JOINT INSTITUTE FOR NUCLEAR RESEARCH
The Bogoliubov Laboratory of Theoretical Physics

FINAL REPORT ON THE SUMMER STUDENT PROGRAM

The application of the reduced density matrix formalism to the problem of decay of metastable state

Supervisor:
Dr. Nikolai Viktorovich Antonenko

Student:
Dmitrii Doroshenko, Russia
Peter the Great St. Petersburg Polytechnic University

Participation period:
June 30 – August 17

Dubna, 2019

Contents

Abstract

The induced nuclear decay is considered as a transport process over the fission barrier underlying dissipative forces. Using quantum master equation for the reduced density matrix, the influence of the number of basis function on the precision of the decay probability and the decay rate of metastable states is studied.

Introduction

A problem of description of an escape of a quantum system from a quasi-stationary state is of interest in various fields of physics: chemical kinetics, diffusion in solids, nucleation, electrical transport, nuclear reactions, etc. The modeling of the escape rate requires the treatment of the dynamics of collective degree of freedom q as a diffusion and dissipative process determined by the interaction of the collective subsystem with the environment formed by many other degrees of freedom [1]. Such a process can be described with the quantum Fokker-Planck diffusion equations or with the Langevin approach or with the path-integral technique, or with the density-matrix formalism. The reduced density matrix for the collective subsystem obeys the following equation [2, 3]:

$$\frac{d}{dt}\rho = -\frac{i}{\hbar}\left[\tilde{H}_c, \rho\right] - \frac{i\lambda_p}{2\hbar}\left[q, \{p, \rho\}_+\right] - \\ -\frac{D_{pp}}{\hbar^2}\left[q,[q,\rho]\right] + \frac{D_{qp}}{\hbar^2}\left[p,[q,\rho]\right] + \left[q,[p,\rho]\right]\frac{D_{qp}}{\hbar^2} \tag{1}$$

where

$$\tilde{H}_c = \frac{1}{2\mu}p^2 + \tilde{U}(q) \tag{2}$$

is the renormalized Hamiltonian which is related to the relevant collective subsystem with the coordinate q and conjugated momentum p, μ is the collective mass parameter, and $\tilde{U}(q)$ is the renormalized collective potential. The renormalization of the potential energy is appeared because of the coupling between the collective subsystem and environment. Here, D_{pp}, D_{qp}, λ_p and are the diffusion coefficient in momentum, mixed diffusion coefficient, and friction coefficient, respectively. Note, that if the subsystem is coupled with the environment through the coordinate, the $D_{pp} = 0$, $D_{qp} = 0$ and $\lambda_p = 0$.

An anharmonic potential $\tilde{U}(q)$ can be approximated at each q by a local harmonic or inverted oscillator potential, using the Taylor expansion up to the second order in q. Since the frequency of local oscillator depends on the coordinate, the obtained diffusion coefficients become coordinate dependent. Therefore, for an anharmonic potential $\tilde{U}(q)$ the use of the constant diffusion coefficients seems to be an approximation which is suitable in the regime of weak dissipation and high temperature.

Our goal is to find the numeric solution of Eq. (1) for modeled potential $\tilde{U}(q) = 0.526q^4 - 0.701q^3 - 1.574q^2$ and to study the escape of initial Gaussian packet from left hand side to right hand side.

Methods

Theoretical realization

To solve the master equation for ρ we can write it in the coordinate representation:

$$\frac{d}{dt}\rho(t,x,y) = L(x,y)\rho(t,x,y) \tag{3}$$

$$L(x,y) = -i\left(\frac{\hbar}{2\mu}\left(\partial_{x,x} - \partial_{y,y}\right) + \tilde{U}(x) - \tilde{U}(y)\right) - \\ -\frac{1}{2}\lambda_p(x-y)\left(\partial_x - \partial_y\right) - \frac{D_{pp}}{\hbar^2}(x-y)^2 - \\ -\frac{i}{\hbar}\left[D_{qp}\left(\partial_x + \partial_y\right)(x-y) + (x-y)\left(\partial_x + \partial_y\right)D_{qp}\right] \tag{4}$$

