Decay of unstable states in macroscopic systems

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A unified treatment of the total time regime of the decay of an unstable macroscopic state is derived by functional integral methods. A new one-variable integral representation for the conditional probability is obtained. Previous results with only a limited range of validity are contained as special cases. Further, the evolution of initial states in the vicinity of the instability point is studied.

The temporal behavior of fluctuations in a macroscopic system which is initially quenched to an unstable stationary state is one of the intriguing phenomena in nonequilibrium statistical mechanics.[1] Such processes are observed in many physical systems, e.g., superfluorescence, the onset of laser activity, spinodal decomposition, and also in many different fields, e.g., chemical reactions, electronics, and biology.

When a system is in an unstable stationary state the decay is initiated solely by stochastic forces and the fluctuations of the observables will rapidly grow. At intermediate times the observables have changed macroscopically and also the fluctuations are of macroscopic order. In this time regime the stochastic forces are small compared to the deterministic forces. In the final time regime, where the system approaches the stable stationary state, the fluctuations shrink to a finite microscopic level. There, we have to take into account the stochastic forces properly again.

Several approximation schemes for such decay processes have been proposed. In the methods of Refs. 2 and 3 the Fokker-Planck equation associated with the stochastic process is solved for the initial and intermediate time regime in different approximations, and the corresponding solutions are matched together at a time t_0 which was determined by fitting the experimental data. In recent approaches[4,5] the separate treatments of initially linear and intermediately deterministic regimes are avoided. However, these methods do not cope with the fluctuations in the final time regime, where equilibrium is approached.

The purpose of this Communication is to present a unified treatment of all time regimes of the decay of an unstable stationary state by functional integral methods. It turns out that some sort of approximate kink solution dominates the functional integral in the final time regime where equilibrium is approached. By a careful treatment of the resulting quasisymmetry mode a new integral representation for the conditional probability of the decay process is obtained. Previous results, being valid only at intermediate times, are recovered by a saddle-point approximation.

To avoid unessential complications I consider the stochastic overdamped motion in a one-dimensional symmetrical bistable potential $U(x)$ with minima at $x=\pm 1$ and a maximum at $x=0$. Hence, the deterministic motion is given by $\dot{x}=-U'(x)$, $x=0$ is the unstable stationary point and $x=\pm 1$ are the stable points of the system. The dynamics of the stochastic system is described by the Fokker-Planck equation

$$\frac{\partial P}{\partial t}=-\frac{\partial}{\partial x_f}[U'(x_f)P]+\frac{\epsilon}{2}\frac{\partial^2 P}{\partial x_f^2} \ , \qquad (1)$$

where $P(x_f,t;x_i)$ is the conditional probability with the initial condition $P(x_f,0;x_i)=\delta(x_f-x_i)$. The diffusion constant ϵ is assumed to be small, $\epsilon \ll \omega_0 \equiv |U''(0)|$ and $\epsilon \ll \omega_1 \equiv U''(1)$. The solution of Eq. (1) is given by the path integral

$$P(x_f,t;x_i)=\frac{\exp[-U(x_f)/\epsilon]}{\exp[-U(x_i)/\epsilon]}K(x_f,t;x_i) \ , \qquad (2)$$

$$K(x_f,t;x_i)=\int_{x_i}^{x_f}Dx(\tau)\exp(-S/\epsilon) \ , \qquad (3)$$

where S is the action

$$S(x_f,t;x_i)=\int_0^t d\tau[\dot{x}^2/2+V(x)] \ , \qquad (4)$$

$$V(x)=U'^2(x)/2-\epsilon U''(x)/2 \ . \qquad (5)$$

In the small-ϵ limit the functional integral (3) is dominated by the stationary points of S, $\delta S/\delta x_c=-\ddot{x}_c+V'(x_c)=0$. These are the paths $x_c(\tau)$ of a particle of unit mass moving in the inverted potential $-V$ with boundary conditions $x_c(0)=x_i$ and $x_c(t)=x_f$. The standard evaluation of Eq. (3) by steepest descent gives

