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A Statistical Mechanical Approximation for the Calculation of Time Auto-Correlation Functions

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ABSTRACT

This paper considers the problem of estimating the time auto-correlation function for a quantity that is defined in configuration space, given a knowledge of the mean-square displacement as function of time in this part of phase space. An approximate formula is derived which reduces the calculation of the time auto-correlation function to a "double canonical" average. In this approximation, the mean-square displacement itself may be evaluated from the "double partition function" in the case of Langevin dynamics. The scheme developed is illustrated by computer simulations of a simple one-dimensional systems, showing a good agreement between the exact time auto-correlation functions and those found by the approximation.

The calculation of a time auto-correlation function [1,2] is a straightforward matter in any computer simulation tracing the time evolution of a system [3-5]. However, computer simulations are not feasible today on time scales longer than microseconds. These time scales are relevant for viscous liquids approaching the glass transition. Therefore, one cannot by simulations calculate a number of experimentally accessible quantities in viscous liquids. Examples are the frequency-dependent viscosity [7], bulk modulus [8], dielectric constant [9], or specific heat [10,11], that all via the fluctuation-dissipation theorem [1,2,6] are given as Laplace transforms of a time auto-correlation function. In this situation one would like to have an approximate theory at hand. Focussing only on time auto-correlation functions of quantities $A(X)$ that are defined in configuration space, $X=(X_1,..,X_n)$, an approximation is proposed below, based on an ansatz for the joint probability of initial point X at $t=0$ and final point X' after time t, $P(X,X';t)$. In terms of the joint probability the time auto-correlation function is given by

$$\langle A(0)A(t)\rangle = \int dXdX'\, A(X)A(X')\ P(X,X';t) \quad . \tag{1}$$

If Z is the configurational partition function, given in terms of $\beta=1/(k_BT)$ and the potential energy $U(X)$ as

$$Z(\beta) = \int dX\, e^{-\beta U(X)} \quad , \tag{2}$$

and $G(X\rightarrow X';t)$ is the Green's function, the exact expression for the joint probability is

$$P(X,X';t) = \frac{e^{-\beta U(X)}}{Z} G(X \rightarrow X';t) \quad . \tag{3}$$

However, Eq. (3) is not very useful unless the Green's function is known. The principle of detailed balance implies that $P(X,X';t)=P(X',X;t)$, a requirement any approximation should also satisfy to ensure time-reversal invariance.

The exact method for calculating $\langle A(0)A(t)\rangle$ is shown in Fig. 1 illustrating the path in configurational space. At a number of times $t_1,\ldots,t_n$ one computes the quantity $A(X(t_j))A(X(t_j+t))$, and $\langle A(0)A(t)\rangle$ is the average of this product as $n\rightarrow\infty$. Assuming here and henceforth that the X_i's are simple rectangular coordinates and that $\langle A\rangle=0$, one always finds $\langle A(0)A(t)\rangle\rightarrow 0$ as $t\rightarrow\infty$. This loss of correlation after long time comes about because the final point X' is far away from the initial point X. A measure of the distance travelled in time t is provided by the mean-square displacement, $\langle \Delta X^2(t)\rangle$: If $X\equiv X(t_j)$, $X'\equiv X(t_j+t)$, and $\langle\rangle$ denotes an average over j, the mean-square displacement is defined by

$$\langle \Delta X^2(t)\rangle = \langle (X-X')^2\rangle \equiv \sum_{i=1}^{n} \langle (X_i-X_i')^2\rangle \quad . \tag{4}$$

Assuming that the mean-square displacement itself is a known function of time, the idea is now to estimate $\langle A(0)A(t)\rangle$ via the "spatial" auto-correlation of A in configurational space evaluated at distances equal to $\sqrt{\langle \Delta X^2(t) \rangle}$. Before proceeding, we briefly discuss the physics of this way of thinking about the time auto-correlation function. A simple case is when the mean-square displacement is proportional to time (for $t \to \infty$ this is, of course, always the case). In this case, if the "spatial" correlation of A has a Gaussian distance decay, the time auto-correlation function is a simple exponential, corresponding to Debye relaxation. If, however, the spatial correlation of A has an exponential distance decay, the time auto-correlation function is a stretched exponential with exponent ½. The latter case gives a reasonable fit to many experiments on viscous liquids [12]. The above picture of decomposing the time auto-correlation function into a) a "geometric" correlation and b) the distance travelled in a given time, is in harmony with another well-known property of viscous liquids. In these systems all linear relaxation functions have roughly the same average relaxation rate, a rate which slows down dramatically upon cooling. In the "geometric" picture, this is simply a consequence of the motion slowing down in configuration space, whereas the "spatial" correlation probably only change little upon cooling in a narrow range of temperatures. The mean-square displacement acts as a "molecular clock".

