Memory effects in Langevin approach to the nuclear fission process

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We present the schematic calculations within the Langevin approach in order to investigate the dependence of fission width on the memory time and the excitation energy at low temperatures where the quantum fluctuations play an important role. For this we consider the simple one-dimensional case with the potential energy given by two parabolic potentials (Kramers potential). For friction and the mass parameters we use the deformation independent values fitted to the results obtained earlier within the microscopic linear response theory. We have found out that at small excitation energies (comparable with the fission barrier height) the memory effects in the friction and random force acts on the fission width in opposite direction. The total effect is not so large, but still quite noticeable (depending on the value of the relaxation time). The use of effective temperature in the diffusion coefficient turns out to be much more important compared with the memory effects. The calculated fission width at very low excitation energies is unrealistically too big.

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I. INTRODUCTION

The Langevin approach is applied to the description of the nuclear fission process already for few decades [1–12]. In these works the one-five dimensional Langevin equations were solved with macroscopic or microscopic transport coefficients. The approach describes quite successfully the mass distributions and kinetic energies of fission fragments, the multiplicities of emitted neutrons. Still, there are few long-standing problems are not described properly up to now. One such phenomenon is the rapid transition of fission fragments mass distribution from symmetric to mass asymmetric in spontaneous fission of Fermium isotopes [14]. As it was shown by Flynn et al [15], the mass distributions of fission fragments of Fermium isotopes are very sensitive to the excitation energy. The mass distributions in spontaneous fission and thermal neutron-induced fission look very different.

This circumstance indicates the necessity to have an accurate description of the fission process at extremely low excitation energies, below the fission barrier. At low excitation energies, quantum effects become important not only in transport coefficients but also in diffusion coefficient and the memory effects in friction and random force.

Below in this preprint, we try to make it clear what is the influence of memory effects on the fission width at low excitation energies. To make it extremely clear we consider the simple one-dimensional case with the potential energy given by two parabolic potentials (Kramers potential). At the same time, for friction and mass parameters we use some results obtained in calculations within the microscopic linear response theory.

As it will be clear from the calculations below, the use of effective temperature turns out to be much more important compared with the memory effects.

In Section II we check how our one-dimensional numerical code reproduces the decay width. In Section III the non-Markovian Langevin equations are solved at constant temperature and dependence of the fission width on the value of relaxation time and excitation energy is clarified. In Section IV the role of effective temperature is investigated. Section VI contains the summary and open questions.

II. CLASSICAL LANGEVIN EQUATIONS

In order to check the numerical code we will solve first the one-dimensional Langevin equations with the "white" noise,

$$\frac{dq}{dt} = \frac{p(t)}{M},$$
$$\frac{dp}{dt} = -\frac{\partial E_{pot}}{\partial q} - \gamma p/M + \sqrt{D}\xi,$$  \hspace{1cm} (1)

where $\xi$ are the normally distributed random numbers with the properties

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(s) \rangle = 2\delta(t-s)$$  \hspace{1cm} (2)

and the diffusion coefficient $D$ is given by Einstein relation, $D = \gamma T$. The temperature here is considered to be time-independent parameter, related to the excitation energy $E^\ast$ by the Fermi-gas relation $E^\ast = aT^2$, and for
the level density parameter $a$ we use the approximation 

$$a = A/14.61(1.0 + 3.114A^{1/3} + 5.626A^{2/3}),$$

where $A$ is the mass number.

For the potential energy, we choose the simplest two-
parabolic (Kramers) potential, see Fig. 1.

$$E_{\text{pot}}(q) = (2V_b/q_0^2)q(q - q_0), \quad 0 < q < q_0,$$

$$= (2V_b/q_0^2)(q - q_0)(2q_0 - q), \quad q_0 < q < 2q_0.$$ 

This potential depends on two parameters, the barrier
height $V_b$ and the barrier width $q_0$. We have fixed the
barrier height as $V_b = 6$ MeV, which is close to the value
of the fission barrier of actinide nuclei. The width of the
barrier is somewhat uncertain. It depends on the
definition of the collective coordinate $q$ and the model
for the potential energy. For simplicity, we have put here
$q_0 = 1.0$. In principle, one should check the dependence
of final results on $q_0$.