$$K=N|\mathrm{Det}\hat{L}(x_c)|^{-1/2}\exp(-S_c/\epsilon) \ , \qquad (6)$$

where $\hat{L}(x_c)=-d^2/d\tau^2+V''(x_c)$ is the second variation operator $\delta^2S/\delta x_c^2$ and N is an appropriate normalization constant. The determinant in (6) is calculated for eigenfunctions $[\hat{L}(x_c)-\lambda_n]x_n(\tau)=0$ with boundary conditions $x_n(0)=x_n(t)=0$. It can be related to the classical motion according to[6,7]

$$N^2/|\mathrm{Det}\hat{L}(x_c)| = \left|\frac{\partial E}{\partial x_f}\right| \Big/ 2\pi\epsilon\dot{x}_c(0) \ , \tag{7}$$

where E is the energy of the path $x_c(\tau)$.

The steepest descent estimate (6) of the path integral is accurate if the fluctuations around the classical path x_c are small. To be more specific, Eq. (6) is appropriate, if $\lambda_n >> O(\epsilon)$ for all n. This condition is generally fulfilled in the case of monostable systems but may break down for dominant trajectories of bistable systems. In the latter case the minima of the potential $V(x)$ at $x=0$ and at $x=\pm 1$ are almost degenerate in energy. $V(\pm 1)=V(0) -(\omega_0+\omega_1)\epsilon/2$. Accordingly, a path connecting $x_i=O(\sqrt{\epsilon})$ and $x_f=\pm 1+O(\sqrt{\epsilon})$ is a kinklike solution with an approximate time translation symmetry.[8] Related to this quasisymmetry there is a nodeless mode $x_0(\tau)$ whose eigenvalue λ_0 decreases exponentially with time to $O(\epsilon)$.[9]

The situation is somewhat reminiscent of the problem of tunneling between degenerate vacua in quantum mechanics.[7,8] The difference lies in the fact that in our problem the degeneracy is removed by a term of order ϵ and that we aim at a result being a function of x_i, x_f, and t. Thus we are concerned with a kinklike solution whose energy explicitly depends on x_i, x_f, and t.

To deal with the quasisymmetry of the action we consider a family of kinklike solutions $\bar{x}(\tau,t_0)$ which have fixed boundaries $\bar{x}(0,t_0)=x_i$, $\bar{x}(t,t_0)=x_f$ and where t_0 indicates the kink position. These trajectories are approximate stationary points of the action. The center t_0 of the kink represents a collective coordinate[10] and serves the elimination of the quasisymmetry mode $x_0(\tau)$. Then, the appropriate generalization of Eq. (6) is given by

$$K = N\int_0^t dt_0 J \frac{\exp(-\bar{S}/\epsilon)}{|\mathrm{Det}'\hat{L}(\bar{x})|^{1/2}} \ , \tag{8}$$

where $\bar{S}$ is the action of the path $\bar{x}(\tau,t_0)$ and Det$'$ has the lowest eigenvalue omitted. In leading order the measure of integration J is independent of t_0 and is given by

$$J^2=[U(x_i)-U(x_f)]/(2\pi\epsilon) \ .$$

At times

$$0\leq t\lesssim t_s \equiv \ln(\omega_0/\epsilon)/(2\omega_0)$$

the range $x_f=\pm 1+O(\sqrt{\epsilon})$ is insignificant to the distribution $P(x_f,\ t;\ x_i=O(\sqrt{\epsilon}))$. Thus, in this time regime the decay of an unstable stationary state is adequately described by Eq. (6). Our general result (8), however, also covers the subsequent time regime $t>t_s$, in which the equilibrium distribution is approached around the stable sites ± 1 of the system.