We now turn to the problem of estimating the joint probability $P(X,X';t)$. In the thermodynamic limit $n \to \infty$ the relative fluctuations in the mean-square displacement go to zero, and therefore the distance between $X=X(t_j)$ and $X'=X(t_j+t)$ is precisely $\sqrt{\Delta X^2(t)}$. Similarly, the relative fluctuations in potential energy go to zero, so the potential energy of both points X and X' is equal to $\langle U\rangle = -\frac{\partial \ln Z}{\partial \beta}$. The ansatz for $P(X,X';t)$ assumes equal probability for all pair of points with the correct distance and the correct potential energy. Thus,

$$P(X,X';t) \propto \delta[(X-X')^2-\langle\Delta X^2(t)\rangle]\,\delta[U(X)-\langle U\rangle]\,\delta[U(X')-\langle U\rangle] \quad . \tag{5}$$

In the thermodynamic limit there is "equipartition" between $U(X)$ and $U(X')$, and the last two delta functions may be replaced by a single delta function,

$$P(X,X';t) \propto \delta[(X-X')^2-\langle\Delta X^2(t)\rangle]\,\delta[U(X)+U(X')-2\langle U\rangle] \quad . \tag{6}$$

The next step is to convert Eq. (6) to a "canonical" form, which is computationally more convenient than the "microcanonical" form. This is done by replacing the first delta function by $\exp[-a(X-X')^2]$ where a is a Lagrangian multiplier adjusted to give the correct mean-square displacement. Similarly, the second delta function is replaced by $\exp(-b[U(X)+U(X')])$ where b is adjusted to ensure that the average of $U(X)+U(X')$ is $2\langle U\rangle$. If the "double partition function"

$$\tilde{D}(a,b) = \int dXdX' \; e^{-a(X-X')^2-b[U(X)+U(X')]} \tag{7}$$

is introduced, the final ansatz for the calculation of the time auto-correlation function is

$$\langle A(0)A(t)\rangle = \int \frac{dXdX'}{D(a,b)} \; A(X)A(X') \; e^{-a(X-X')^2-b[U(X)+U(X')]} \quad . \tag{8}$$

In the thermodynamic limit Eq. (8) is equivalent to the average Eq. (1) over the distribution Eq. (5).

The two parameters a and b are determined in the following way. First, $b=b(a)$ is found from the condition that the average joint potential energy of initial and final point is $2\langle U\rangle$. Thus, $b(a)$ is determined from the condition that this average is independent of a:

$$\frac{d}{da}\frac{\partial \ln D}{\partial b} = 0 \quad . \tag{9}$$

Since $\frac{d}{da}=\partial_a+\frac{db}{da}\partial_b$ [with the standard abbreviated notation for partial derivatives], the expansion of Eq. (9) leads to the following first order differential equation for $b(a)$

$$\frac{db}{da} = \frac{\partial_a D\,\partial_b D - D\,\partial^2_{ab}D}{D\,\partial^2_b D - (\partial_b D)^2} \quad . \tag{10}$$

Once the function $b(a)$ has been determined, $a=a(t)$ is found from requiring the mean-square displacement calculated from $D(a,b(a))$ to be correct:

$$-\frac{\partial \ln D}{\partial a} = \langle \Delta X^2(t) \rangle \quad . \tag{11}$$

The short and long time limits are determined as follows. For $a(t)$ one clearly has

$$\begin{aligned} a(t=0) &= \infty \\ a(t=\infty) &= 0 \end{aligned} \quad . \tag{12}$$

In the limit of large times X and X' are far apart and $U(X)$ is uncorrelated with $U(X')$. In this limit $b=\beta$:

$$b(a=0) = \beta \quad . \tag{13}$$

In the short time limit the points X and X' are forced together. Thus, $P(X,X';t) \propto \delta(X-X')\exp[-2bU(X)]$ for $t \to 0$ and Eq. (1) yields

$$\lim_{t\to 0} \langle A(0)A(t) \rangle = \frac{\int dX\, A^2(X)\, e^{-2bU(X)}}{\int dX\, e^{-2bU(X)}} \quad . \tag{14}$$

