantity varies strongly with density, as to be expected: The strong density dependence of this quantity is related to the divergence of the viscosity on solidification. It is now interesting to look at the time dependence of the memory function $M_q(t)$. As stated in the beginning, in the time of the pioneers of liquid dynamics (neutron scattering and simulations) the $S(q, \omega)$ data were fitted by expression (3) with empirical forms for $M_q(t)$. It appeared, that taking a single exponential

$$M_q(t) = M_q(t{=}0)\, e^{t/\tau_q} \tag{16}$$

gave very bad fits to the data. It was found first for a simulation of liquid Lennard-Jones argon [23] that an expression of the form

$$M_q(t) = M_q(t{=}0) \left((1 - a)\, e^{t/\tau_q^{(1)}} + a\, e^{t/\tau_q^{(2)}} \right) \tag{17}$$

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[3] In real materials the ergodicity is restored at macroscopic time scales by activated processes [18].

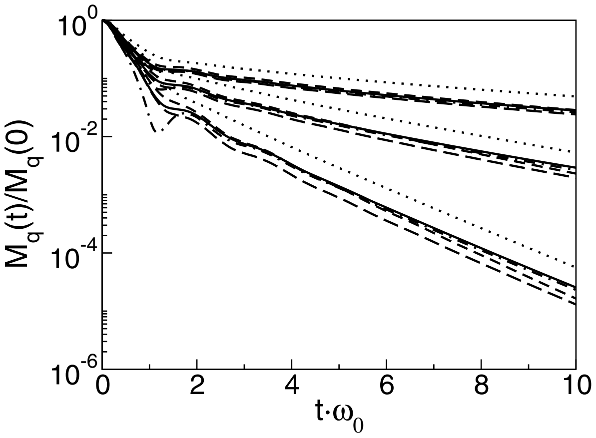

Fig. 3. Normalised Memory functions for (from bottom to top) $\varphi = 0.40$, $\varphi = 0.45$, $\varphi = 0.49$, $\varphi = 0.52$, $\varphi = 0.55$, $\varphi = 0.60$ and for wavenumbers $q\sigma = 1$ (dots), 3 (short dashes), 5 (long dashes) 7 (lines), 9 (dash-dots). The maximum of $S(q)$ is at $q\sigma \approx 7$.

fitted the data quite well. A number of $S(q,\omega)$ data on liquid metals, obtained by inelastic X-ray scattering, as well as pertinent simulational data could also fitted quite well by this expression [6,24–27]. In all cases it turned out that the "fast" relaxation time $\tau_q^{(1)}$ was almos temperature independent, whereas the "slow" relaxation time $\tau_q^{(2)}$ was strongly temperature dependent and much larger than $\tau_q^{(1)}$.

In Fig. 3 we have plotted the memory functions $M_q(t)$, normalised to their initial value for different values of q and φ. First we recognize that MCT produces the double-exponential structure of the form (17) as postulated in the literature. We also note that — once the q-dependent prefactor is scaled out — there is no appreciable q dependence. another remarkable observation is that indeed the decay constant $\tau_q^{(2)}$ strongly depends on φ, whereas $\tau_q^{(1)}$ is almost density independent. In fact, $\tau_0^{(2)}$ can be identified with the so-called α relaxation time, which is proportional to the viscosity, i.e. it diverges also at the liquid-to-glass transition[4]. The second time regime obviously describes already in the dense liquid regime the onset of the *cage effect* [18], i.e. the fact that one particle, which moves in the liquid, cannot escape immediately from the cage the other particles are forming around the given particle. $1/\tau_0^{(2)}$ is then the escape rate from the cage.