Making the following coordinate transformations:

$$x = q + \frac{z}{2} \\ y = q - \frac{z}{2} \tag{5}$$

we obtain the equation for reduced density matrix

$$\frac{d}{dt}\rho(t,q,z) = L(q,z)\rho(t,q,z)$$

$$L(q,z) = i\frac{\hbar}{\mu}\partial_{q,z} - iz\tilde{U}'(q) - i\frac{1}{24}z^3\tilde{U}'''(q) - \\ -\lambda_p z\partial_z - \frac{D_{pp}}{\hbar^2}z^2 - \frac{i}{\hbar}\left(D_{qp}z\partial_q + \partial_q z D_{qp}\right) \tag{6}$$

To solve the equation (6) we use oscillator basis:

$$\rho(t,q,z) = \sum_{k=0}^{n} f_k(t,q)B_k(\sigma,z) \\ B_k(\sigma,z) = \frac{i^k}{k!}\left(\frac{k}{2}\right)!e^{-z^2/8\sigma^2}H_k\left(\frac{z}{2\sigma}\right) \tag{7}$$

Solving the master equation we obtain the time-dependent density matrix in coordinate representation and the probability $P(t)$ of penetrability of the Gaussian packet through the barrier at $q = q_b$:

$$P(t)=\int_{q_b}^{\infty}\rho(t,q,0)=\sum_{k=0,2,4,\ldots}\int_{q_b}^{\infty}f_k(t,q)dq \tag{8}$$

as well as the time-dependent probability rate

$$\Lambda(t)=\frac{1}{1-P(t)}\frac{dP(t)}{dt} \tag{9}$$

Practical realization

For solving differential equation previous Wolfram Mathematica program was used. It was checked and debugged. Model potential with the form $\tilde{U}(q)=0.526q^4-0.701q^3-1.574q^2$ are presented on the Figure 1.