In order for this to give the correct canonical average one must have $b=\beta/2$, i. e.,

$$b(a=\infty) = \frac{\beta}{2} \quad . \tag{15}$$

The short time behavior of $a(t)$ may be derived directly from the equations of motion, as briefly sketched below. In the case of Newtonian dynamics, the Green's function at short times is easily found from the integrated equations of motion where the momentum is Gaussianly distributed (for simplicity it is assumed that all particles have the same mass m),

$$G(X \to X'; t) \propto \exp\left[-\frac{\beta}{2m} \sum_{i=1}^{n} \left(\frac{m}{t} \ (X_i' - X_i) + \frac{1}{2} \partial_i U \ t\right)^2\right] \ . \quad (16)$$

To first order in t this yields

$$G(X \to X'; t) \propto \exp\left[-a(t) \ (X - X')^2 - \frac{\beta}{2} [U(X') - U(X)]\right] \ , \quad (17)$$

where

$$a(t) = \frac{\beta m}{2t^2} \qquad (\textit{Newtonian dynamics}, t \to o) \ . \quad (18)$$

Note that via Eq. (3) this Green's functions confirms the form of the ansatz Eq. (8) for $t \to 0$, as well as the boundary condition Eq. (15). Next we consider the case of Langevin dynamics,

$$\dot{X}_i = -\mu \frac{\partial U}{\partial X_i} + \xi_i(t) \ , \quad (19)$$

with the standard Gaussian white noise term [14] $\langle \xi_i(t) \xi_j(t') \rangle = 2 \ \mu \ k_B T \ \delta_{i,j} \ \delta(t - t')$. From the equations of motion one finds that, because the integrated noise term is Gaussianly distributed,

$$G(X \to X'; t) \propto \exp\left[-\frac{\beta}{4\mu t} \sum_{i=1}^{n} \left(X_i' - X_i + \mu \ \partial_i U \ t\right)^2\right] \ . \quad (20)$$

At short times this again leads to Eq. (17), where however now

$$a(t) = \frac{\beta}{4\mu t} \qquad (\textit{Langevin dynamics}, t \to 0) \ . \quad (21)$$

In the case of Langevin dynamics Eq. (8) may be applied to the calculation of the force-force time auto-correlation function. This leads to an equation that in principle allows a calculation of $\langle \Delta X^2(t) \rangle$ directly from the double partition function. The mean-square displacement in time t is given by (sum over i)

$$\langle \Delta X^2(t) \rangle = \int_0^t dt' \int_0^t dt'' \langle \dot{X}_i(t') \dot{X}_i(t'') \rangle \quad . \tag{22}$$

Since the noise terms are uncorrelated at different times, Eqs. (19) and (22) imply

$$\frac{d^2}{dt^2} \langle \Delta X^2(t) \rangle = 2 \langle \dot{X}_i(0) \dot{X}_i(t) \rangle = 2 \mu^2 \langle \partial_i U(0) \partial_i U(t) \rangle \quad . \tag{23}$$

From Eq. (8) the force-force time auto-correlation function is rewritten as

$$\langle \partial_i U(0) \partial_i U(t) \rangle = \frac{1}{b^2} \int \frac{dX dX'}{D(a,b)} \left[\partial_i e^{-bU(X)}\right] \left[\partial'_i e^{-bU(X')}\right] e^{-a(X-X')^2} \tag{24}$$

By partial integrations one finds

$$\begin{aligned} \langle \partial_i U(0) \partial_i U(t) \rangle &= \\ - 4 \frac{a^2}{b^2} \int \frac{dX dX'}{D(a,b)} & (X-X')^2 e^{-a(X-X')^2 - b[U(X) + U(X')]} \\ &= 4 \frac{a^2}{b^2} \frac{\partial \ln D}{\partial a} \end{aligned} \tag{25}$$

Thus, the equation for $a(t)$ is from Eqs. (11), (23) and (25)

$$\left(\frac{d^2}{dt^2} + 8 \mu^2 \frac{a^2}{b^2} \right) \frac{\partial \ln D}{\partial a} = 0 \quad . \tag{26}$$

The expansion of Eq. (26) is straightforward, though tedious.

In order to check the validity of Eq. (8) a simple systems was studied numerically obeying Langevin dynamics. The system was chosen to be so simple that the integral in Eq. (8) may be evaluated "exactly", thus avoiding the noise of Monte Carlo simulations. No attempts were made to verify that Eq. (26) gives the correct $a(t)$. Instead the following procedure was followed. At a number of fixed a-values $b(a)$ was found from the requirement that the average joint potential energy is $2\langle U\rangle$. Then the mean-square displacement was evaluated for each a from Eq. (11) and also as function of time from the dynamical simulations, allowing an identification of the times corresponding to the fixed a-values. Finally, the time auto-correlation function was calculated from Eq. (8) at the fixed a-values. Figure 2 shows the results for $\langle X^3(0)X^3(t)\rangle$ for the Langevin motion of a particle in a double-well potential [14]. The full curve is the exact time auto-correlation function found by solving the Smoluchowski equation [13] and the dots give the prediction of Eq. (8). Results are shown for $\beta=2$ and for $\beta=8$ in dimensionless units.