For the potential one can define the stiffness $C =
d^2E_{\text{pot}}/dq^2 = 4V_b/q_0^2$ and the frequency of harmonic vi-
bervations $\omega_0 = \sqrt{C/M}$. In present work we fix $h\omega_0 =
1$ MeV, what is close to the frequency of collective vibrations calculated for $^{235}U$ in [16] within the microscopic linear response theory.

Thus, we will have for the mass parameter the defor-
mation and temperature independent value

$$M = 4V_b/(\omega_0 q_0^2),$$

For the remaining parameter, friction coefficient $\gamma$, we
will use a slightly modified approximation of [16]

$$\gamma/M = 0.6(T^2 + h^2\omega_0^2/\pi^2)/(1 + T^2/40)$$

(here $T$ is in MeV). Now all the parameters of Eqs. 1 are
fixed.

For the initial values of $q$ and $p$ we chose $q_{in} =
q_0/2, p_{in} = 0$. I.e., we start from the ground state de-
formation and assume that all the excitation energy is
put into the intrinsic degrees of freedom.

By integration of (1) from $t$ to $t + \Delta t$ one gets

$$p(t + \Delta t) = p(t) - F(t)\Delta t + \sqrt{D} \int_{t}^{t+\Delta t} \xi(s)ds.$$  

with

$$F(t) \equiv \partial E_{\text{pot}}/\partial q + \gamma p(t)/M$$

At each step of integration, we will need the integral
$$\int_{t}^{t+\Delta t} \xi(s)ds,$$ which is a sum of Gaussian random num-
bers, and thereby is itself a Gaussian random number. Its average and variance can be calculated with the sta-
tistical properties of $\xi(t)$, as

$$\int_{t}^{t+\Delta t} \langle \xi(s)\rangle ds = 0,$$

$$\int_{t}^{t+\Delta t} \int_{s}^{t+\Delta t} \langle \xi(s)\xi(s')\rangle dsds' = 2\Delta t.$$  

Thus, we can describe $\int_{t}^{t+\Delta t} \xi(s)ds$, by a new Gaussian random number $\omega_1(t)$,

$$\int_{t}^{t+\Delta t} \xi(s)ds = \omega_1(t)\sqrt{\Delta t},$$

such that $\omega_1(t)$ have the properties

$$\langle \omega_1 \rangle = 0, \quad \langle \omega_1^2 \rangle = 2.$$  

The random numbers $\omega_1$ can be constructed by Box-
Muller transform [17], then Eq. 1 turns into

$$p(t + \Delta t) = p(t) - F(t)\Delta t + \sqrt{D\Delta t} \omega_1.$$  

That is the integration schema of the classical Langevin
equations that we are using at present.

In what follows we will be interested in the fission
width of the system bound by the potential $V_b$. The fission
width $\Gamma_f$ is defined assuming the exponential de-
crease in time of the number of "particles" in the potential
well

$$P(t) = e^{-\Gamma_f t/h}$$

From here we will get

$$\Gamma_f = -h \ln[P(t)]/t$$

By solving the Langevin equations one will get the set of
time moments $t_b$, at which some trajectories would cross
the barrier, namely reach the value $q = 2q_0$. The total
probability to get out of the potential well will be equal to

$$P_b(t) = \sum_{t_b} \Theta(t - t_b)/N_t,$$

with

$$\Theta(x) = \begin{cases} 
0, & \text{if } x < 0, \\
1, & \text{if } x \geq 0.
\end{cases}$$
where \( N_{tr} \) is the number of all trajectories taken into account. Since the sum of probabilities to stay or get out of the potential well should be equal to unity \( P(t) + P_b(t) = 1 \), for \( P(t) \) one gets

\[
P(t) = 1 - \sum_{t_b} \Theta(t - t_b)/N_{tr}
\]

(17)

The fission width \( \Gamma_f \) is defined then by the fit of \(-\ln P(t)\) by linear in \( t \) function

\[
\int \left[ -\ln P(t) - \Gamma_f t/\hbar \right] dt - \min,
\]

(18)

From (18) one gets

\[
\Gamma_f = -\hbar \int_0^{t_{\text{max}}} t \ln P(t) dt / \int_0^{t_{\text{max}}} t^2 dt
\]

(19)