Another very important characteristic of collective excitations in a liquid is the (renormalised) dispersion

$$\Omega(q) = \mathrm{Max}\{\omega^2 S(q,\omega)\} \tag{18}$$

which is also the maximum of the current-current correlation function. It turns out, that this function, calculated in MCT, is almost density independent [20]. This means, that on the frequency scale given by $\Omega(q)$ the liquid just reacts elastically as the frozen solid (glas). In Fig. 4 we have plotted the dispersions of the six liquid metals referred to in Fig. 1 in units of ω_0 against $q\sigma$. We note that like the structure factors these curves collapse to a single one. Together with these data we have also plotted the (renormalised) dispersion $\Omega(q)$ as calculated in MCT for two values of φ corresponding to the dense regime. The reason for the scaling behavior predicted by MCT is that the dispersion is governed by the value of the sound velocity and the atomic diameter and nothing else.

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[4] Near the transition the exponential transforms into a *stretched* exponential [18].

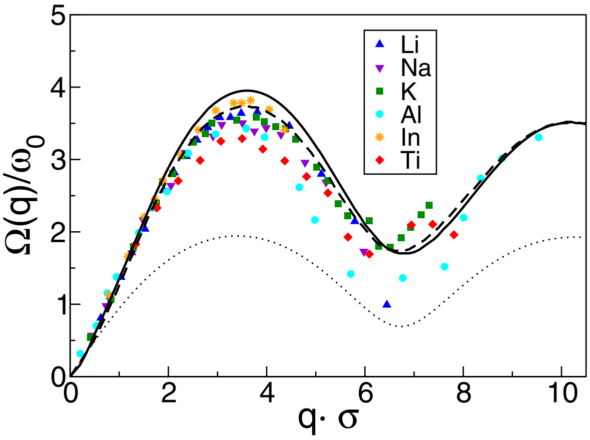

Fig. 4. Dispersion of the maxima of $\omega^2 S(q,\omega)$ of several liquid metals [6,28,29] together with the MCT results for $\varphi = 0.40$ (dashes) and $\varphi = 0.45$ (full line). The lower thin dotted line is $\Omega_0(q)$ for $\varphi = 0.4$ as given in Eq. (4).

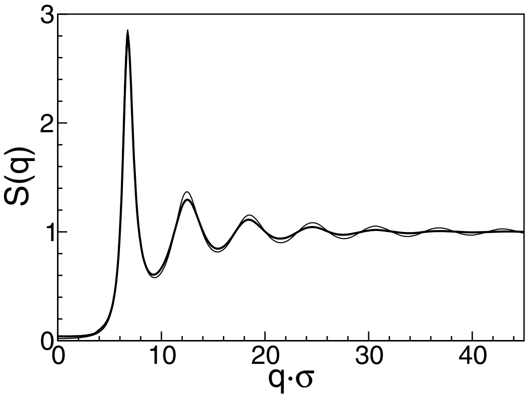

Fig. 5. Thick line: Static structure factor of a simulation of Lennard-Jones Argon by Levesque et al. [23]. Thin line: Hard sphere PY static structure factor with $\sigma_{eff} = 1.026\sigma$ and $\varphi = 0.48$.

For comparison we have also plotted the unrenormalised dispersion $\Omega(q)$ as given by formula (4). The renormalization effect is a nontrivial result of MCT.

3.2 Liquid Lennard-Jones argon

In the previous section we found that the MCT memory function has a two-relaxation time structure. As mentioned above, this property of the memory function has already been found in a computer simulation of liquid Argon by Levesque et al. [23]. So we want to compare the results of MCT with the results of this computer simulation. The simulation is based on a Lennard-Jones potential

$$U\left(r\right) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right). \tag{19}$$

The temperature used for the simulation is $T = 0.723\varepsilon/k_B$ and the density is $n = 0.844\sigma^{-3}$ which corresponds to Argon at 86.5 K with a density of 1.418g/cm^3. As

