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Path Integral Approach to Spontaneous Fission

Zastosowanie całek po trajektoriach w rozszczepieniu jąder atomowych

Приближение интегралов по траекториям в случае спонтанного деления

Dedicated to Professor
Stanisław Szpikowski on occasion
of his 60th birthday

1. INTRODUCTION

Many of papers dealing with the spontaneous fission process describe it as a penetration of the nucleus through the potential barrier in a deformation space [1 , 2]. In order to have the penetrability (the barrier penetration probability) $\bar{P}$ one usually assumes WKB formula

$$\bar{P} = \left[1 + \exp\left(2S_{12}\right)\right]^{-1} , \qquad (1)$$

where S_{12} is the reduced action given by the formula

$$S_{12} = \int_{(1)}^{(2)} \sqrt{2 \mid V - E \mid B_a}\ da \qquad (2)$$

and it is taken along some trajectory given in prepared deformation space. Here $V = V(a)$ is the potential energy, $B_a = B_a(a)$ is the effective mass parameter (effective inertia) and E is the energy of the fissioning nucleus. The parameter "a" specifies the position of a point on the trajectory with a_1 and a_2 being the classical turning points corresponding to given energy E ($V(a) = E$). It might be the arc length of the trajectory considered.

The effective inertia B_a associated with the fission motion along this trajectory is

$$B_a = \sum_{k,l} B_{q_k q_l}(a) \frac{dq_k}{da} \frac{dq_l}{da}, \qquad (3)$$

where $B_{q_l q_k}$ are components of the inertia tensor and q_k ($k=1,2,\ldots n$) are deformation parameters specifying n-dimensional deformation space admitted in the description of the fission motion.

The fission half life time T_{sf} is calculated from the formula

$$T_{sf} = \frac{\ln 2}{n} \frac{1}{P} \qquad (4)$$

where n is the number of assaults of the nucleus on the fission barrier in time unit and is equal to the frequency $\omega_f/2\pi$ of vibrations in the direction of fission degree of freedom. Further we shall assuming $\hbar\omega_f = 1$ MeV [1 , 2].

There are two basic methods of selecting the path to fission in the case of multidimensional deformation space.

i) The static method. The fission trajectory is taken to be that minimizing the potential energy $V(\{q\})$ [3].

ii) The dynamic method. This method suggested originally in paper [4] and developed for practical approaches in references [2, 5, 6] assumes that the fission path is that which minimizes the total action S_{12}. This allows to include the influence of B_a parameter on the process in a dynamic way. In effect the fission path differs from static one calculated in i) and the penetration probability $\bar{P}$ reaches its higher value leading to the decrease of the spontaneous fission half life T_{sf} [2, 5]. The minimization of S_{12} might be realized in practice by applying Ritz method (see ref.[5, 6]) or by dynamical programing methods (see ref.[2, 5, 6]).

In both cases described above the penetrability $\bar{P}$ is calculated along single path in deformation space.

From the quantum mechanical point of view such a description of the fission process is incomplete. One may consider the fission as a penetration of multidimensional fission barrier going through the all possible paths leading to a fragmentation of the nucleus. Each path should be taken properly with specific weight and the total penetrability should be a sum of all partial probabilities of fragmentation. Here the statistical mechanics comes into play and the method of averaging observables should be used. How to do all of that is the basic problem of our paper.

In Section 2 the method of integration over the paths is proposed and the algorithm of calculating spontaneous fission half lives is described.

Section 3 discuss the results of realistic model calculation. Different effects connected with the applied metropolis algorithm used in evaluating path integrals are considered. The results obtained in present work are compared with other ones derived on the basis of static i) and dynamic ii) approaches (see eq. refs. [1, 2, 5, 6]).

2. PATH INTEGRAL FORMULATION OF FISSION PROCESS

2.1. Path integrals

In this section we follow closely the way presented in paper [7].

Our basic expression is the Euclidean (imaginary time) version of Feynman path integral [7, 8, 9]

$$Z = \int D\bar{q}\; e^{-S[\bar{q}]/\hbar} \tag{5}$$

The role of imaginary time plays an arc length "a" of the trajectory in n-dimensional (deformation) space $\{\bar{q}\}$. The action $S[\bar{q}]$ is calculated on the actual path in deformation space and its form is given by eq. (2).

Making the "a" axis discrete we adopt the following notation

$$\bar{q}(a_j) = \bar{q}_j\,, \qquad j = 0,1,\ldots,N \tag{6}$$

where $-\infty < q_j^k < \infty$, $k=1,\ldots,n$.