A demonstration of Eq. (19) is shown in Fig. 2.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{The probability \([18]\) of ”particle” to stay within the potential well (black) and its fit by the linear function (red).}
\end{figure}

The fission width \( \Gamma_f \) calculated by Eqs. (12), (19) is shown in Fig. 3 as a function of the excitation energy \( E^* \). For the comparison we show also the Kramers decay width \( \Gamma_K \),

\[
\Gamma_K = \frac{\hbar \omega_0}{2\pi} e^{-V_0/T} (\sqrt{1 + \eta^2} - \eta), \quad \text{with } \eta \equiv \gamma/2M\omega_0,
\]

(20)

and the quantity inversely proportional to the so called ”mean first passage time” \( \Gamma_{mft} = \hbar/\tau_{mft} \) (dashed line in Fig. 3), where

\[
\tau_{mft} = \gamma/\sqrt{2q_1 \int_{q_2}^{q_2} dq_1 e^{E_{pot}(q_1)/T}} \int_{-\infty}^{q_1} dq_2 e^{-E_{pot}(q_2)/T},
\]

(21)

and \( q_1 \) and \( q_2 \) are the solutions of the equation \( E_{pot}(q) = E^* \). As one can see, above \( E^* = 3 \text{ MeV} \) the fission width \( [18] \) is very close to Kramers approximation. The inverse mean first passage time is slightly larger. For smaller excitation energies \( \Gamma_f \) is very small and the computations are too time-consuming.

The solid line marked by filled dots in Fig. 3 is the decay width calculated within WKB-approximation, \( \Gamma_{WKB} \), where the decay rate \( r_{WKB} \) is given by [21],

\[
r_{WKB} = \frac{\omega_0}{2\pi} \exp \left[ -\frac{2}{\hbar} \int_{q_1}^{q_2} p(q) dq \right]
\]

(22)

For the collective momentum \( p(q) \) we used

\[
p^2(q) = 2(E^* - E_{pot})/M.
\]

(23)

As one can see, the quantum tunneling is dominant at rather small excitation energies, \( E^* \leq 0.6 \text{ MeV} \).

\section{III. NON-MARKOVIAN LANGEVIN EQUATIONS}

The estimates of the memory effects on the nuclear dynamics are rather contradictory. In earlier publications, one can find both the opinion that non-Markovian effects have a substantial influence on the fusion or fission processes [22, 24] and the statement that non-Markovian effects are very small [3].

To clarify this question, we will consider the non-Markovian Langevin equations that contain the memory effects, see [22], Eqs. 376-377,

\[
dq/dt = p(t)/M,
\]

(24)

\[
dp/dt = -\partial E_{pot}/\partial q - \int_{-\infty}^{t} \beta(t - t')p(t') dt' + \zeta(t),
\]

with \( \beta(t - t') = (\gamma/M) \exp (-|t - t'|/\tau)/\tau. \)

In the present work we will use a particular type of random numbers \( \zeta(t) \), that satisfy the equation

\[
d\zeta(t)/dt = -\zeta(t)/\tau + \xi/\tau
\]

(25)

