NUCLEAR DISSIPATIVE DYNAMICS IN LANGEVIN APPROACH

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ABSTRACT

NUCLEAR DISSIPATIVE DYNAMICS IN LANGEVIN APPROACH

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In this thesis Langevin approach is applied to analyze the nuclear dissipative dynamics in fission and fusion reactions. In these investigations, the nuclear elongation coordinate and the corresponding momentum are chosen as collective variables. By considering changes in these variables the decay rate of fission and the formation probability of fusion for heavy ion reactions are calculated. These calculations are performed using simulation techniques and the results thus obtained are compared with the corresponding results of analytic solutions.

Keywords: Dissipative nuclear dynamics, Brownian motion, decay rate, fission, fusion, heavy-ion fusion

ÖZ

LANGEVIN YAKLAŞIMI ÇERÇEVESİNDE ÇEKİRDEKSEL DAĞITICI HAREKETLER

Tanrıverdi, Vedat
Yüksek Lisans, Fizik Bölümü
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Bu tezde fizyon ve füzyon tepkimelerinde çekirdeklerinin çarpışma dinamiğini analiz etmek için Langevin yaklaşımı uygulandı. Bu araştırmalarda nükleer uzama koordinatı ve karşılık gelen momentum kollektif değişkenler olarak seçildi. Bu değişkenlerdeki değişimler göz önüne alınarak fizyonun bozunma hızı ve ağır iyonlar için oluşum olasılığı hesaplandı. Bu hesaplar simülasyon teknikleri kullanılarak yapıldı ve elde edilen sonuçlar analitik çözümlerin sonuçlarıyla karşılaştırıldı.

Anahtar Sözcükler: Atom çekirdeklerinin çarpışma dinamiği, Brown tipi hareket, bozunma hızı, fizyon, füzyon, ağır iyon füzyonu

To My Family...

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CHAPTER 1

INTRODUCTION

It is known that a nucleus is made up with protons and neutrons together known as nucleons. The main difference between them is their charges. Proton is a positively charged particle. On the other hand, neutron is a chargeless particle. In addition, there is a small difference between their masses. Of course their quark structure is different, however this is out of the scope of this thesis. The main interaction between the nucleons is strong interaction and this interaction holds nucleons together in a nucleus [1]. Also there is another interaction between the protons due to the their charges, electromagnetic interaction. Since proton charges are of the same sign, the electromagnetic interaction shows itself as a repulsion. Although the strong force is more powerful than the electromagnetic force, it is short ranged force. On the other hand, the range of electromagnetic force is infinite. So this electromagnetic interaction results with instabilities on nuclei with high atomic number. In order to learn more on these instabilities we should study them from the point of view of energy considerations.

Fig. 1.1 shows the dependence of binding energy per nucleon B/A on the mass number A. It is seen from the figure that for $A > 16$ binding energy per nucleon is in the range 7.3-8.7 MeV. Maximum binding energy is seen around $A \simeq 60$. So a

