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A model solution of the generalized Langevin equation: Emergence and Breaking of Time-Scale Invariance in Single-Particle Dynamics of Liquids**

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It is shown that the solution of generalized Langevin equation can be obtained on the basis of simple comparison of the time scale for the velocity autocorrelation function of a particle (atom, molecule) and of the time scale for the corresponding memory function. The result expression for the velocity autocorrelation function contains dependence on the non-Markovity parameter, which allows one to take into account memory effects of the investigated phenomena. It is demonstrated for the cases of liquid tin and liquid lithium that the obtained expression for the velocity autocorrelation function is in a good agreement with the molecular dynamics simulation results.

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Relaxation processes in a complex system can be characterized by the pronounced memory effects, which are manifested in the non-exponential decay or oscillatory behavior of the time correlation functions (TCF's) for the corresponding dynamical variables [1, 2]. Hence, one can reasonably assume that the direct accounting for the memory effects could simply the theoretical description of the system behavior. The convenient way to examine this is to consider a system, in which the origin of the memory effects is well studied. As an example of such the physical system one can take a high-density (viscous) liquid, a supercooled liquid or/and a glass [3], where the memory effects appear in single-particle dynamics as well as in collective particle dynamics [4–6].

From theoretical point of view, the convenient way to take these effects into account most adequately is to use in the description the so-called memory function formalism [7], which is associated with the projection operators technique of Zwanzing and Mori [8, 9] as well as with the recurrent relations method suggested by Lee [10]. Remarkably, the memory function formalism allows one to represent the equation of the motion for a variable (originally, for the velocity of a particle in liquid) in the form of a non-Markovian integro-differential equation, which contains a characteristic component – a memory function. For the case when the velocity of a particle represents such the variable, the integro-differential equation is known as the generalized Langevin equation (GLE). Herein, if time behavior of the memory function is defined, then the solution of the GLE will determine the evolution of the variable (the velocity) and the corresponding TCF – the velocity autocorrelation function (VACF) – can be computed [4, 5]. Nevertheless, although the technique of projection operators gives a prescription to calculate the memory function, the direct computations are very difficult to be realized for real physical systems [10–12]. In this work, we shall demonstrate that a solution of GLE can be derived by simple interpolation of its solutions for the memory-free

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**Dedicated to the memory of Prof. Renat M. Yulmetyev
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case, the strong-memory case and the case with a moderate memory. Further, the resulted solution will contain the parameter which represents a quantitative measure of the memory effects.

Let us take the velocity v_α of a α-th particle in liquid as a dynamical variable. Then, GLE can be written as [6, 8, 9]

$$\frac{dv_\alpha(t)}{dt} = -\Omega_1^2 \int_0^t d\tau M_1(t-\tau) v_\alpha(\tau) + f(t), \quad (1)$$

where $f(t)$ is the random force per unit mass, $M_1(t)$ is the normalized first order memory function, which is related to the random force $f(t)$ by the second fluctuation-dissipation theorem [8, 9], and Ω_1^2 is the first-order frequency parameter arising from normalization of $M_1(t)$. Note, it is assumed that $\langle v_\alpha(0) f(t)\rangle = 0$. Multiplying Eq. (1) by $v_\alpha(0)$, taking an appropriate ensemble average $\langle \ldots \rangle$ and applying further the projection operators technique, it is possible to obtain a hierarchical chain of integro-differential non-Markovian equations in terms of TCF's:

$$\frac{dM_{i-1}(t)}{dt} + \Omega_i^2 \int_0^t d\tau M_i(t-\tau) M_{i-1}(\tau) = 0, \quad (2)$$

$$i = 1,\ 2, \ldots\ .$$

If VACF is chosen as an initial TCF of this hierarchy, then GLE will be the first equation (i.e. $i = 1$) of this chain[a]. In the case,

$$M_0(t) = \frac{\langle v_\alpha(0) v_\alpha(t)\rangle}{\langle v_\alpha(0)^2\rangle}$$

is VACF; $M_i(t)$ is TCF of the corresponding dynamical variable, which has meaning of the ith-order memory function [13], whereas Ω_i^2 is the i-th-order frequency parameter. Note that all TCF's of chain (2) including VACF are normalized to unity for convenience, i.e.

