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A note on the time evolution of the fission decay width under the influence of dissipation

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Abstract

The claim put forward in a recent paper by Jurado, Schmidt and Benlliure that the transient effect of nuclear fission may be described simply as a relaxation process in the upright oscillator around the potential minimum is refuted. Some critical remarks on the relevance of this effect in general are added.

In the paper [1] it has been claimed that "a new, highly realistic analytical approximation to the exact solution of the Fokker–Planck equation" has been presented. In this Letter we should like to raise some questions about the justifications of the approximations used there, in particular with respect to its application to the decay of a metastable state. Before we address details of the approach a few remarks of more general nature are in order.

It has become customary to look at nuclear fission as a time dependent process. As the current j_b across the barrier shows a "transient behavior", simply because it takes some finite time before j_b reaches a quasi stationary value, one likes to interpret the result in terms of a time dependent decay width $\Gamma_{\rm f}(t)$, modifying in this way the one originally deduced by Kramers using *essentially the same picture*. This transient time seemingly implies a delay of fission during which light particles might be emitted *in addition* to those given by the conventional ratio $\Gamma_n/\Gamma_{\rm f}^{\rm st}$ of the partial widths Γ_n for neutron evaporation to the stationary value $\Gamma_{\rm f}^{\rm st}$ for fission, even if for the latter the Bohr–Wheeler expression $\Gamma_{\rm BW}$ is replaced by the smaller value $\Gamma_{\rm K}$ of Kramers' rate formula. In arguments in favor of such a procedure it is often claimed that the time dependence comes in only if fission is considered as a transport process underlying dissipative forces. In this one forgets that the transition state method is also based on "collective motion" which, in principle, like particle emission, is a time dependent event. It is only that for these processes one has become accustomed to apply widths calculated in a time *independent* picture, in which, in addition, inherent averaging procedures are applied. Truth is that also Kramers' rate formula does not represent anything other than an inverse *average decay time*. This can directly be seen by exploiting the concept of the "mean first passage time" (MFPT). For over-damped motion an analytic formula for the $\tau_{\rm mfpt}$ can be derived

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from which, under the usual conditions for Kramers' rate formula, it follows that $\Gamma_{\mathrm{K}} = \hbar/\tau_{\mathrm{mfpt}}$, see, e.g., [2]. Interestingly enough, the value of the τ_{mfpt} does not depend much on the initial position of the system, in clear distinction to the transient effect [3]. In [3] and [4] the concept of the MFPT has been applied to nuclear fission to examine, for the limit of over-damped motion, if more light particles may be emitted than given by the ratio $\Gamma_n/\Gamma_{\mathrm{K}}$. In [4] it has been demonstrated that Kramers' rate formula is valid only for simple potentials and under favorable conditions for the temperature. For potentials having some structure in addition to just one pronounced minimum and one barrier the fission lifetime was seen to be considerably longer than the $\tau_{\mathrm{K}} = \hbar/\Gamma_{\mathrm{K}}$ associated to Kramers' rate. This feature may already by inferred from the form

$$\tau_{\mathrm{K}} = \frac{2\pi\gamma}{\sqrt{C_{\mathrm{a}}|C_{\mathrm{b}}|}} \exp(E_{\mathrm{b}}/T) \tag{1}$$

the τ_{K} takes on for over-damped motion. Any uncertainty in the product of the two stiffnesses at the minimum and the barrier, C_{a} and C_{b}, respectively, reflects itself in a corresponding error of their geometric mean, and hence in τ_{K}. Indeed, these stiffnesses are known at best in the immediate neighborhood of the extrema. Realistically, however, the potentials are hardly symmetric about these extrema. In cases that beyond the top of the barrier, for instance, the potential becomes wider this property may effectively imply a smaller $|C_{\mathrm{b}}|$ and, hence, a larger value of τ_{K}.

We agree with the authors of [1] that the understanding of nuclear dissipation is of great importance, in particular its variation with shape and temperature. After all, these are perhaps *the* decisive features through which different models or theories of nuclear transport can be distinguished [5]. It may perhaps be of interest to mention that, in addition to the papers cited in [1], quite some work has been done, both experimentally [6,7] as well as theoretically [8], in which such questions have specifically been addressed.

The main concern of [1] is that in previous analyses of experimental results uncertainties of a factor of two showed up in the so-called reduced friction coefficient β. There can be no question that the ultimate goal must be to improve our understanding about this problem, but it is questionable that the uncertainties and ambiguities of the method used in [1] imply progress. To begin with, one should not trace all problems back to *just the one constant* β. Even discarding possible inaccuracies in the height of the barrier, which enters the decay rate in exponential fashion, there are crucial problems with the transport coefficients themselves. The β, for instance, only stands for the ratio of friction γ to inertia M. For obvious physical reasons, these two quantities must be expected to exhibit a totally different variation with temperature. Moreover, for a coordinate dependent inertia, Kramers' formula has to get an additional factor involving the square root of the ratio of the inertias at barrier and minimum [8,9]. For truly over-damped motion, on the other hand, any quantity which involves the inertia looses any meaning. Indeed, the latter does not appear in formula (1).