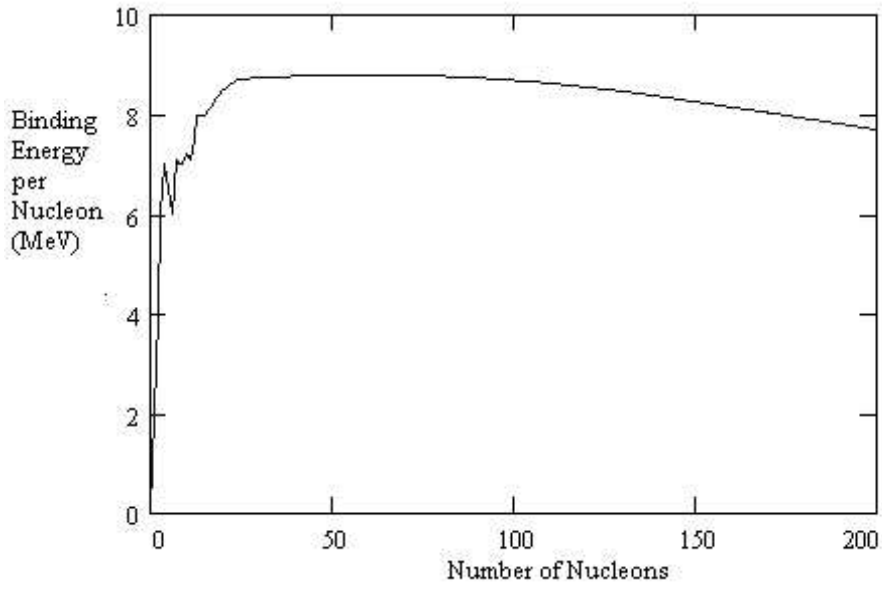

Figure 1.1: *Binding energies per nucleon as function of A.* This figure represents binding energy per nucleon with respect to mass number. The maximum of this figure is seen for $A \simeq 60$. For $A < 60$ there are local maximums, which can be explained by shell model [2].

nucleus with $A \simeq 60$ is more stable than the nuclei $A > 60$. Therefore, if a mother nucleus with mass number $2A$ is divided into two daughter nuclei with mass number A some energy is released, that is the sum of the masses of the daughter nuclei is not equal to the mass of the mother nucleus. The released energy in this process is explained by the Einstein's mass-energy relation $E = mc^2$. This process is called fission. Such a process is observed firstly in the neutron-induced fission in 1939 by O. Hahn and F. Strassman in Germany and explained by L. Meitner as: "After absorbing a neutron, the excited uranium divides into two fragments with about equal masses" [2]. Before this experiment there were other observations about nuclear decays. In 1896 Becquerel observed radioactivity and some other physicist performed other experiments on nuclear decays. However, they had not had the knowledge about structure of atom and quantum physics,

and they had not been able to recognize the physics behind these observations.

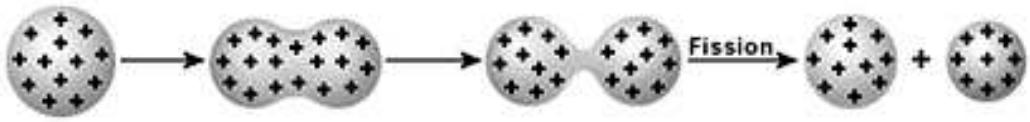

Figure 1.2: *Nuclear deformation in the fission process.* This figure represents fission process schematically. First we see a sphere, which represents a stable mother nucleus. The next ones are drawn to represent fluctuations of this mother nucleus. At the last figure we see two daughter nuclei.

Today it is known that these radioactive processes are nuclear reactions. These nuclear reactions occur due to the interactions between the nucleons. Fission process is represented in Fig. 1.2 schematically. A mother nucleus is firstly fluctuating and after some time these fluctuations overcome the barrier due to the strong interactions and the mother nucleus splits into two daughter nuclei. In fact fission can take place in many different ways, and this figure is only a schematic representation. For a mother nucleus ^{205}At undergoing fission we have 205 interacting particles. Even with the help of computers the solution of such a problem nearly impossible. There are some simulation techniques such as Molecular Dynamics which consider every particle in the system. However, in such a techniques one considers firstly one particle in the system and finds the interaction of this particle with the others by using a potential which defines the interactions between these particles. Then one finds the resultant interaction and then studies the motion of that particle in the effect of this resultant interaction

in the time interval $\triangle t$. One then repeats the same procedure for all particles in the system. By this simulation technique one can find configuration of the system at time t corresponding to an initial condition of the system [3, 4, 5]. In this thesis, we will follow a different approach to this problem.