The integral (5) reads then

$$Z = \int_{-\infty}^{\infty} \prod_{j=1}^{N} d\bar{q}_j \exp\left(-\frac{1}{\hbar} S\left[\{\bar{q}_j\}\right]\right). \tag{7}$$

The last expression is identical to the partition function for a statistical mechanics problem. The action S which couples nearest neighbour sites on a lattice $\bar{q}_{j-1}$, $\bar{q}_j$ and $\bar{q}_{j+1}$, plays the role of the hamiltonian of the considered system (e.g. a crystal). The Boltzmann factor is

$$e^{-1/\hbar\, S[\bar{q}]}$$

and the Planck constant $\hbar$ is equal to the temperature kT. The limit $\hbar \longrightarrow 0$ picks out the classical configuration of the system (the single classical trajectory in our case).

Having the partition function it is simple to write average of any observable O. In terms of the path integral one has

$$\langle O \rangle = \frac{\int D\bar{q}\ e^{-S/\hbar}\ O(\bar{q})}{\int D\bar{q}\ e^{-S/\hbar}} . \qquad (8)$$

The last form is equivalent to the more explicite expression

$$\langle O \rangle = \frac{\int_{-\infty}^{\infty} \prod_{i=1}^{N} d\bar{q}_i\ O(q_1, q_2, \ldots, q_N)\, e^{-S/\hbar}}{\int_{-\infty}^{\infty} \prod_{i=1}^{N} d\bar{q}_i\ e^{-S/\hbar}} . \qquad (9)$$

Here $d\bar{q}_i$ stays for the product $dq_i^1, dq_i^2, \ldots dq_i^n$.

2.2. Averaged spontaneous fission half life time

In the case of fission the quantity of interest is the spontaneous fission half life time T_{sf} or shorter $\bar{T}_{sf}$ which we define as

$$\bar{T}_{sf} = \frac{\int D\bar{q}\ e^{-S/\hbar}\ T_{sf}[\bar{q}]}{\int D\bar{q}\ e^{-S[\bar{q}]/\hbar}} . \qquad (10)$$

The quantity T_{sf} appearing on the RHS of the formula (10) is the spontaneous fission half life time as calculated in accord to the WKB prescription (4). The equation (10) is a statistical expression which contains all the informations about the nature of the potential energy V and the mass parameters $B_{q_k q_l}(\bar{q})$ entering the expression for the action S (eq. (2)).
All global characteristics and the quantal features of the fission scenery are already contained in (10).

The average $\bar{T}_{sf}$ contains contributions from all possible trajectories to fission each of which contributes with proper weight determined by the action $S[\bar{q}]$.

2.3. Monte Carlo tools

The technique for evaluating the sum over trajectories is based on the Monte Carlo method of Metropolis [7 , 10 , 11 , 12]. In this method an integral of the type

$$\int f(\bar{q})\, D\bar{q} \tag{11}$$

is approximated by a sum of a finite number of terms

$$\sum_i f(\bar{q}_i)\, \Delta\bar{q}_i \tag{12}$$

The points $\bar{q}_i$ in (10) are not selected at random, but are distributed in that region of deformation space giving the dominant contributions to the integral. In the case of integrals given by Eqs.(8-10) the points $\bar{q}_i$ have to be selected according to the distribution

$$P(q)D(\bar{q}) = \frac{\exp\left[-S[\bar{q}]/\hbar\right] D\bar{q}}{\int D\bar{q}\; e^{-S/\hbar}} . \tag{13}$$

If such a selection of $\bar{q}_i$ is done the Monte Carlo estimate O for the observable O simply reduces to an arithmetic average

$$O \cong \frac{1}{M} \sum_{i=1}^{M} T_{sf}(\bar{q}_i), \tag{14}$$

where M is the total number of configurations (trajectories) generated in the Monte Carlo sequence.

The method of selection of important configurations is called "an importance sampling" [7 , 10 , 11]. Its realization is possible using a Markov process to generate M configurations $\{\bar{q}_i\}$ in equation (14). The process is constructed so that in the limit of large M the probability of occurence of a given configuration $\{\bar{q}_i\}$ is done by the Boltzmann distribution (13).

In the following we sketch only the practical rules of the Metropolis algorithm [7] used in evaluating the $\bar{T}_{sf}$ of eq.(10).