Let us turn now to the more formal problems of [1]. The authors aim at delivering a simple way of calculating the time dependent prefactor which supposedly relates $\Gamma_{\mathrm{f}}(t)$ to Kramers' stationary value Γ_{K}. The essential approximation is to calculate this prefactor *not from a global* solution of Kramers' equation, which would properly account for the *motion across the barrier*, but from a solution of the same transport equation *restricted to the upright oscillator* by which the fission potential may be approximated in the *neighborhood of the minimum*. A moments reflection tells one that at the barrier, where the current j_b is to be calculated, the height of the artificial potential in this region may easily exceed the barrier height several times. The very fact that in this region the stiffness of this auxiliary potential has the wrong sign is most crucial for the current, in particular at large times. Whereas for the inverted oscillator the $j_b(t)$ eventually turns into the stationary one already found by Kramers, the current for an upright oscillator tends to zero exponentially. In other words, replacing already in ([1]-6) (which is to say in Eq. (6) of Ref. [1]) the correct distribution W_n by the one for an upright oscillator, called W^{par} in Eq. ([1]-9), leads to a vanishing denominator in this basic formula.

To circumvent this problem some intermediate steps are performed to finally end up with formula ([1]-8) for which the W^{par} of ([1]-9) is to be inserted. One basic assumption for this is specified in Eq. ([1]-7). It implies that, for any time t and at the barrier top, the dependence of the distribution on coordinate and velocity is identical to the one at infi-

nite time. For an oscillator this statement is easily seen to be incorrect, both for under-damped as well as for over-damped motion (for which it is claimed to be exact). Take the distribution given in ([1]-9), namely[1]

$$W^{\mathrm{par}}(x = x_b; t) = \frac{1}{\sqrt{2\pi}\sigma(t)} \exp\left(-\frac{x_b^2}{2\sigma^2(t)}\right), \qquad (2)$$

which for an oscillator delivers the correct form for the density in coordinate space. For over-damped motion this statement is evident, for under-damped motion one first needs to integrate over velocity. Putting the form (2) into ([1]-7) the $C(t)$ of ([1]-7) turns out to be

$$C(t) = \frac{\sigma(t \to \infty)}{\sigma(t)} \times \exp\left(-\frac{x_b^2}{2}\left[\frac{1}{\sigma^2(t)} - \frac{1}{\sigma^2(t \to \infty)}\right]\right), \qquad (3)$$

which evidently is *not only a function of time* but varies with x_b. As the upright and inverted oscillator turn into each other by analytic continuation (changing only the sign of the stiffness) [5] the proof just given also applies to the motion of a Gaussian across a barrier, if simulated by a parabola.

For the $\sigma^2(t)$ needed for the $W^{\mathrm{par}}(x = x_b; t)$ of Eq. (2) a form is given in Eq. ([1]-10) which corresponds to zero initial width. On the other hand, the authors claim it to be more suitable to start from ground state fluctuations and they try to simulate this feature by introducing[2] a time shift t_0. It is meant to represent the "time shift needed for the probability distribution to reach the width of the zero-point motion in deformation space", which is supposed to be "equal to the time that the average energy of the collective degree of freedom needs to reach the value $(1/2)\hbar\omega_1$ associated to the zero-point motion". Obviously, the authors seem to understand t_0 as a kind of relaxation time to the equilibrium of the oscillator, as represented by the ground state. It may be noted in passing that for a genuine quantum system any application of ([1]-10) is prohibited anyway as the distribution can never have zero width. In any case, it remains unclear why it should be the ground state and, hence, why there is no influence of the large intrinsic excitations which are produced in the first stage of the reaction; after all the authors work with a finite temperature.

At this stage it may be worth while to remind the reader of some basic features of transport theory, which may help to clarify a few critical steps used in [1]. To begin with, let us look how quantum features may be accounted for. As it stands, Eq. ([1]-10) describes relaxation to the equilibrium specified by the equipartition theorem of classical mechanics, represented here by the prefactor of the curly bracket. For a damped oscillator this may be generalized to represent quantum fluctuations correctly (see, e.g., [5]). In equilibrium they are *not* given by those of the ground state $\hbar/2\mu\omega_1$ used here, for instance in Eq. ([1]-12). In fact for over-damped motion just the opposite is true: there the correct quantum equilibrium is indeed given by the classical limit, see [5] for the oscillator and [10] for the general case.