In this paper a statistical mechanical approximation for the calculation of time auto-correlation functions was derived. The formalism assumes a knowledge of the mean-square displacement in configurational space as function of time; the mean-square displacement acts as the "molecular clock". The remaining "spatial" auto-correlation calculation is a "double canonical" average (Eq. (8)). Note that the corresponding double partition function, $D(a,b)$, contains the ordinary configurational partition function as a special case, $Z^2(\beta)=D(0,\beta)$.

The approximation is only useful if $\langle\Delta X^2(t)\rangle$ is known. Experimentally, this quantity is accessible via the intermediate incoherent scattering function. In some cases a phenomenological estimate of the mean-square displacement may be given. Thus, for hopping in a rugged energy landscape where all minima are equal, the mean-square displacement is **universal** at low temperatures (except for trivial scalings), i.e., it is independent of the barrier height probability distribution. This has been shown recently [15] by effective medium calculations and by computer simulations of the frequency-dependent conductivity, which is simply related to the mean-square displacement [16]. Finally, there is the possibility that the mean-square displacement may be found approximately from Eq. (26) if Langevin dynamics is assumed, as is common, e. g., in polymer dynamics [17].

Equation (26) signals that Langevin dynamics plays a special role in the proposed scheme for calculation of time autocorrelation functions. A question of considerable interest is if and when Langevin dynamics can be expected to give the same time auto-correlation functions as Newtonian dynamics [18]. If the ansatz is correct, two different dynamics give the same time auto-correlation functions for any quantity defined in configuration space, if just the two dynamics give the same mean-square displacement. In this way the ansatz provides a mechanism for the consistency of any two types of dynamics.

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FIGURE CAPTIONS

Fig. 1:

Path in configuration space with coordinates $X=(X_1,..,X_n)$ illustrating the exact definition of the time auto-correlation function. At a number of times $t_1,..,t_n$ one computes the quantity $A(X(t_j))A(X(t_j+t))$, and the time auto-correlation function is obtained as the average of this product as $n\to\infty$. In the thermodynamic limit the distance between the points $X(t_j)$ and $X(t_j+t)$ is the same for all j, because the relative distance fluctuations go to zero as the number of degrees of freedom go to infinity. This distance is the square root of the mean-square displacement in time t. In the approximation for evaluating the time auto-correlation function proposed here, equal probability is given to all pairs of initial (t=0) and final points after time t, that have the correct distance and where each point has the correct potential energy.

Fig. 2:

Log-log plot of $\langle X^3(0)X^3(t)\rangle$ as function of time for a Langevin particle in a double-well potential given in dimensionless units as $U(X)=(1/4)X^4-(1/2)X^2$. The full curve is the exact time auto-correlation function evaluated by solving the Smoluchowski equation. The symbols give the predictions of Eq. (8); the system is so simple that no Monte Carlo simulation is necessary to evaluate Eq. (8). Results are shown for $\beta=2$ and for $\beta=8$.