$$\lim_{t\to 0} M_{i-1}(t) = 1,$$

$$i = 1,\ 2,\ \ldots .$$

Moreover, applying the operator of Laplace transformation $\hat{\mathcal{L}} = \int_0^\infty dt\ e^{-st}[\ldots]$ to equations of chain (2), one obtains the infinite fraction [7]:

$$\widetilde{M}_0(s) = \frac{1}{s + \Omega_1^2 \widetilde{M}_1(s)} = \cfrac{1}{s + \cfrac{\Omega_1^2}{s + \cfrac{\Omega_2^2}{s + \cfrac{\Omega_3^2}{s + \ldots}}}}. \quad (3)$$

It is necessary to note that the ith-order memory function $M_i(t)$ corresponds to a concrete relaxation process, the physical meaning of which can be established directly from consideration of the analytical expression for $M_i(t)$. On the other hand, the squared characteristic time scale τ^2 of the relaxation process can be defined as [1]

$$\tau_{i-1}^2 = \left| \int_0^\infty t M_{i-1}(t)\, dt \right| = \left| \lim_{s\to 0} \left(-\frac{\partial \widetilde{M}_{i-1}(s)}{\partial s} \right) \right|, \quad (4)$$

$$i = 1,\ 2,\ \ldots .$$

The time scales τ_{i-1} corresponding to TCF's of chain (2) form the hierarchy, which has the following peculiarity: the quantity τ_i defines a memory time scale for TCF $M_{i-1}(t)$, the relaxation time of which is τ_{i-1}. As a quantitative measure of memory effects for the ith relaxation level it is convenient to use the dimensionless parameter [1]

$$\delta_i = \frac{\tau_{i-1}^2}{\tau_i^2}, \quad i = 1,\ 2,\ \ldots, \quad (5)$$

where τ_i^2 is defined by Eq. (4). This simple criterion allows one to determine whether the considered process is characterized by a strong statistical memory, or it has a memoryless behavior. Namely, one has

$$\begin{array}{rl} \delta \to 0 & \text{for a strong memory limit,} \\ \delta \simeq 1 & \text{for a case of moderate memory,} \\ \delta \to \infty & \text{for a memory-free limit.} \end{array} \quad (6)$$

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[a] Originally, the equation (1) written for the variable-velocity was called as the GLE. Nevertheless, the related integro-differential equation written for the corresponding time correlation function is also mentioned as the GLE in the modern studies [7].

It is remarkable that for the three cases determined by (6) there are known exact solutions of the GLE written for the VACF [14, 15]:

$$\frac{dM_0(t)}{dt} + \Omega_1^2 \int_0^t d\tau M_1(t-\tau)M_0(\tau) = 0,$$

where the first frequency parameter of a many-particle system (say, for a liquid), where atoms/moleculs interact through a spherical potential $U(r)$, can be written as [16–18]

$$\Omega_1^2 = \frac{4\pi n}{3m} \int_0^\infty dr\, g(r) r^3 \times \left[\frac{d}{dr}\left(\frac{1}{r}\frac{dU(r)}{dr}\right) + \frac{3}{r^2}\frac{dU(r)}{dr} \right]. \qquad (7)$$

Here n is the numerical density, m is the particle mass, and $g(r)$ is the pair distribution function; and Eq. (7) is the first equation of the chain (2), i.e. at $i = 1$. Let us consider these three cases in detail.

First, one assumes that Eq. (7) describes the behavior of the system without memory, i.e. $\tau_0^2 \gg \tau_1^2$. For the case one has $\delta \to \infty$. Here, the memory function $M_1(t)$ has to decay extremely fast; and, therefore, it can be taking in the following form:

$$M_1(t) = 2\tau_1 \delta(t), \qquad (8)$$

where $\delta(t)$ is the Dirac Delta-function, τ_1 is the time scale of $M_1(t)$. By substituting Eq. (8) into Eq. (7) and solving the resulted equation, one obtain the VACF $M_0(t)$ with ordinary exponential dependence:

$$M_0(t) = e^{-\Omega_1^2 \tau_1 t}. \qquad (9)$$

As known, such the dependence is correct for the velocity correlation function of the Brownian particle with the relaxation time $\tau_0 = (\Omega_1^2 \tau_1)^{-1} = m/\xi_\beta$, m and ξ_β are the mass and the friction coefficient, correspondingly. As for the self-diffusion phenomena in a liquid, where particle (α) moving with the velocity $v_\alpha(t)$ is identical to all others, exponential relaxation of the VACF is rather strongly idealized model [19].