Before explaining this approach let us turn back to Fig. 1.1. It is noted above that as a result of the binding energy difference, some energy is released in the fission of a nucleus with high mass number. In Fig. 1.1 it is seen that there is also binding energy difference between binding energy per nucleon for nuclei with small mass number if one climbs the curve from low A side. This means that if two small nuclei combine into a nucleus with larger mass number, again some energy is released and this reaction is named fusion process. In this case released energy per nucleon is much larger than that of in the fission process. In fact the source of the energy of the stars is mainly the fusion reactions. Nuclei should firstly overcome the Coulomb barrier to participate in fusion. In the stars fusion takes place with the help of their huge temperature and gravitational attraction. The energy to overcome the Coulomb barrier is high and one of the ways of obtaining this energy is the fission process. Therefore, yet there is no practical way of using fusion in order to obtain energy for everyday life. In this thesis fusion is not considered as an energy supply. We will discuss it to synthesize super heavy elements. So we will deal with heavy ion fusion reactions. In the Fig. 1.3 fusion process and potentials are schematically represented for the formation of super heavy elements. It is seen from the figure that there are two potential barriers. One of them is Coulomb barrier and the other barrier shows

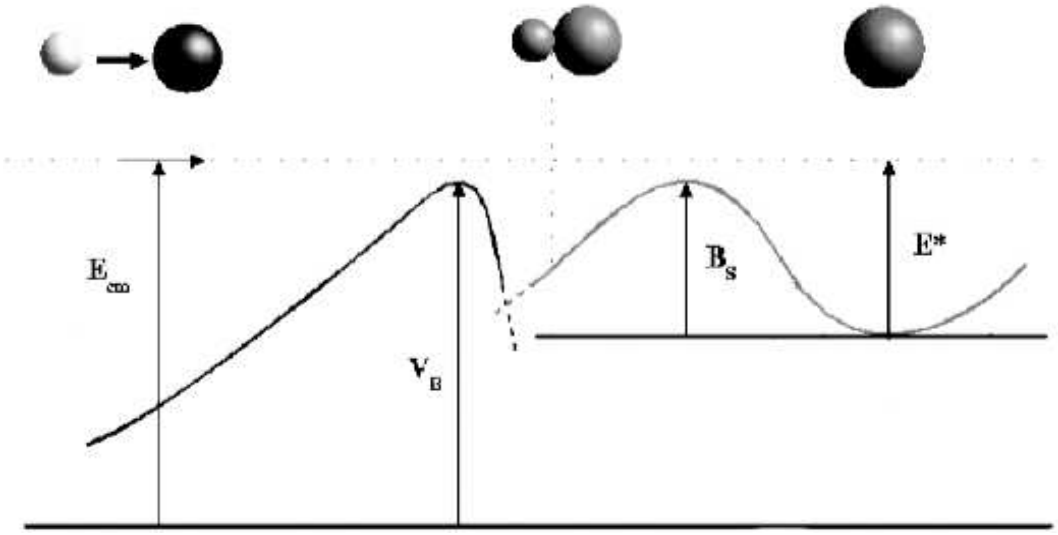

Figure 1.3: *Fusion potentials and shapes of nuclei.* This figure represents shapes and potentials for the fusion process. The drawings at the top represent nuclei in the fusion process with respect to the position. First, we see nuclei which will participate in the fusion. The next one represents touching configuration and the last one represents the product of the fusion process, a stable large nucleus. The curves represent potential for fusion process with respect to the position. The local maximum of the first curve occurs due to the electromagnetic interactions, called the Coulomb barrier. In this figure, its height is shown as V_B. Total energy of nuclei shown with E_{CM} on the left. In the second curve strong interaction is added and the local maximum represents saddle point for the formation. Its height with respect to the local minimum is represented by B_S. Local minimum occurs at the position A, at which energy of stable nucleus is shown by E^* [6].

itself due to the strong interactions in the diffusion process. As a result we can say that to form a super heavy element the system of particles should overcome these two barriers. Therefore, we can say that fusion probability is multiplication of two probabilities: sticking probability that is passing probability of the system over the Coulomb barrier, and formation probability that is passing probability of the system over the barrier due to the strong interaction [7]. Hence fusion probability can be written as

$$P_{fusion} = P_{stick} * P_{form}. \tag{1.1}$$

In this thesis we will deal with only the formation probability. In order to calculate the formation probability we will follow same technical procedure in the case of solution of fission reaction.