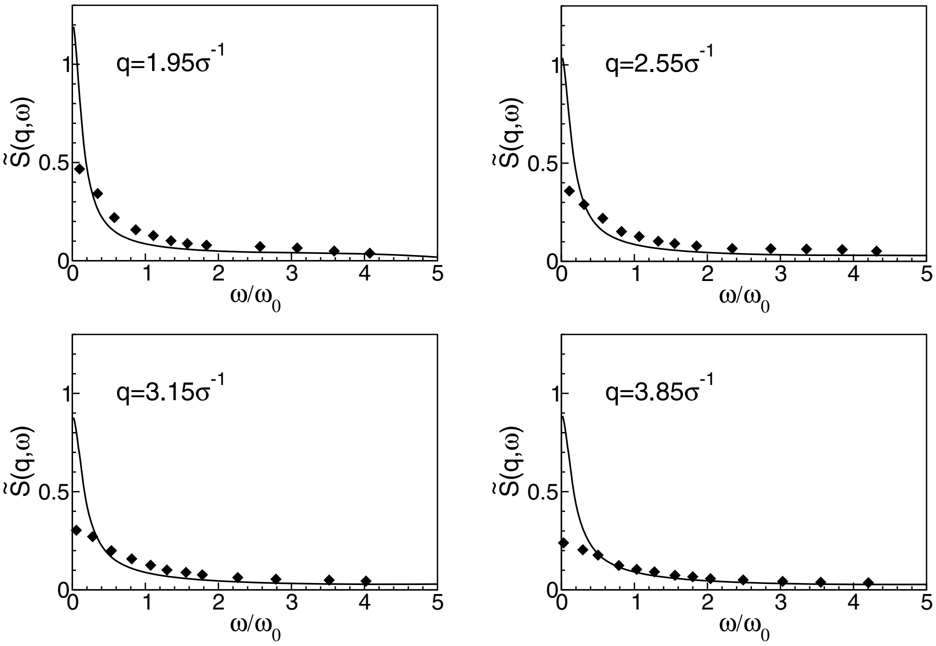

Fig. 6. MCT result for $\tilde{S}(q,\omega) \equiv S(q,\omega)/S(q) \cdot \omega_0$ (lines) compared with the result of a computer simulation by Levesque et al. [23] (diamonds).

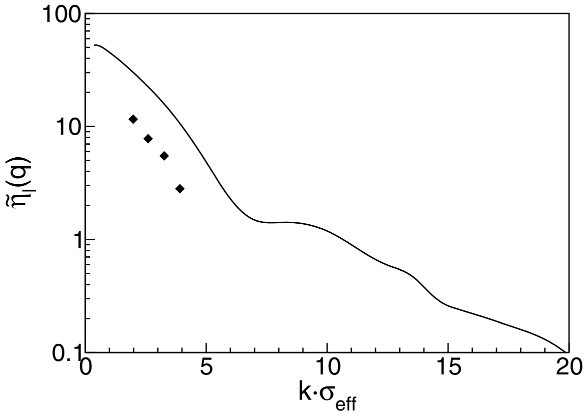

Fig. 7. MCT result (line) for the viscosity $\tilde{\eta}_\ell(q)$ as defined in equation (15) compared with the simulation by Levesque et al. [23] (diamonds).

input for MCT calculation we took the static structure factor from the simulation by Verlet et al. [30] for a system in the same state. This structure factor is compared in Fig. 5 to the Percus-Yevick structure factor of hard spheres. The simulated structure factor is very similar to the one of hard spheres with a packing fraction of $\varphi = 0.48$.

In Fig. 6 we compare our result for the dynamic structure factor with that of the computer simulation. There is some agreement for higher frequencies, but there is also quite a big deviation for the zero-frequency limit. Because the zero-frequency limit of the dynamic structure factor is related to the generalised viscosity (Eq. (15)), this also leads to quite some deviations in the q dependent viscosity between the MCT result and the simulation, as can be seen in Fig. 7.