Second, one considers the opposite situation appropriate to the system, the single-particle dynamics of which is characterized by a strong memory, i.e. $\tau_0^2 \ll \tau_1^2$. For the case one obtains from definition (5) that $\delta \to 0$. The most relevant form of the *non-decaying* memory function can be taken as

$$M_1(t) = H(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}, \qquad (10)$$

where $H(t)$ is the step Heaviside function. By substituting Eq. (10) under the convolution integral of Eq. (7), one obtains

$$\frac{dM_0(t)}{dt} = -\Omega_1^2 \int_0^t d\tau M_0(\tau). \qquad (11)$$

After solving this equation one finds that

$$M_0(t) = \cos(\Omega_1 t). \qquad (12)$$

It should be noted that no the characteristic time-scale τ_0 is included into solution (12) as well as that $M_0(t)$ does not satisfy the condition of attenuation of correlation at $t \to \infty$ [20]. Actually, the system with an *ideal memory* "remembers" its initial state and returns periodically to this state, functionally reproducing it with precision.

These two above considered cases are limiting ones. However, it is known that single-particle dynamics of real systems is characterized by a memory, albeit the memory is not ideal. Therefore, for the case one can write that the parameter δ takes values from the range $0 < \delta \ll \infty$. There is also the physically correct solution of Eq. (7) for this region of δ, and the solution was firstly obtained by Yulmetyev (see Ref. [21]). Let us consider the case, when the time scales of the initial TCF and of its memory became comparable, i.e.

$$\delta \simeq 1.$$

The case can be realized at the time-scale invariance of the relaxation processes in many-particle systems [13]. In addition, if the time-dependencies of the VACF and of its memory function are approximately identical, then one can write

$$M_1(t) \simeq M_0(t). \qquad (13)$$

Taking into account relation (13) and applying Laplace transformation to Eq. (7), we obtain ordinary quadratic equation:

$$\Omega_1^2\widetilde{M}_0^2(s) + s\widetilde{M}_0(s) - 1 = 0. \tag{14}$$

By solving the last equation and by applying the operator of the inverse Laplace transformation $\hat{\mathcal{L}}^{-1}$, we find the VACF

$$M_0(t) = \frac{1}{\Omega_1 t} J_1(2\Omega_1 t), \tag{15}$$

where $J_1(\ldots)$ is the Bessel function of the first kind. Then, for the squared characteristic time scales of the VACF and of its memory function one obtains from definition (5) and Eq. (14) that

$$\tau_0^2 = \tau_1^2 = \frac{1}{2\Omega_1^2}. \tag{16}$$

Thus, the quantity proportional to the inverse frequency parameter determines both the squared time scales. Solution (15) describes the damped oscillated behavior of the function $M_0(t)$. It is worth nothing that the TCF's scenario is observed frequently in such the physical systems as electron gas models, linear chain of the neighbor-coupled harmonic oscillators and others [10, 22] as well as in collective particle dynamics in simple liquids [13], where the TCF of the local density fluctuations is considered.

The three considered cases allow one to find solution of Eq. (7) at the three different values of the memory parameter: $\delta = 1$ with solution (15); the memory-free case with solution (9) corresponds to $\delta \to \infty$, whereas solution (12) was obtained for the system with ideal memory at $\delta \to 0$. So, if we shall generalize Eqs. (9) and (12) in a unified functional dependence, then we can obtain the following solution of Eq. (7) in terms of the Mittag-Leffler function [23]:

$$M_0(t) = \sum_{k=0}^{\infty} \frac{(-\Omega_1^2 \tau_1^{1-\nu} t^{\nu+1})^k}{\Gamma(\nu k + k + 1)}, \tag{17}$$

where Γ is the Gamma function, τ_1 is the time scale of the memory function $M_1(t)$, the frequency parameter is determined by (7), and the dimensionless parameter ν is the redefined memory measure:

$$\nu = (2/\pi)\arctan(1/\delta), \tag{18}$$

and $\nu \in [0; 1]$. For an strong memory case, i.e. $\delta \to 0$, Eq. (17) gives expansion in series of Eq. (12), whereas for a memory-free limit with $\delta \to \infty$ we obtain expansion of Eq. (9). Relation (17) has a stretched exponential behavior at short times and demonstrate an inverse power-law relaxation at long times. It should be noted that the similar solution of integro-differential equations was proposed earlier by Stanislavskii in Ref. [12] on the basis of applying the fractional calculus technique.