Fig.1

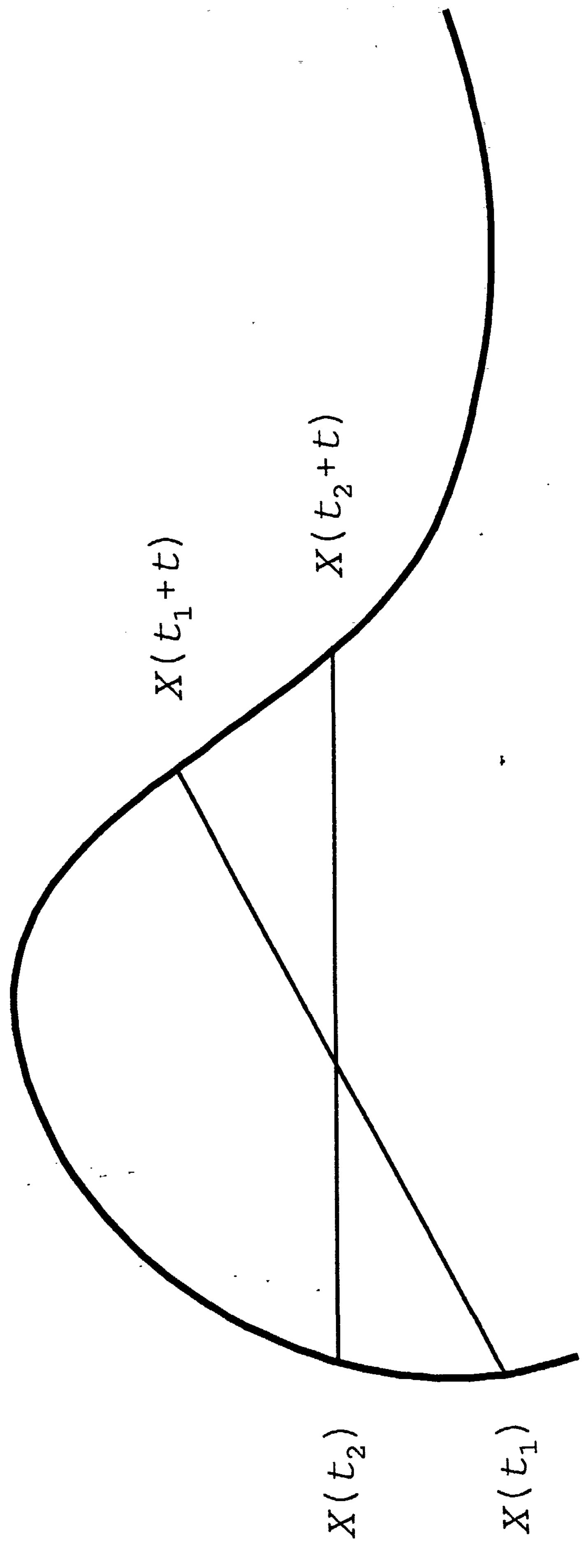
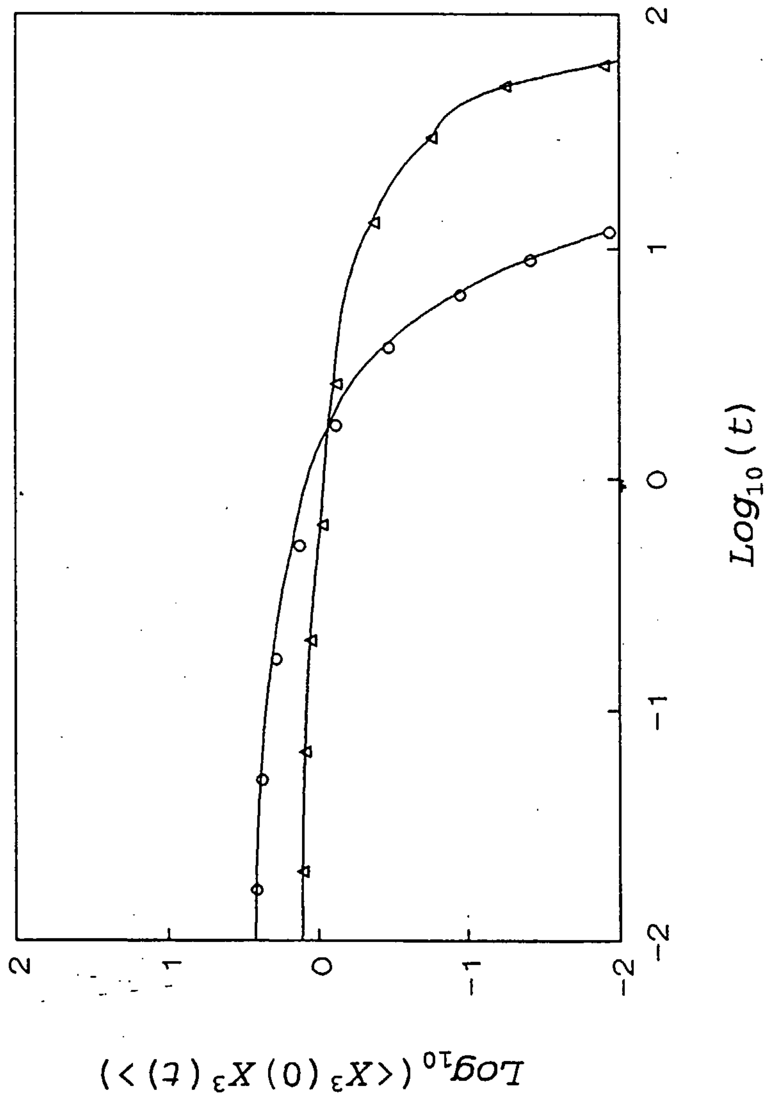


Fig. 2



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