Let $\{\bar{q}_j\}$, $j=1,\ldots,N$ denote some initial (e.g. taken at random) trajectory. Let us now select randomly a new value for $\bar{q}_j$ (for a specific j) with uniform probability. Denote this new $\bar{q}_j$ by $r_{\bar{q}_j}$. If the action S is lowered by the replacement of $\bar{q}_j$ by $r_{\bar{q}_j}$ the variable at the site j is set to the new value $r_{\bar{q}_j}$. If however the change $\Delta S \geq 0$ then a random number r' with uniform probability distribution between 0 and 1 is generated and $\bar{q}_j$ is changed to $r_{\bar{q}_j}$ only if

$$\exp(-\Delta S) > r'. \tag{15}$$

In the last expression ΔS denotes the difference

$$\Delta S = S[r_{\bar{q}}] - S[\bar{q}] \tag{16}$$

where $S[r_{\bar{q}}]$ is the new action calculated along the new trajectory passing through the point $r_{\bar{q}_j}$ and S is the action taken along the starting path. If the relation given by eq. (15) is not fulfilled the lattice variables at the site j retain their previous values $\bar{q}_j$ $(= q_j^1, \ldots q_j^n)$.

The next site $(j+1)$ is probed in analogous manner and so on through the lattice. If this is made for all lattice points $j=1,2,\ldots,N$ the one Monte Carlo step is done and a new trajectory $\{\bar{q}_j\}$ is obtained. Repeating this process M times and then using eq. (10) the Monte Carlo average $\bar{T}_{sf}$ can be calculated.

The Metropolis algorithm described above is a one possible method of evaluating the path integral. Among other methods the 'Heat Bath' method is known [3] and 'stochastic quantization' method based on Langevin equation are in use especially in the field theoretical implementations of path integrals [15, 16].

Problems of convergence of the process of generating configurations have been discussed widely in the literature [7, 11, 12, 15] and will be discussed in the concrete case of $\bar{T}_{sf}$ calculation in the next section.

3. REALISTIC CALCULATIONS

3.1. A model

We consider a fission process in a 3-dimensional deformation space $\{\varepsilon_{24}, \Delta_p, \Delta_n\}$ where ε_{24} is an average path to fission in the Nilsson $(\varepsilon_2, \varepsilon_4)$ - space given by [2]

$$\begin{aligned} \varepsilon_2 &= 0(0.05)1.00 \\ \varepsilon_4 &= 0.2\,\varepsilon_2 - 0.06 \end{aligned} \tag{17}$$

The parameters Δ_p and Δ_n are pairing field parameters for protons and neutrons respectively.

The potential energy V of the nucleus is obtained by the Strutinsky [18] prescription

$$V = E_{LD} + (E_{BCS} - \tilde{E}) \tag{18}$$

where E_{LD} is the liquid drop energy and the expression in brackets on the RHS is called a shall correction and it is a difference between the BCS model energy and corresponding 'smooth' energy of the nucleus (see e.g., refs.[4 , 5 , 1]). In the following we do not add a zero point energy to the potential energy surface [19]). Mass parameters B_{ij} are obtained in the cranking approximation. The corresponding formulae is [3 , 4]

$$B_{ij} = 2\hbar^2 \sum_{\nu\nu'} \frac{|\langle\nu|\partial H/\partial q^i|\nu'\rangle|^2}{(E_\nu + E_{\nu'})^3}(u_\nu v_{\nu'} + v_\nu u_{\nu'})^2 + P_{ij}. \tag{19}$$

Here H is the single particle hamiltonian, u_ν and v_ν are the BCS occupancy parameters and E_ν is the quasi particle energy corresponding to the single particle state $|\nu\rangle$. The term P_{ij} describes the effect of the collective motion in the pairing field [4].

A discussion of mass parameters coupled to the neutron and proton degrees of freedom Δn and Δp is given in ref. [17].

The effective mass parameter as appearing in the action S (eq. (2)) reads in our case

$$B = B_{\varepsilon_{24}\varepsilon_{24}} \dot{\varepsilon}_{24}^2 + B_{\Delta_p \Delta_p} \dot{\Delta}_p^2 + B_{\Delta_n \Delta_n} \dot{\Delta}_n^2$$

$$+ 2\left(B_{\varepsilon_{24}\Delta_p} \dot{\varepsilon}_{24} \dot{\Delta}_p + B_{\varepsilon_{24}\Delta_n} \dot{\varepsilon}_{24} \dot{\Delta}_n\right) \qquad (20)$$

where dot means the derivative taken over the path variable 'a'.