In this thesis we will study nuclear dynamics in the framework of Langevin approach which includes fluctuation dissipation theorem. For this purpose Langevin equation is used which is historically first investigated to explain Brownian motion. Brownian motion is firstly examined by the Scottish botanist Robert Brown at 1827 [8]. He discovered that pollens ceaselessly move in a irregular way. However this can not have a biological explanation because pollens are not living things. This subject is later studied by some physicist and now it is known as Brownian motion, which for small dust particles immersed in a fluid occurs due to the random collisions of the dust particles with the molecules of the fluid. Fig. 1.4 shows a two dimensional Brownian motion. One of scientist who studied the Brownian motion is Albert Einstein. Related to this subject Einstein wrote that "I discovered that there would have to be [observable] movement of suspended particles without knowing the observations concerning Brownian motion were already long familiar" in 1905 while investigating atomic theory [9]. Another physicist who studied Brownian motion is Paul Langevin. While studying this subject in order to explain this motion Langevin investigated the following equation

$$m\frac{dv}{dt} = F_f(t) - \beta v. \tag{1.2}$$

This equation is a stochastic equation because it contains the random force $F_f(t)$

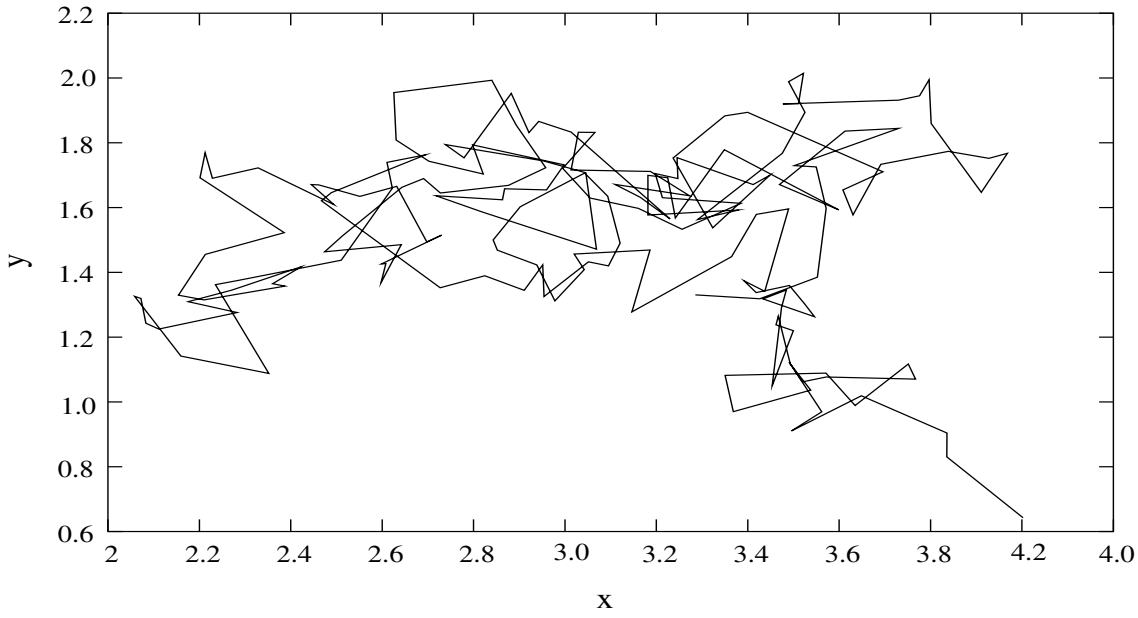

Figure 1.4: *Two-dimensional Brownian motion.* This figure represents two dimensional Brownian motion. The fluctuations of the dust particle results in a change of its position. This zigzag line in the figure shows changes in position of dust particle.