and are used by the description of the so called Ornstein-Uhlenbeck processes.
The formal solution of Eq. (25) is
\[
\zeta(t) = \zeta(t_0)e^{-t/t_0} + \frac{1}{\tau} \int_{-\infty}^{t} e^{(t-s)/\tau} \xi(s) ds. \tag{26}
\]
Putting \( t_0 = -\infty \) one gets
\[
\zeta(t) = \frac{1}{\tau} \int_{-\infty}^{t} e^{(t-s)/\tau} \xi(s) ds. \tag{27}
\]
With help of Eq. (27) one can easily get the correlation \( \langle \zeta(t)\zeta(t') \rangle \),
\[
\langle \zeta(t)\zeta(t') \rangle = \frac{1}{\tau^2} \int_{-\infty}^{t} ds e^{(t-s)/\tau} \int_{-\infty}^{t'} ds' e^{(t'-s')/\tau} \langle \xi(s)\xi(s') \rangle = e^{-|t-t'|/\tau}. \tag{28}
\]
Here parameter \( \tau \) characterizes the strength of the memory effects. The correlation function (28) was used earlier in (22, 23). The more complicated form of the correlation function was derived in (22, 24). Here we will use the simplest form (28). In this case the Langevin equations we will have
\[
\frac{dq}{dt} = p(t)/M, \tag{29}
\]
\[
\frac{dp}{dt} = -\frac{\partial E_{pot}}{\partial q} - \frac{1}{\tau} \int_{0}^{t} dt' e^{-|t-t'|/\tau} \gamma p(t')/M + \sqrt{D} \zeta, \tag{30}
\]
Now we will introduce for the retarded friction \( R(t) \) the notation,
\[
R(t) = \frac{1}{\tau} \int_{0}^{t} dt' e^{-|t-t'|/\tau} \gamma p(t')/M. \tag{31}
\]
It can be easily checked that \( R(t) \) obeys the differential equation
\[
\frac{dR}{dt} = -\frac{R}{\tau} + \frac{1}{\tau} \gamma p(t)/M. \tag{32}
\]
Then non-Markovian equations (29) turn into the set of Markovian equations
\[
\frac{dq}{dt} = p(t)/M, \tag{33}
\]
\[
\frac{dp}{dt} = -[\partial E_{pot}/\partial q + R(t)] + \sqrt{D} \zeta, \tag{34}
\]
\[
\frac{dR}{dt} = -R/\tau + (\gamma p/M)/\tau, \tag{35}
\]
\[
\frac{d\zeta}{dt} = -\zeta/\tau + \xi/\tau. \tag{36}
\]
That is this set of equations that we will solve numerically below.

The integration of second Langevin equation (32) results in
\[
p(t+\Delta t) = p(t) - [\partial E_{pot}/\partial q + R(t)] \Delta t + \sqrt{D} \int_{t}^{t+\Delta t} \zeta(s) ds, \tag{37}
\]
For the evaluation of the integral on the right we will write down the solution of equation for \( \zeta(t) \) (32) in two ways
\[
\zeta(t+\Delta t) = \zeta(t) - \frac{1}{\tau} \int_{t}^{t+\Delta t} \zeta(s) ds + \frac{1}{\tau} \int_{t}^{t+\Delta t} \xi(s) ds, \tag{38}
\]
\[
\zeta(t+\Delta t) = \zeta(t)e^{-\Delta t/\tau} + \frac{1}{\tau} \int_{t}^{t+\Delta t} e^{-|t-t'|/\tau} \xi(s) ds. \tag{39}
\]
By subtracting the second line from the first one will find
\[
\int_{t}^{t+\Delta t} \zeta(s) ds = \tau[1 - e^{-\Delta t/\tau}] \zeta(t) + \int_{t}^{t+\Delta t} \frac{1}{1 - e^{-\Delta t/\tau}} \xi(s) ds. \tag{40}
\]
This relation is exact. The integral in (40) can be calculated in the same way as it was done for (11). Then one will get
\[
\int_{t}^{t+\Delta t} \zeta(s) ds = \tau[1 - e^{-\Delta t/\tau}] \zeta(t) + \sqrt{\Delta t - 2\tau(1 - e^{-\Delta t/\tau}) + \tau(1 - e^{-2\Delta t/\tau})}/2 \omega_1. \tag{41}
\]
The main order term of (41) in \( \Delta t/\tau \) is:
\[
\int_{t}^{t+\Delta t} \zeta(s) ds \approx \zeta(t) \Delta t, \quad \text{for} \quad \Delta t << \tau. \tag{42}
\]
It looks like the colored noise can be integrated like an analytical function.

The iterations for the third equation on (32) would give
\[
R(t+\Delta t) = R(t) - [R(t) - \gamma p(t)/M] \Delta t/\tau. \tag{43}
\]
To get a reasonable accuracy with (43), \( \Delta t \) should be much smaller than \( \tau \). The limit \( \tau \to 0 \) can not be obtained with (43). Instead one can use the formal solution of (41),
\[
R(t+\Delta t) = R(t)e^{-\Delta t/\tau} + \frac{1}{\tau} \int_{t}^{t+\Delta t} dt' e^{-|t-t'|/\tau} \gamma p(t')/M. \tag{44}
\]
The integral in (44) can be calculated assuming that \( p(t') \) does not change much on the time interval \( \Delta t \). Then
\[
R(t+\Delta t) = R(t)e^{-\Delta t/\tau} + [\gamma p(t)/M](1 - e^{-\Delta t/\tau}). \tag{45}
\]
For \( \tau \to 0 \) one easily gets the Markovian limit, \( R(t) = \gamma p(t)/M \).