One can see that terms of the type $B_{\Delta_p \Delta_n}$ are absent. This is the effect of no mixing between proton and neutron pairing interactions which we assumed here.

3.2. Monte Carlo experiment. Results and discussion

In order to begin the Monte Carlo experiment we have to prepare the starting path to fission. From the calculations done early [2 , 5 , 17] it is known that curves of a physical significance are

i) static trajectory (represented by a dashed line in Fig. 2),
ii) dynamic trajectory (solid line in Fig. 2).

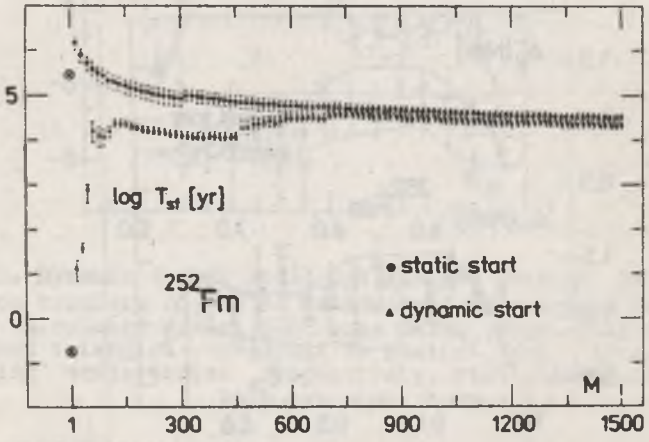

Fig. 1. The convergence of the Metropolis algorithm. Full circles correspond to the logarithm of the averaged spontaneous fission half life time T_{sf} as calculated after M Monte Carlo steps for the case of static starting path. Full triangles give the ln T_{sf} for the dynamic start. Error bars for both cases are also displayed.

This two different starts give us the possibility to check the convergence of the Metropolis algorithm. The convergence process is illustrated in Fig. 1. One can observe the change in the logarithm of the mean value of T_{sf} as calculated after M Monte Carlo steps for both considered cases. On the beginning of the numerical experiment the values corresponding to static and dynamic trajectories differ among themselves on about 6 units in $\log T_{sf}$. After $M \cong 800$ Monte Carlo steps (MCS) both logarithms of averaged T_{sf} values coincide. The corresponding value of $\log T_{sf}$ is equal to 4.70. This result changes to the value 4.40 in the successive 700 MCS. The overlap reached gives an evidence that the Monte Carlo process applied is fairly convergent. However the increasing of M may lead to the unexpected jumps in the $\log T_{sf}$ values which increase slightly the result 4.40. Such a behaviour of the Monte Carlo process is a consequence of the appearance of some "wild" trajectories on which the action S is very large one. This leads in consequence to the increase of average T_{sf}. The influence of such undesired curves can be eliminated after a very long runs of the Monte Carlo program. On the other hand in long runs the periodic nature of the pseudo random

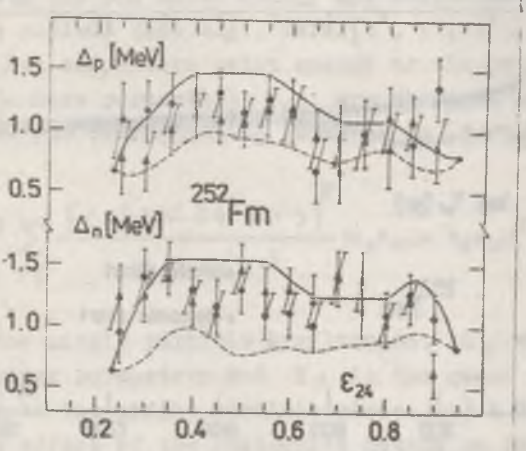

Fig. 2. Dynamic (solid line) and static (dashed line) paths to fission in (ε_{24}, Δ_p, Δ_n) space for ^{252}Fm. Full circles represent the average path to fission as calculated after 1500 Monte Carlo steps starting from the static path. Full triangles represent the average trajectory for which the starting curve was the dynamic path to fission.

number generators may cause the additional complications. Therefore we have stopped the Monte Carlo process at 1500 steps.

All results presented here are obtained for ^{252}Fm nucleus for which the experimentally known value of $\log T_{sf}$ is equal to 2 and our predicted value differs on two units from it. At the same time the Monte Carlo result is smaller than the static value of $\log T_{sf}^{stat} = 5.5$.