and it has fluctuation and dissipation parts. The relation between these parts should be determined in accordance with the equipartition theorem. In order to solve this equation statistical methods of physics should be used, because random force is known with its statistical properties. Hence Langevin equation can be applied problems having fluctuation and dissipation parts in a statistical way [10, 11]. In this thesis we will apply Langevin equation to the nuclear reactions. Firstly we will choose a Brownian coordinate in the nucleus. The size and the mass associated this coordinate should be larger than those of the medium. In our case the medium or the heat bath consist of nucleons and we take as the Brownian coordinate the distance between the centers of the daughter nuclei in fission process. This coordinate changes as mother nucleus fluctuates. The

elongation coordinate which is the distance between the centers of daughter nuclei is represented schematically in Fig. 1.2. It is noted above that nucleons are held in the nucleus by the strong interaction so there is a potential which effects particles in the nuclear medium due to the interactions between the nucleons. The calculation of this potential is performed by using the liquid drop model because the shape can be used as a parameter during calculations of the potential. In this thesis we employ the potential suggested by Y. Abe et al. [12]. With a few simple considerations we can draw some conclusions on the form of the potential. Firstly, the existence nuclei in nature shows us that there should be a well in the shape of this potential. Secondly since this nucleus can be divided, then there should be a saddle point, representing interaction between the daughter nuclei. Also we know that strong interaction is short ranged, thus away from the saddle point there should be a quick decrease. Hence shape of the potential looks like as in Fig. 1.5. Using this potential we will solve the Langevin equation and calculate decay rate for fission process. In order to calculate the decay rate by simulation we take ensembles which are initially distributed with respect to their elongation coordinate and corresponding momentum. Then the corresponding Brownian particles will move by the effect of the random force and under the friction in the potential which is shown in Fig. 1.5. This motion will continue in time interval $\triangle t$ and after this time interval another random force will effect the Brownian particle. This will be repeated n times and after n step we will reach the Brownian particle's position at time t which is given by $t = n \cdot \triangle t$. Due to the nature of this position we will conclude whether the nucleus is compound

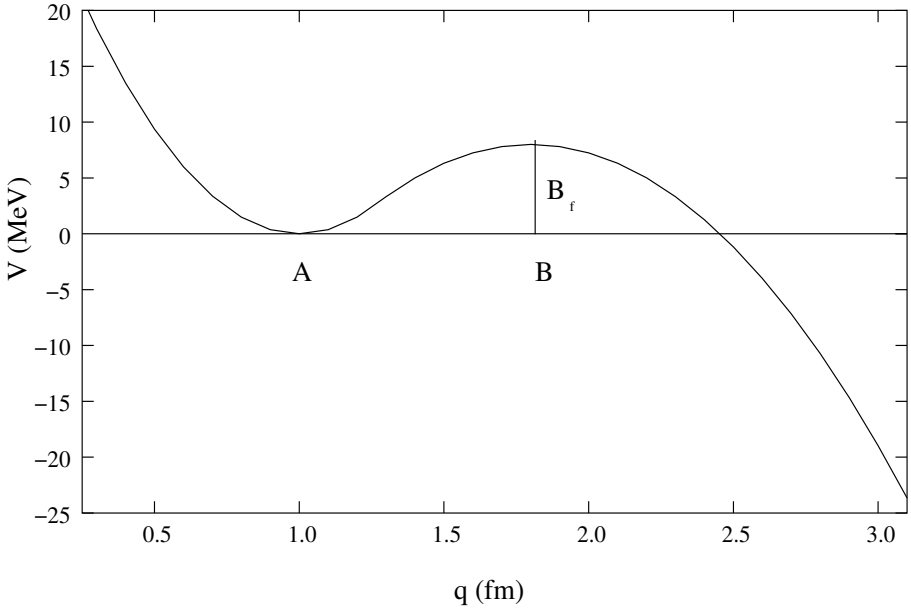

Figure 1.5: *Fission potential.* This figure represents potential with respect to the elongation coordinate for the fission process. Around the local minimum A mother nucleus is stable. Local maximum at B represents saddle point of fission process, and height of this barrier is shown by B_f.

or not i.e. if position of particle is grater than the saddle point, nucleus is not compound and vice versa. We will repeat the same procedure for all ensembles and in order to calculate decay rate we will perform the ensemble average.