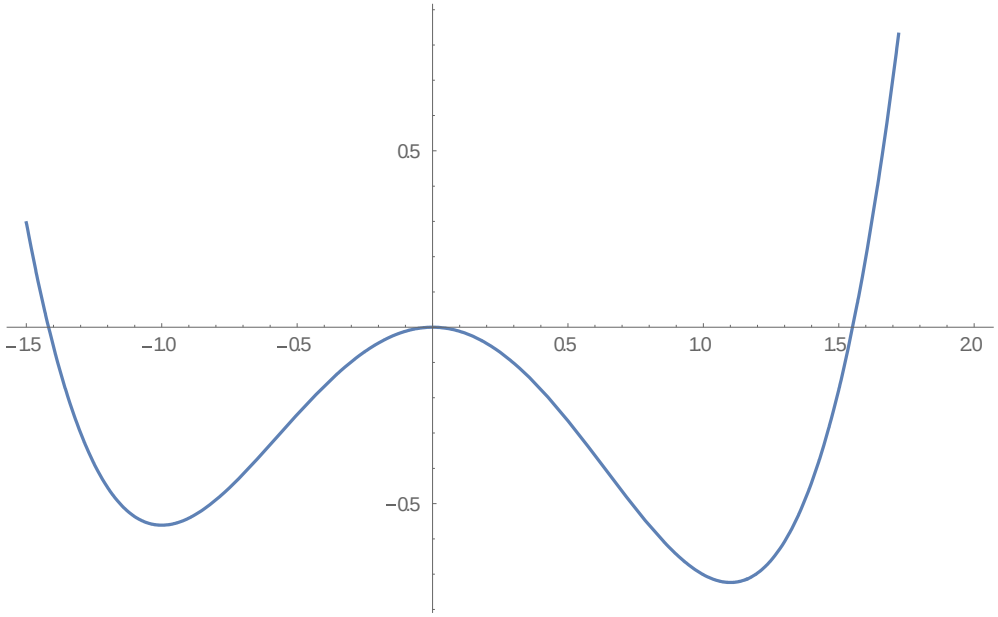

Fig. 1 Model potential

Others initial parameters are $T=1\,MeV$, $p=0\,MeV$, $\hbar\lambda_p=1\,MeV$ and starting point $q_0=-1\,fm$. To check the accuracy of the found solution, we integrate the density matrix over q in all region of the coordinate. Note, that the deviation of this value from unity shows the quality of our calculations. We use different times for the check. The obtained results for different number of basis functions are presented below. Here P_b and P_a means the probabilities at t=0 and t=3, respectively.