Prior to the further evaluation of Eq. (8) we now first consider Eq. (6). The well-known difficulty in handling the problem of classical mechanics in Eq. (6) for an anharmonic potential is avoided by a deterministic approximation in that range where the anharmonic terms are relevant. To be explicit, the energy of the path $x_c(\tau)$ from $x_i=0$ to $x_f>0$ is approximately determined by the expression[11]

$$t=\int_0^{x_f} dx[2(V_0+E)]^{-1/2}-\Theta_0(x_f,0) \ , \tag{9}$$

$$\Theta_0(z,y)=\int_y^z dx[|1/U_0'(x)|-|1/U'(x)|] \ , \tag{10}$$

where $V_0=(U_0'^2-\epsilon U_0'')/2$ with $U_0'=-\omega_0 x$ is the harmonic approximation of V about $x=0$. If it were $V=V_0$, Eq. (9) would be exact. The additional term $\Theta_0(x_f,0)$ is the amount of time accounting for the anharmonic deviation $V-V_0$. In the deterministic approximation $x_c(\tau)=x_d(\tau)$, where $\dot{x}_d=-U'(x_d)$, Θ_0 is given by Eq. (10). As a consequence of the approximation (9), x_f is restricted to $0<x_f\leq a$ and $0<x_f\leq b(t)$, where $1-a>>O(\sqrt{\epsilon})$ and $b(t)$ is obtained from $T_0(b)\equiv t+\Theta_0(b,0)=0$. We finally obtain from Eqs. (6) and (7)

$$\begin{aligned} P(x_f,t;0) &= \frac{\omega_0\sqrt{G}\exp(-G)}{\sqrt{\pi}|U'(x_f)|} \ , \\ G &= (\omega_0/\epsilon)x_f^2/\{\exp[2\omega_0 T_0(x_f)]-1\} \ , \end{aligned} \tag{11}$$

where $T_0(x_f)=t+\Theta_0(x_f,0)$. At short times, $0\leq t\lesssim(2\omega_0)^{-1}$, Eq. (12) reduces to the exact solution of the harmonic problem $U(x)=U_0(x)$. At times $(2\omega_0)^{-1}<<t\lesssim t_s$ one obtains from Eq. (11)

$$\begin{aligned} P(x_f,t;0) &= F'\exp(-F^2)/\sqrt{\pi} \ , \\ F &= (\omega_0/\epsilon)^{1/2}x_f\exp[-\omega_0 T_0(x_f)] \ , \end{aligned} \tag{12}$$

which is exactly the "scaling" solution of Suzuki.[11,12] Equation (12) describes the formation of the double peaks of the distribution $P(x_f;t;0)$ in the intermediate time regime, where the system is controlled by the deterministic forces and the stochastic forces are negligible.

Let us next consider the further evaluation of Eq. (8). Three remarks are appropriate. (1) Since we now assume $|x_i|\leq O(\sqrt{\epsilon})$ and $|1-x_f|\leq O(\sqrt{\epsilon})$, both the harmonic regions of V around $x=0$ and $x=1$ are relevant. (2) The path $\bar{x}(\tau,t_0)$ is only an approximate stationary point of the action. Thus, the conservation of energy is violated as a function of the kink position t_0. (3) Let E_0 and E_1 be the energies of the path $\bar{x}$ in the harmonic region around $x=0$ $(V=V_0)$ and $x=1$ $(V=V_1)$, respectively. Then, using the deterministic approximation in the intervening anharmonic region of V, E_0 and E_1 are obtained by inverting the expressions

$$t_0=\int_{x_i}^{x_m} dx[2(V_0+E_0)]^{-1/2}-\Theta_0(x_m,x_i) \quad ,$$
$$t_1=\int_{x_m}^{x_f} dx[2(V_1+E_1)]^{-1/2}-\Theta_1(x_f,x_m) \quad , \tag{13}$$

where $t_1=t-t_0$ and x_m is fixed somewhere in the valley of the inverted potential $-V(x)$, $x_m>0$. Calculating $\mathrm{Det}[\hat{L}(\bar{x})]$ and $\lambda_0(\bar{x})$ in the corresponding approximation it turns out that $\mathrm{Det}'[\hat{L}(\bar{x})]$ is factorized.[13] Equation (13) assumes the form

$$K(x_f,t;x_i)=\int_0^t \frac{dt_0}{2\pi\epsilon}\left\{\left|\frac{\partial E_0}{\partial x_i}\right|\left|\frac{\partial E_1}{\partial x_f}\right|\right\}^{1/2}\exp(-\bar{S}/\epsilon) \quad . \tag{14}$$