Moreover, one can obtain the general solution of Eq. (7) by interpolation of all three solutions (9), (12) and (15). Assuming the smooth parabolic crossover from the strong memory and memory-free limits to a case of the moderate memory ($\delta = 1$) we obtain

$$M_0(t) = 4\left(\nu - \frac{1}{2}\right)^2 \sum_{k=0}^{\infty} \frac{(-\Omega_1^2 \tau_1^{1-\nu} t^{\nu+1})^k}{\Gamma(\nu k + k + 1)} + \left[1 - 4\left(\nu - \frac{1}{2}\right)^2\right] \sum_{k=0}^{\infty} \frac{(-2\Omega_1^2 t^2)^k}{k!(k+1)!}, \tag{19}$$

where the parameter ν is defined by (18). The significance of the first contribution increases at approaching δ to the zeroth value or at $\delta \to \infty$. Thus, for example, Eq. (19) gives a standard exponential relaxation in the memory-free limit with $\delta \to \infty$. The second contribution in (19) provides the Gaussian behavior for the short-time range $t < \Omega_1^{-1}$. Further, the numerical coefficient before sum in the second contribution of Eq. (19) dominates in the intermediate region, where the time scales of memory function and of the VACF are comparable. This contribution becomes maximal at $\delta = 1$, whereas the first item turns into zero[b].

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[b] Notice that the second contribution in expression (19) can be considered as a particular case of the Mainardi function [24] (or the Wright function [23]), which includes such functions as the Gaussian function, the Dirac delta-function and others.

Both the memory-free situation with absolutely uncorrelated particle motions and the strong-memory case with the pronounced correlations in the particle velocities related with the vibrational particle dynamics are only limit ones for a real liquids. A real liquid (a fluid) tends to the first one at high temperatures and low density, whereas it approaches to another limit at low temperatures with large values of the density. Moreover, it is realized a regime of dense fluids, where the surrounding medium with neighbor particles has an appreciable impact on a forward moving particle (α), causing the so-called vortex diffusion [25] and existence of the power law decay of $M_0(t)$ with time. This indicates on the memory effects in single-particle dynamics, albeit the memory is far to be strong. Our numerical estimations of the memory effects for self-diffusion processes in the Lennard-Jones fluids [14] have found that the parameter δ at the reduced temperature $T^* \approx 1$ and the reduced density $n^* = 0.5$ has a value ≈ 5.9, and then it increases with the growth of temperature and the decreasing of density. The parameter δ achieves value ≈ 8.7 at the temperature $T^* \approx 4.8$ and the density $n^* = 0.5$, and demonstrates non-linear smooth Markovization. For more visibility of aforesaid we present in Fig. 1 the density- and the temperature-dependence of the memory parameter δ calculated for the VACF of Lennard-Jones fluids [14].

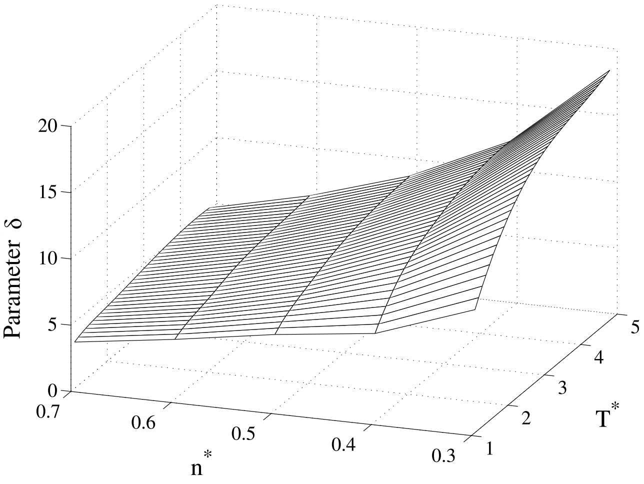

FIG. 1. Density- and temperature-dependence of the memory parameter δ computed on the basis of molecular dynamics simulation results for the VACF of the Lennard-Jones liquid for the following region of the (n^*, T^*)-phase diagram: $0.3 \leq n^* \leq 0.7$ and $1 \leq T^* \leq 4.7$, $n^* = n\sigma^3$, $T^* = k_B T/\epsilon$, where σ and ϵ are the parameters of the Lennard-Jones potential [14].