Let us examine now the derivation of Eq. ([1]-12), $t_0 = \hbar\beta/(4\omega_1 T)$, meant to determine the time lapse t_0. This equation is obtained by assuming a linear dependence between the $\sigma^2(t)$ and time t. This approximation is justified by arguing that the "influence of the potential on the diffusion process" may be "neglected" as it "is anyhow small in the range of the zero-point motion". To see the catch in this argument let us simply write the correct equation for $\sigma^2(t)$, as it comes out of the Smoluchowski equation for the oscillator:

$$\frac{d}{dt}\sigma^2(t) + 2\frac{C}{\gamma}\sigma^2(t) = 2D_{\mathrm{ovd}}. \qquad (4)$$

Here, C is the stiffness of the potential $U(x)$, such that the latter may be written as

$$U(x) = \frac{C}{2}x^2 \quad \text{with } C = \mu\omega_1^2, \qquad (5)$$

and D_{ovd} is the diffusion coefficient, which according to (4) is determined by the equilibrium fluctuation σ^2 through

$$D_{\mathrm{ovd}} = \frac{C}{\gamma}\sigma^2(t \to \infty) \equiv \frac{C}{\gamma}\sigma_{\mathrm{eq}}^2 \approx \frac{T}{\gamma}. \qquad (6)$$

Eq. (4) implies that the "influence of the potential on the diffusion process" is given by the second term on the left *which has the same size independent* of the

[1] It is properly normalized, also in the sense of Eq. ([1]-5) if one only makes the common assumptions that x_b is sufficiently far away from the minimum such that the tiny tail beyond x_b does not influence the normalization integral.

[2] It remains unclear why the authors did not simple generalize the analytic form ([1]-10) to one valid for any initial condition, such as (7), shown below for over-damped motion.

"range" of the coordinate. The solution of Eq. (4) for $t \geqslant 0$ is given by

$$\sigma^2(t) = \left(\sigma^2(t=0) - \sigma_{\rm eq}^2\right) \exp\left(-\frac{2C}{\gamma}t\right) + \sigma_{\rm eq}^2, \qquad (7)$$

showing that relaxation to the equilibrium value happens on the time scale $\tau_{\rm ovd} = \gamma/2C$ independent of the initial fluctuation. Of course, for $t \ll \tau_{\rm ovd}$ and zero initial fluctuations the $\sigma^2(t)$ becomes linear in t, but the reason why such a $\sigma^2(t)$ should be identified as the *ground state fluctuation* of the *undamped* oscillator remains unclear. Put in the context mentioned above: it is unclear why such a value of $\sigma^2(t) \equiv \hbar/2\mu\omega_1$ should be relevant if *reached by a process of strong damping*.

Next we turn to the value found for t_0 from Eq. ([1]-12). It turns out so small that the introduction of this quantity and the associated fluctuation cannot explain why the $\Gamma_{\rm f}(t)$ starts to become finite only at about 0.7×10^{-21} s. Indeed, for $\beta = 2 \times 10^{21}$ s^{-1}, $\hbar\omega_1 = 1$ MeV and $T = 3$ MeV one gets the very small number of $t_0 \simeq 0.06 \times 10^{-21}$ s. The explanation given in [3] comes much closer: there, by simulating the whole fission process by a Langevin equation, it was demonstrated that such a shift is related to the relaxation of the initial distribution to the quasi-equilibrium in the minimum. For the numbers just used the relaxation time $\tau_{\rm ovd}$ becomes $\tau_{\rm ovd} \simeq 0.36 \times 10^{-21}$ s—provided one makes use of the relation (5). The value of $\tau_{\rm ovd}$ becomes even *very* close to the $\simeq 0.7 \times 10^{-21}$ s at which in Fig. [1]-1 the $\Gamma_{\rm f}(t)$ is seen to rise if the relation of frequency to stiffness is replaced by the *incorrect* one given in Eq. ([1]-13) where the stiffness K is assumed to be only half the correct value given in (5), in accord with the common definition used in text books not only on nuclear physics but on classical and quantum mechanics as well. It is true that, for the cases discussed in Fig. [1]-1, the motion is not really over-damped (for $\hbar\omega_1 = 1$), but the $\tau_{\rm ovd}$ may nevertheless be taken as a fair estimate.

As indicated before, it is left unclear why in the general case the system should start with a small fluctuation. Indeed, formula ([1]-8) together with ([1]-9) implies any transient effect (of the type discussed here) to be absent if one chooses to start out of the quasi-equilibrium, which is to say for $W^{\rm par}(x = x_b, t = 0) = W^{\rm par}(x = x_b, t \to \infty)$. For a bound system, like the upright oscillator, such an initial condition implies that the system stays in equilibrium for ever. For over-damped motion this may be seen from Eq. (7) together with (2). For a metastable situation like fission, on the other hand, the situation is different: then there will be a finite current outwards. Exactly this feature is not described correctly by formulas ([1]-8) and ([1]-9). Please recall that in many cases an initial condition like that of the quasi-equilibrium specified before is not at all unrealistic. For sufficiently large fission barriers, as they are required for Kramers's rate formula anyhow, the system may well have enough time to reach such a stage around the first well before it decays by fission.

Let us finally comment on the feature that for certain cases the present construction seems to represent fairly well the numerically obtained global solutions of the transport equation for the full fission potential. In our opinion this feature should be considered accidental rather than supply a decent basis for trustworthy applications in future work of the approximations advertised in this Letter. There are simply too many inconsistencies to warrant applicability to the general case.

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