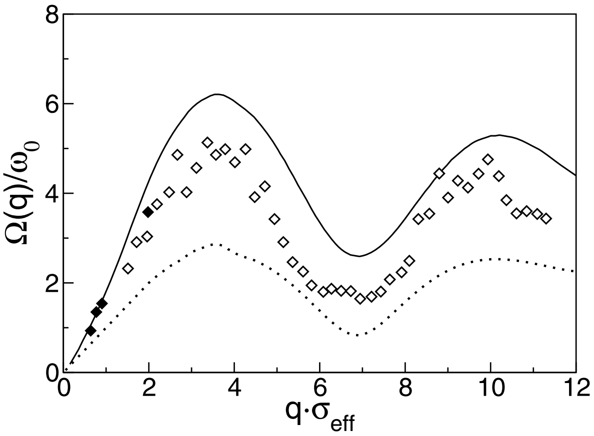

Fig. 8. MCT result (line) for the dispersion of the current correlation function compared with the result of the simulation by Levesque et al. [23] (full diamonds) and Rahman [31] (empty diamonds). The dotted line is $\Omega_0(q)$ for as given in Eq. (4).

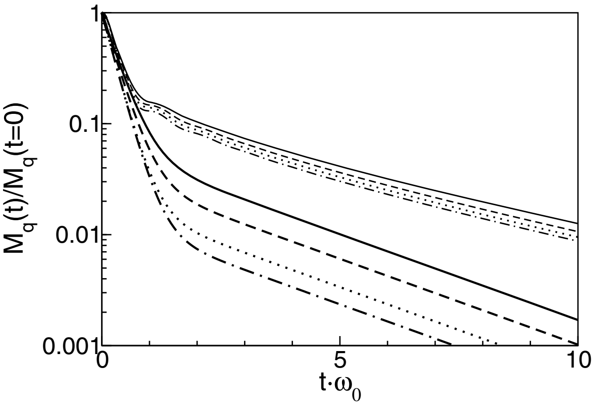

Fig. 9. MCT result (thin lines) for the memory function compared with the result of the computer simulation by Levesque et al. [23] (thick lines) for $q\sigma = 1.95$ (solid lines), $q\sigma = 2.55$ (dashed lines), $q\sigma = 3.15$ (dotted lines), $q\sigma = 3.85$ (dash-dotted lines).

The quantitative deviation is related to the well-known fact that MCT underestimates the critical packing fraction at which the glass transition occurs. So the MCT result describes a state which is much closer to the glass transition. This leads to an overestimation of the viscosity.

In Fig. 8 we compare the generalised sound dispersion from MCT with the sound dispersion of the computer simulation. Because the simulation by Levesque et al. only covered a limited q-range, we also included a different computer simulation of Lennard-Jones Argon by Rahman [31] in a similar state ($T = 76$K, $\rho = 1.408\,\mathrm{g/cm}^3$). As can be seen, there is again at least some qualitative agreement.

Finally, in Fig. 9 there is a comparison between the memory functions of MCT and the computer simulation by Levesque et al. [23]. The memory function of the computer simulation cannot be obtained directly. It can only be obtained by postulating a two-relaxation time structure for the memory function and by using the two relaxation times to obtain the best fit for the dynamic structure factor. In MCT the memory function is obtained directly by solving the mode-coupling equations. The quantitative deviation between simulation and mode coupling theory in the relaxation time can again be explained by the fact that MCT describes a state closer to the glass transition.

4 Conclusions

We were able to obtain a MCT description of the collective dynamics of simple liquids by using smoothed Percus-Yevick structure factors of hard spheres as input. These depend essentially only on one single parameter, which is the packing fraction φ. With this parameter the difference of the state of the liquid with respect to its melting point can be described, where it usually takes values near 0.45. The result of MCT is that the dispersion of the longitudinal sound-like excitations as given by the maximum of the current correlation spectrum depends only very weakly on φ. This means that at reduced densities the dispersion remains essentially the same as that of the dispersion in the undercooled and even glassy state. The relaxation as described by MCT consists of two distinct time regimes. The fast relaxation which is on microscopic time scales is almost independent of the density. The slower relaxation in an extended time regime is equivalent to the alpha-relaxation known from the dynamics close to the glass transition. The theory is able to describe the experimentally observed relaxation times and the dispersion of sound modes in simple liquids, even though the coupling to heat diffusion and transverse degrees of freedom is neglected. They obviously ar not of crucial importance in the collective dynamics of simple liquids in the ps^{-1} frequency and Å^{-1} wavenumber regime.

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