Moreover, as known, the Bessel function of Eq. (15) has the following asymptotic behavior [26]:

$$J_1(z) = \sqrt{2/\pi z}\left\{\cos\left(z - (3\pi/4)\right) + \mathcal{O}(|z|^{-1})\right\}.$$

Then, returning to Eq. (19), it is easy to make sure that in a case of moderate memory this equation yields the following long-time tail:

$$M_0(t) \propto t^{-3/2}, \qquad (20)$$

which is a well-known feature of the VACF's of liquids [27, 28]. The long-time tails of the VACF of a simple liquid can be reproduced within the microscopic *mode coupling theories* (see, for example, [5]), according to which where it is related to a viscous mode. The approach presented in this study is consistent with the mode-coupling theories and provides a theoretical description, in which information about complex correlated vibrational-diffusive motions of the particles is included into a single parameter δ. Furthermore, it is seen that Eqs. (17) and (19) contain such the characteristics of a many-particle system as the characteristic time scale of the memory τ_1 and the averaged frequency Ω_1^2, which is defined through the radial distribution function $g(r)$ and the particle's interaction potential $U(r)$. These quantities can be calculated from their definitions for concrete systems, or may be taken from molecular dynamics simulations (see, for example, [29]). On the other hand, while analysing experimental data, the term δ may be used as a fitting parameter to do the quantitative estimation of the memory effects in the considered system.

As an example, we demonstrate in Fig. 2 results of Eq. (19) for a model system with the frequency parameter $\Omega_1^2 = 5$ ps^{-2}. The memory

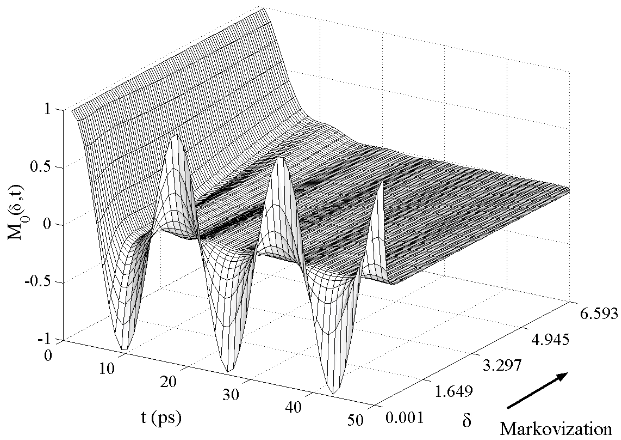

FIG. 2. Velocity autocorrelation function $M_0(\delta, t)$ as a function of the time t and of the memory parameter δ computed from Eq. (19) for model case: $\delta \in [0.001;\ 6.593]$, where $\Omega_1^2 = 5\,\text{ps}^{-2}$ and the time scale $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$. The arrow points to the direction of Markovization.

parameter δ varies within the interval from 0.001 to 6.593, whereas the memory time scale τ_1 has been defined here as $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$. Thus, the presented results include situations of a system with a strong memory when the ratio between the time scales of the VACF and of its memory function archive the value 0.001, and situations when these time scales are comparable. One can see from this figure that the oscillations in the VACF disappear with attenuation of the memory effects (at Markovization) [14]. These oscillations will disappear completely at $\delta \to \infty$. The stronger memory effects in the single-particle dynamics of a system, the more considerable the amplitude of fluctuations and their decay.

The dependence presented by Eq. (19) is supported by experimental results. Experimental and molecular dynamic studies of simple liquids such as liquid tin [30], liquid germanium and lithium [31], liquid selenium [32], liquid sodium [33], Lennard-Jones fluids [34] and other systems [29, 35] have allowed one to discover the relaxation of the VACF with the signatures of the pronounced memory effects, which is manifested, in particular, in algebraic decay of the VACF.