21 functions

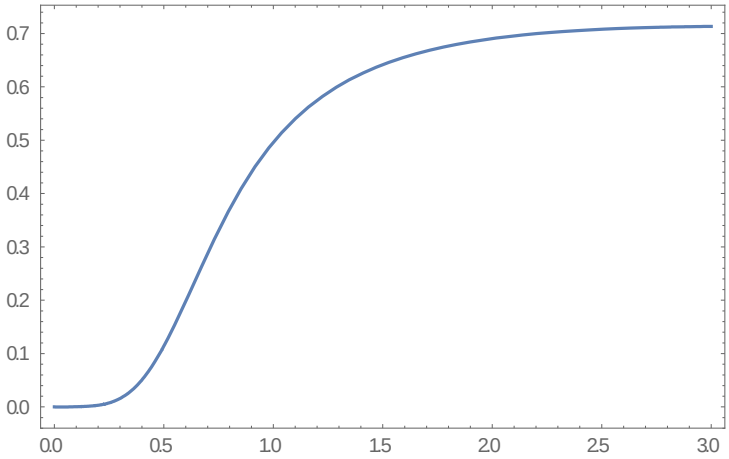

Fig. 2 Probability-time dependence for n=21

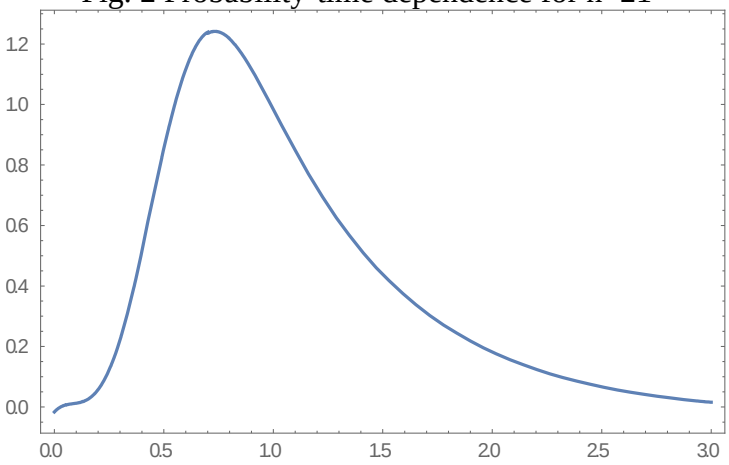

Fig. 3 Probability rate-time dependence for n=21

$P_b = 1$

$P_a = 0.999285$

22 functions

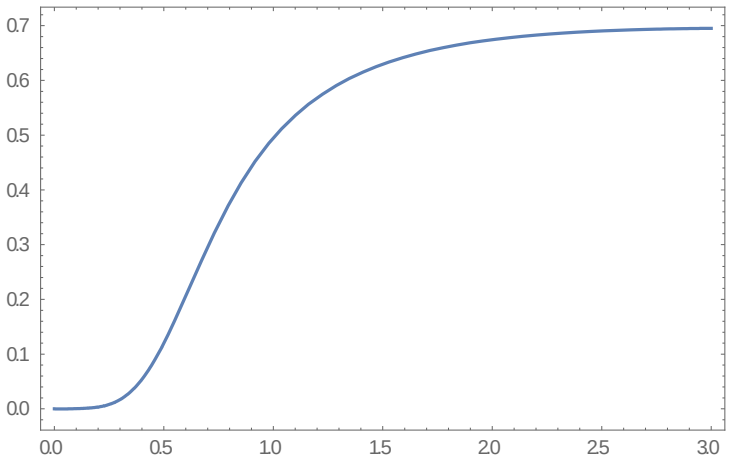

Fig. 4 Probability-time dependence for n=22

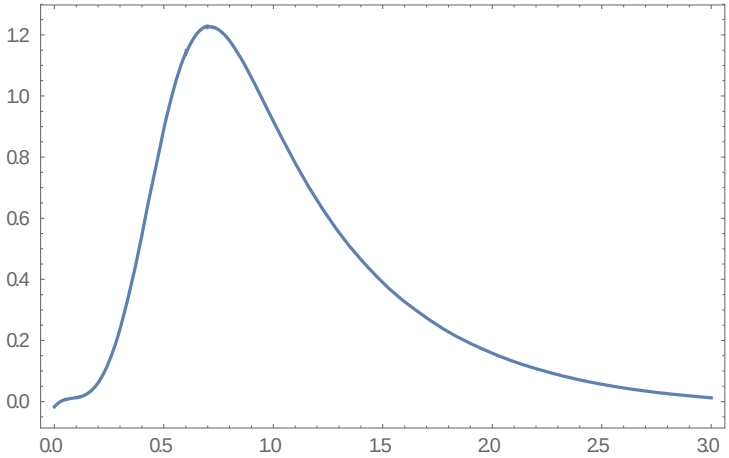

Fig. 5 Probability rate-time dependence for n=22

$P_b = 1$

$P_a = 0.999643$

41 functions

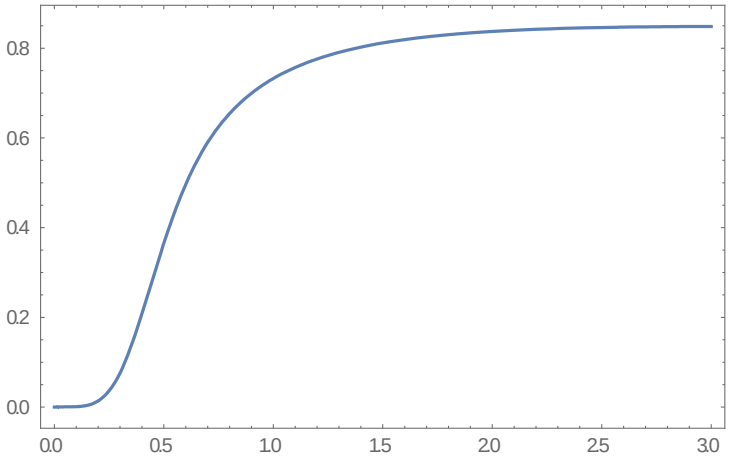

Fig. 6 Probability-time dependence for n=41

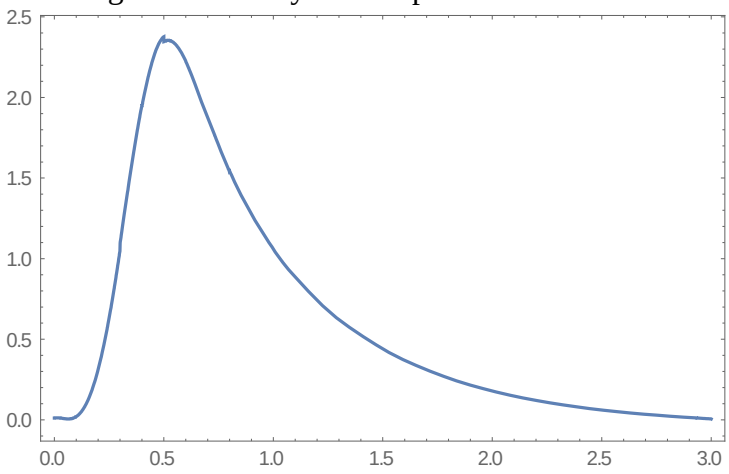

Fig. 7 Probability rate-time dependence for n=41

$P_b = 1$

$P_a = 0.999712$

61 functions

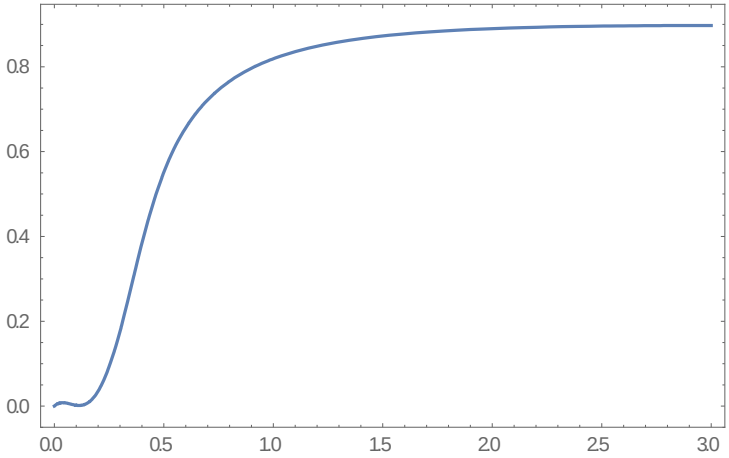

Fig. 8 Probability-time dependence for n=61

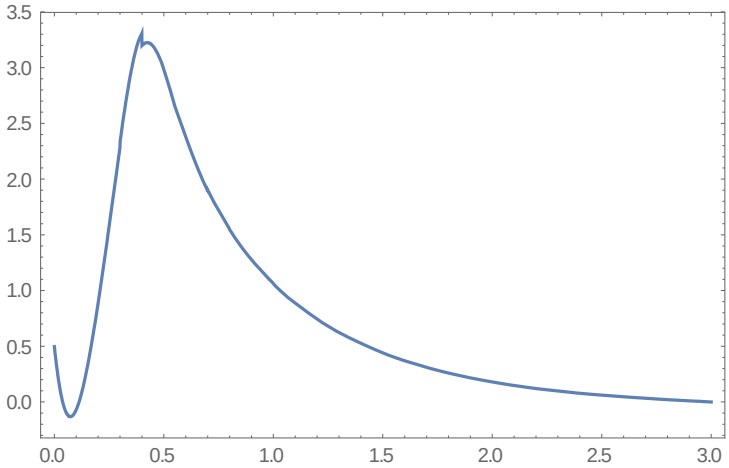

Fig. 9 Probability rate-time dependence for n=61

$$P_b = 1$$

$$P_a = 0.999998$$

Analysis of P_a shows that it tends to 1 when the number of basis function increases, and the optimal number is 61.

Conclusion

The program that calculates the decay probability of the metastable state in the model potential was studied and debugged. It was obtained that:
1. The number of basis function influence on the values of decay probabilities.
2. The results of calculated probabilities become stable with number of basis functions larger than 61.
3. The program can be used to model real physical systems and to study the decay processes in these systems.

References

1.Применение теории открытых квантовых систем к задачам ядерной физики В.В. Саргсян, З. Каноков, Г.Г. Адамян, Н.В. Антоненко Физка элементарных частиц и атомного ядра 2016. Т. 47 Вып. 2

2. Fission rate and transient time with a quantum master equationV. V. Sargsyan, Yu. V. Palchikov, Z. Kanokov, G. G. Adamian, and N. V. AntonenkoPhys. Rev. C **76**, 064604

3.Coordinate-dependent diffusion coefficients: Decay rate in open quantum systems V. V. Sargsyan, Yu. V. Palchikov, Z. Kanokov, G. G. Adamian, and N. V. Antonenko Phys. Rev. A 75, 062115