In a similar way we will find the passing probability over the barrier for fusion. For this case we will begin with initially sticking two nuclei. In other words we will not include Coulomb barrier in our calculations. This means that there is only one barrier for the potential and if sticken system goes over this barrier, we assume that fusion takes place. Second barrier in the Fig. 1.3 represents this potential barrier. So this is not a realistic fusion probability calculation. This is the calculation of the passing probability over the barrier which occur due to the strong interactions between the nucleons.

CHAPTER 2

FORMALISM

In this chapter, we present the theoretical framework for decay rate and passing probability calculations. We develop firstly Langevin equation and then Fokker-Planck equation and Kramers equation. We give the solution of the Langevin equation and the derivation of the Kramers decay rate.

2.1 Langevin Equation

To develop Langevin equation we start with the motion of a small particle with mass m which is immersed in a fluid. This particle will move under a friction force due to the collisions between that particle and the molecules of the fluid. The expression for this force is given by the Stokes' law

$$F_c = -\beta v \tag{2.1}$$

and equation of motion given by

$$m\frac{dv}{dt} = -\beta v \tag{2.2}$$

where β is friction coefficient. In this motion if the only force is this friction force then particle should stop at some point. However for a small enough particle, dust or Brownian particle, it is known from the Brownian motion that it does not

stop. So to explain this motion we need another force. We insert a fluctuation force into this equation. Hence the equation of motion becomes

$$m\frac{dv}{dt} = F_f(t) - \beta v \tag{2.3}$$

where $F_f(t)$ is fluctuation force. Dividing Eq. (2.3) by mass m we get

$$\frac{dv}{dt} = \Gamma(t) - \gamma v \tag{2.4}$$

where Γ is fluctuating force per unit mass and $\gamma = \frac{\beta}{m}$. In this equation Γ is a stochastic quantity so this equation is a stochastic equation. This stochastic quantity Γ can be known in its average properties. As noted before fluctuating force occurs due to the collisions between the dust particle and the molecules of the fluid. These collisions occur at all directions with equal probability because dust particle is surrounded with the molecules of liquid and these molecules move. Hence we can assume that ensemble average of the fluctuation force given by

$$< \Gamma(t) >= 0. \tag{2.5}$$

Other property of this force is average of multiplications. Average of multiplication of two fluctuation force is given by

$$< \Gamma(t)\Gamma(t') >= 0, \tag{2.6}$$

provided that the duration time τ_0 of a collision is much smaller than the relaxation time $\tau = \frac{1}{\gamma}$ of the velocity of the dust particle. In other words the time passing between two collisions is larger than the time in which the dust particle is contact with the molecule, which plays a role in first collision. However if second collision occur while the interaction, which occurs due to the first collision,

between the dust particle and molecule is still effective, then there is a relation between the average of this multiplication. In the limit $\tau \rightarrow 0$, it is given as

$$< \Gamma(t)\Gamma(t') >= q_k \delta(t - t'). \tag{2.7}$$

In this equation the term on the right hand side q_k will be determined in the later parts of this section. Now we continue with the moments of fluctuation force. Higher moments of this stochastic force can be found in terms of second moments by using properties Gaussian distribution function [13]. Then we obtain

$$\begin{aligned} < \Gamma(t_1)\Gamma(t_2)\ldots\Gamma(t_{2n}) > &= \sum_{i_1 \ldots i_n} < \Gamma(t_{i_1})\Gamma(t_{i_2}) > \ldots < \Gamma(t_{i_{2n-1}})\Gamma(t_{i_{2n}}) > \\ < \Gamma(t_1)\Gamma(t_2)\ldots\Gamma(t_{2n+1}) > &= 0 \end{aligned} \tag{2.8}$$

where sum denotes summations on all possible combinations. Even moments give an expected result as summations of the multiplications of second moments. Here it is assumed that the collisions with three particles, one of them is dust particle and the other two are molecules of the liquid, can be ignorable. On the other hand odd moments vanish because the one of the random force remains and average of it is zero.