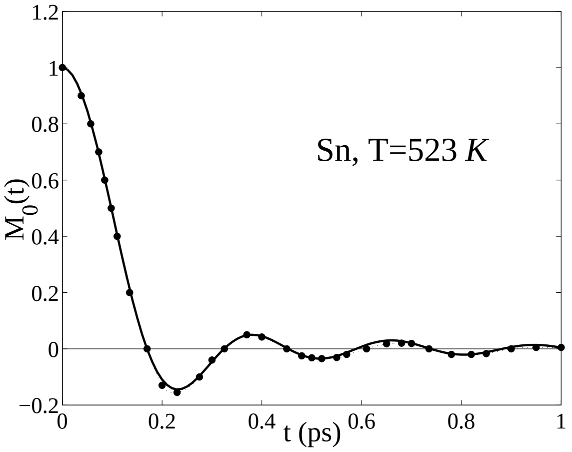

FIG. 3. VACF of liquid tin at the temperature $T = 523$ K (the melting temperature is $T_m = 505.08$ K) calculated from Eq. (19) with parameters $\Omega_1^2 \simeq 130$ ps^{-2}, $\delta \simeq 0.75$ and $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$ (solid curve) and obtained from the classical molecular dynamics simulations [30] (dotted line). The value of the memory parameter confirms the presence of strong memory effects in the single-particle dynamics, which appear due to the specific ion-ion interaction and the correlated disorder in the structure of the melting metal.

To test Eq. (19) for the liquids, we perform the compuations for the cases liquid tin and liquid lithium, for which the VACF's were found before from molecular dynamics simulations [30, 31]. In Figs. 3 and 4, numerical solutions of Eq. (19) are compared with the results of molecular dynamics simulations [30, 31]. As for Fig. 3, the full circles represent the VACF of liquid tin at $T = 523$ K (the melting temperature $T_m = 505.08$ K) calculated by the classical molecular dynamics [30] and the solid curve shows solution of the GLE (19) with $\Omega_1^2 \simeq 130$ ps^{-2}, $\delta \simeq 0.75$ and $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$. It is seen that Eq. (19) well agrees with the molecular dynamics simulations over the whole time interval. The value of the memory parameter reveals the pronounced memory effects in self-diffusion phenomena in liquid tin near its melting point. Strong memory effects, which take place in single-particle dynamics of liquid near its melting point, can be related with the structural transformations of the system [36]. Fig. 4 shows the VACF of liquid lithium at $T = 1073$ K (the

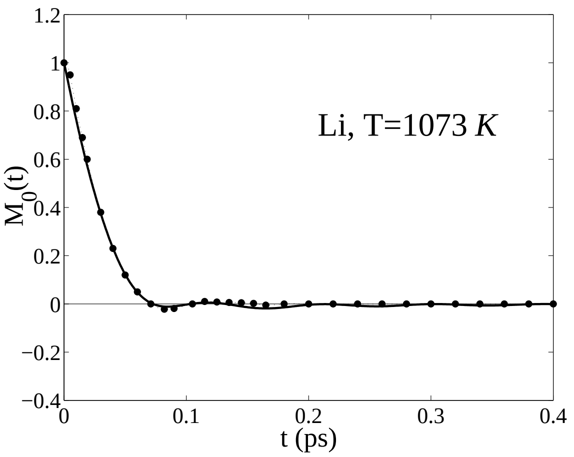

FIG. 4. VACF of liquid lithium at the temperature $T = 1073$ K (the melting temperature is $T_m = 453.65$ K) found from Eq. (19) with the parameters $\Omega_1^2 \simeq 120\,\mathrm{ps}^{-2}$, $\delta \simeq 10$ and $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$ (solid curve) and from molecular dynamics simulations [31] (dotted line). The value of the memory parameter δ reveals a weak memory in single-particle dynamics in liquid lithium for this thermodynamic state, that can be related with a weak influence of the "cage effects" [5] as well as with a low ordering in the system. As a result, a tagged diffusing atom can propagate over larger distances without collisions with neighboring atoms.

melting temperature $T_m = 453.65$ K) determined from the molecular dynamics simulations [31] as full circles, whereas the solid line corresponds to the solution of Eq. (19) with the frequency parameter $\Omega_1^2 \simeq 120\,\mathrm{ps}^{-1}$, the memory parameter $\delta \simeq 10$ and the time scale of the memory function $\tau_1 = 1/\sqrt{2\Omega_1^2\delta}$. As may be seen from Fig. 4, the theoretical results and the data of the molecular dynamics simulations [31] are in good agreement. The VACF of liquid lithium at this temperature does not practically oscillate. This is direct indications of weak memory effects in the system, that can be caused by the absence of structural order in the the system and by the diffusive character of the single-particle dynamics [37].

Finally, the presented approach may also be used to investigate microscopical dynamics in more complex liquids, whose interatomic potentials include angular-dependent contributions. The memory function $M_1(t)$ of these systems, which represents the TCF of the stochastic force $f(t)$, will represent a combination of certain relaxation coupling modes. As a result, the VACF will have a more complex time behavior.

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