Finally, for the fourth equation of (32) one can use the second line of (41). The integral in (41) is a sum of Gaussian random numbers, and thereby is itself a Gaussian random number
\[
\frac{1}{\tau} \int_{t}^{t+\Delta t} e^{-|t-t'|/\tau} \xi(s) ds = a_\omega(t). \tag{46}
\]
Here the random quantity $\omega_1(t)$ has the properties \(11\). The coefficient $a$ is defined calculating the average of left and right part of \(11\) squared,

\[
a^2 \langle \omega_1^2(t) \rangle = 2a^2 = \frac{1}{\tau^2} \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' e^{-\frac{2(s-s')}{\tau^2}} \langle \xi(s)\xi(s') \rangle
\]

The integral in \(12\) is easily calculated with help of \(2\)

\[
\frac{1}{\tau^2} \int_t^{t+\Delta t} ds \int_t^{t+\Delta t} ds' e^{-\frac{2(s-s')}{\tau^2}} \langle \xi(s)\xi(s') \rangle = \frac{[1-e^{-2\Delta t/\tau}]}{\tau}.
\]

Thus,

\[
\int_t^{t+\Delta t} e^{-\frac{2(s-s')}{\tau^2}} \xi(s) ds = \sqrt{\frac{\tau}{2}} \sqrt{1-e^{-2\Delta t/\tau}} \omega_1 \tag{44}
\]

and Eq. \(44\) turns into

\[
\tilde{\xi}(t+\Delta t) = \tilde{\xi}(t)e^{-\Delta t/\tau} + \frac{1}{\sqrt{2\tau}} \sqrt{1-e^{-2\Delta t/\tau}} \omega_1 \tag{45}
\]

Below we investigate separately the influence of the memory effects in the friction and random force on the fission width.

Let us clarify first the influence of retarded friction on the fission width $\Gamma_f$. For this we will keep in Eq. \(29\) the white noise \(2\),

\[
dq/dt = p(t)/M, \tag{46}
\]

\[
dp/dt = -\partial E_{pot}/\partial q - R(t) + \sqrt{D} \xi,
\]

The integration of second Langevin equation \(40\) results in

\[
p(t+\Delta t) = p(t) - [\partial E_{pot}/\partial q + R(t)] \Delta t + \sqrt{2D\Delta t} \omega_1 \tag{47}
\]

The fission width calculated with Eqs. \(41\, 17\) for $E^* = V_5$ is shown by red line in Fig. 4. As one can see, the account of memory effects in the friction force makes $\Gamma_f$ much larger.

The blue line in Fig. 4 is the calculation with memory effects in the random force alone and Markovian friction coefficient. As one can see, the memory effects in the random force make fission width much smaller.

The fission width calculated with \(43\, 46\, 10\) (memory effects both in friction and random forces) is shown by black line in Fig. 4. The memory effects in the friction and random forces almost cancel each other, and the variation of the black curve with $\tau$ is much smaller.

Clearly, the memory effects depend on the magnitude of relaxation time $\tau$.

Since at present the theoretical estimates for $\tau$ vary in very board region, we will choose in calculations below the two values of $\tau$ close to those used in \(26\), namely $\tau = 5 \cdot 10^{-22}$ sec and $\tau = 10^{-21}$ sec. For smaller $\tau$ the role of memory effects will be smaller.

The dependence of the fission width $\Gamma_\tau$ calculated with \(43\, 45\, 10\) on the excitation energy $E^*$ for the values of the memory time $\tau = 5 \cdot 10^{-22}$ sec and $\tau = 10^{-21}$ sec is shown in Fig. 5. For these values of $\tau$, the memory effects have a noticeable effect on the fission width $\Gamma_f$, especially large at small excitation energies.

\[
\text{IV. EFFECTIVE TEMPERATURE}
\]