Fig. 2 shows starting paths to fission: static (dashed line) and dynamic (solid line). Full circles and full triangles show the average trajectories obtained after M = 1500 MCS starting from static and dynamic curves respectively. Averaged trajectories in $(\varepsilon_{24}, \Delta_p, \Delta_n)$ space differ insignificantly. The corresponding standard deviations are also shown.

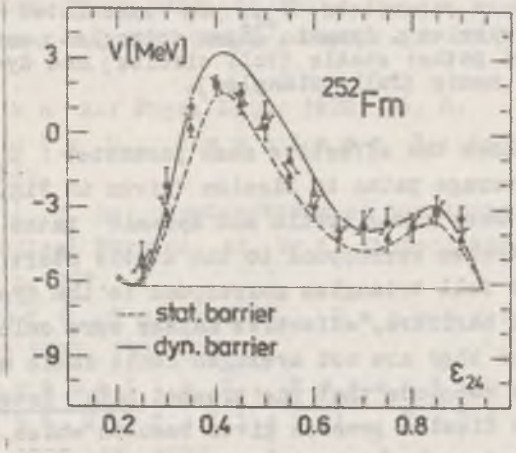

Fig. 3. Dynamic (solid line) and static (dashed line) fission barriers for ^{252}Fm as compared to averaged barriers calculated after 1500 Monte Carlo steps. Full circles and triangles correspond to static and dynamic starting trajectories respectively. Statistical error bars are also shown.

In Fig. 3 corresponding fission barriers are displayed as a function of elongation coordinate ε_{24}. One can see that both averaged barriers agree well within an accuracy given by the standard deviations. Averaged barriers are situated between static and dynamic barriers.

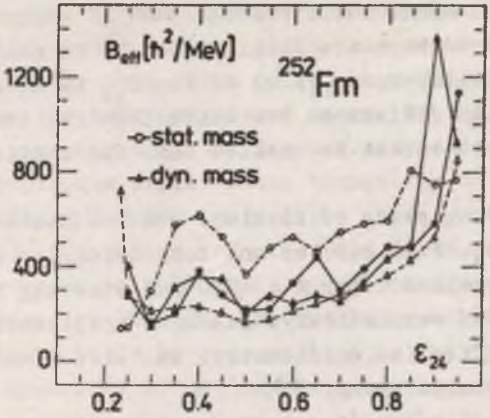

Fig. 4. Effective mass parameters B_{eff} as calculated along static (open circles), dynamic (open triangles) and Monte Carlo averaged paths: static (full circles) and dynamic (full triangles).

The next Fig. 4 shows the effective mass parameter B_{eff} calculated along the average paths to fission (given in Fig. 2) as compared to masses taken along static and dynamic paths to fission. Again, full circles correspond to the static start of Monte Carlo process and full triangles correspond to the dynamic start. In opposition to barriers, effective masses were calculated on average paths and they are not averaged Monte Carlo masses.

It is too early to conclude that the present path integral approach to spontaneous fission process gives results which are better then that reported early [2-5, 17]. However, statistical model of the process may lead to the more correct insight into the fission fenomenon and may indicate the way for many dimensional analysis of it.

The investigations connected to a systematics of spontaneous fission half life times, hights of fission barriers, an asymptotic behaviours of effective masses etc. are in progress.

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STRESZCZENIE

W pracy zaproponowano metodę obliczenia połówkowych czasów życia jąder atomowych ze względu na rozszczepienie spontaniczne stosując formalizm całek po drogach i mechanikę statystyczną. Obliczenia przeprowadzono w trójwymiarowej przestrzeni parametrów Δ_p, Δ_n oraz ε_{24}, gdzie Δ jest przerwą energetyczną typu BCS, a ε_{24} jest parametrem deformacji przestrzennej jądra.

Otrzymane czasy życia są większe niż te, które obliczano wcześniej stosując minimalizację całkowitego działania i biorąc w rezultacie tylko jedną drogę do rozszczepienia.

РЕЗЮМЕ

В работе предлогается метод вычисления времен жизни атомных ядер по отношению к спонтанному делению с применением формализма интегралов по траекториям и статистической механики. Расчеты проводились в трехмерном пространстве параметров Δ_p, Δ_n и ε_{24}, где Δ - это энергетическая шель типа ВКШ, а ε_{24} - параметр пространственной деформации ядра.

Полученные времена жизни больше тех значений, которые вычислялись раньше с помощью минимизации полного действия и рассмотрения только одного канала деления.