By a look at Eqs. (6) and (7) this result can be interpreted as a folding of two kernels,

$$K=\int_0^t dt_0\,\dot{\bar{x}}(t_0)K(x_f,t_1;x_m)K(x_m,t_0;x_1) \quad . \tag{15}$$

For $t \gg (2\omega_0)^{-1}$ and $x_f>0$, Eq. (14) leads to the explicit result

$$P(x_f,t;x_i)=\frac{\sqrt{\omega_0\omega_1}}{\pi\epsilon}\frac{U_1'(x_f)}{U'(x_f)}\int_0^\infty dy\exp(-R/\epsilon) \quad ,$$
$$R=\omega_0(y-x_i)^2+\omega_1(1-x_f-ry^{-\omega_1/\omega_0})^2 \quad , \tag{16}$$
$$r=(1-x_m)x_m^{\omega_1/\omega_0}\exp(-\omega_1 T) \quad ,$$

where $T=t+\Theta_0(x_m,0)+\Theta_1(x_f,x_m)$. In Eq. (16) we have changed over to the integration variable

$$y=x_m\exp\{-\omega_0[t_0+\Theta_0(x_m,0)]\} \quad .$$

Here, the error caused by extending the bounds of the integral to zero and infinity is exponentially small. Note that Eq. (16) is independent of the intermediate point x_m, as follows directly by use of Eq. (11). A similar expression holds for $x_f<0$.

The integral representation (16) is the main result of this Communication. It is the semiclassical solution of the decay of the system which is initially in the harmonic range around the instability point. Equation (16) covers the intermediate and the subsequent time regime where equilibrium is approached separately at the sites $x=+1$ and $x=-1$.

Let us comment on three aspects of our result (16). (1) Evaluating Eq. (16) for $x_i=0$ and $t \lesssim t_s$ by steepest descent at the saddle point $z=1-x_f$ the previous result (12) is recovered. (2) For times $t>t_s$, where the range of x_f around the stability points is important, the integral in Eq. (16) cannot be done by steepest descent. (3) In the limit $t \gg t_s$ Eq. (16) approaches the expression

$$P=\{1+\mathrm{erf}[(\omega_0/\epsilon)^{1/2}x_i]\}P_0(x_f) \quad ,$$

where $P_0(x_f)$ is the equilibrium distribution of the system in the harmonic range around $x_f=+1$. Thus, the proper result for the occupation probability[14] of the site $+1$,

$$p_+=\{1+\mathrm{erf}[(\omega_0/\epsilon)^{1/2}x_i]\}/2$$

is obtained.

Let us remark that Eq. (16) can also be verified by the mode decomposition method.[13] By considering appropriate integral representations of the corresponding mode functions the sum over all mode contributions can be performed explicitly and the result can be written in the form (16).

Recently, de Pasquale, Tartaglia, and Tombesi[15] have treated the decay of an unstable state by the method of stochastic differential equations and have obtained explicit results for the moments. The same results also follow from our Eq. (16) after only a slight modification has been performed.[13]

A final remark is in order. Exchange of probability between the sites $x=-1$ and $x=+1$ happens on a very huge time scale.[16] The basic object to be considered in this case is an approximate double kink solution with boundaries $x_i=-1$ and $x_f=+1$, where the kink positions represent two collective parameters. With the appropriate generalization of Eq. (14) we directly obtain a repulsive kink-kink interaction.[17] Thus, contrary to Ref. 11, we need not change over to an integration path in the complex plane of the relative kink position.[18] The proper value of the inverse transition time

$$t_K^{-1}=\sqrt{\omega_0\omega_1}\exp\{-[U(0)-U(1)]/\epsilon\}/\pi$$

is obtained by this method.

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