The only quantity in the Langevin approach \(32\) that was not changed so far is the diffusion coefficient $D$. In principle, the diffusion coefficient also can contain the quantum effects. As it was shown by H. Hofmann and D. Kiderlen \(30\) in the quantum regime the classical Einstein relation for the diffusion coefficient $D = \gamma T$ should be modified to

\[
D = \gamma T \rightarrow D^* = \gamma T^* \tag{48}
\]

with

\[
T^*(\omega_0) = (\hbar \omega_0/2) \coth (\hbar \omega_0/2T). \tag{49}
\]
for the positive stiffness. The parameter $\omega_0$ is the local frequency of collective motion \[30\]. The minimal value of the effective temperature $T^*$ is given by $\hbar \omega_0/2$. For the negative stiffness Eq. \[49\] takes the form \[31\]

\[ T^*(i\omega_h) = (\hbar \omega_b/2) \cot (\hbar \omega_b/2T). \] (50)

Here $\omega_b$ is the frequency of collective motion around the fission barrier, $\omega_b^2 = |C|/M$. Since $T^*$ should be positive, the application of \[30\] will break down at a critical temperature $T_c$,

\[ T_c = \hbar \omega_b/\pi. \] (51)

Now, we simply replace the diffusion coefficient $D$ in \[32\] by $D^*$. The analog of Fig. 4 is shown in Fig. 4. As one can see from Fig. 6, the effect of effective temperature \[45\] is huge. Depending on the excitation energy, $\Gamma_f$ is getting larger by few orders of magnitude, compared with the value calculated with $D = \gamma T$.

Fig. 6 looks very similar to the Fig. 2 of \[24\] for the probability of compound nucleus formation. It was stressed in \[24\] that the quantum effects increase the compound nucleus formation probability at low excitation energies. At $T = 0.5$ MeV the quantum enhancement of probability of compound nucleus formation in \[24\] and the enhancement of fission width in present work ($T = 0.5$ MeV corresponds to $E^* = 6$ MeV) is approximately the same - one order of magnitude. But the effect of $T^*$ on the fission width increases rapidly at a lower temperature (excitation energies). At $E^* = V_b/2$ ($T = 0.335$ MeV) the fission width calculated with $T$ or $T^*$ differ by three orders of magnitude. It is difficult to believe that such a huge effect makes sense.

The excitation energies shown in Fig. 6 are restricted by the condition \[31\]. In order to go to smaller $E^*$ one may try to avoid using the effective temperature. For this let us note that the diffusion coefficient \[45\] can be identically written as

\[ D^*(\omega) = \gamma(\omega)T^*(\omega) = \frac{\chi''(\omega)}{\omega} \frac{\hbar \omega}{2} \coth \frac{\hbar \omega}{2T} = \frac{1}{2} \Psi''(\omega). \] (52)

Here for the friction coefficient we used the common relation from the linear response theory, $\gamma(\omega) = \chi''(\omega)/\omega$ and the relation between the imaginary parts of the response $\chi''(\omega)$ and the correlation $\Psi''(\omega)$ functions

\[ \Psi''(\omega) = \hbar \chi''(\omega) \coth(\hbar \omega/2T). \] (53)

The correlation function $\Psi''(\omega)$ can be calculated within the linear response theory for any shape, for any temperature, like it was done in \[32\], even with pairing effects taken into account.

The calculations within the Langevin approach with the microscopic transport coefficients will be the subject of the next studies.

V. SUMMARY AND OPEN QUESTIONS

From the results obtained above in a schematic onedimensional model, we can make a few quite general conclusions.

- The presented schematic calculations give a chance to investigate the dependence of fission width on the memory time and the excitation energy at low temperatures where the quantum fluctuations play an important role.
- At small excitation energies (comparable with the fission barrier height) the memory effects in the friction and random force acts on the fission width in opposite direction. The total effect is not so large, but still quite noticeable (depending on the value of $\tau$). The $\Gamma_f$ grows with increasing of the memory time $\tau$. At $\tau = 10^{-21}$ sec and $E^* = V_b$, the memory effects make the fission width 4 times larger as compared with $\tau = 0$.
- The replacement of the temperature by the effective temperature in the diffusion coefficient increases the fission width at low excitation energies by few orders of magnitude. This effect seems unreasonable too big.
- For the further investigation of the role of effective temperature it would be good to carry out the Langevin calculations with all transport coefficients defined within the microscopic approach, say, linear response theory.

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