Up to this point Langevin equation is obtained in its simple form and the properties of the moments of random force is determined. It is seen that Eq. (2.4) is a differential equation and as noted have an stochastic term. It can be solved by the help of the computer techniques by using the properties of the stochastic term. One of the techniques will be explained in a detailed form in the next chapters. However this stochastic force and its effects on this equation should be determined

in a detailed way. In this equation the velocity shows stochastic properties due to the stochastic force. In the motion of the dust particle, it is assumed that collisions happen one after the other and these collisions show themselves in the Langevin equation as random force and friction. Hence random force and friction force have same microscopic origin. Then there should be a relation between them. This relation can be expressed as the fluctuation dissipation theorem and it can be found by using the fact that Brownian particles come into the equilibrium with the heat bath after some time passed over the contact time. This situation is expressed by Eq. (2.4) and its solution for the initial velocity v_0 is

$$v(t) = v_0 e^{-\gamma t} + \int_0^t e^{-\gamma(t-t')}\Gamma(t')dt'. \tag{2.9}$$

By using Eq. (2.5) and Eq. (2.7) the correlation function of the velocity can be found as

$$< v(t_1)v(t_2) >= v_0^2 e^{-\gamma(t_1+t_2)} + \frac{q_k}{2\gamma}(e^{-\gamma(t_1-t_2)} - e^{-\gamma(t_1+t_2)}). \tag{2.10}$$

For large times, in the case of the equilibration, velocity correlation function reduces to

$$< v(t_1)v(t_2) >= \frac{q_k}{2\gamma} e^{-\gamma(t_1-t_2)}. \tag{2.11}$$

Then in the equilibrium, average energy of the Brownian particle is obtained as

$$\begin{aligned} < E > &= \frac{1}{2} m < [v(t)]^2 > \\ &= \frac{1}{2} m \frac{q_k}{2\gamma} \end{aligned} \tag{2.12}$$

and from the equipartition law of the classical statistical mechanics, average energy is given by

$$< E >= \frac{1}{2}kT. \tag{2.13}$$

Hence the relation between the friction coefficient and the random force obtained as

$$q_k = 2\gamma kT/m. \tag{2.14}$$

Up to this point we considered a dust particle without any potential. If a potential effects to dust particle, another term should be inserted to the equation of motion. This term should have position dependence due to the position dependence of the potential. After inserting this term, derivative of velocity is a function of position in the Langevin equation and we know that velocity is the derivative of position. Then Langevin equation becomes a coupled equation as

$$\begin{aligned} \frac{dp}{dt} &= -\frac{\partial V}{\partial q} - \beta p + F_f(t) \\ \frac{dq}{dt} &= \frac{1}{m}p. \end{aligned} \tag{2.15}$$

With the help of the given properties of the random force Langevin equation can be solved in its simplest form.

2.2 Fokker-Planck Equation and Kramers Equation

In this section Fokker-Planck equation will be derived from the Langevin equation. As noted before in the Langevin equation there is a random force. From Eq. (2.4) it is seen that velocity depends on this force so sadden changes occur in the velocity. This means that velocity is not a continuous quantity. If

it is not a continuous quantity it can be considered in an interval. Taking into account these consideration one can think distribution in the velocity space and for this case Fokker-Planck equation is given as [12]

$$\frac{\partial}{\partial t}w(v,t) = -\frac{\partial}{\partial v}\left[\beta v + \frac{1}{2}\frac{q_k}{m^2}\frac{\partial}{\partial v}\right]w(v,t). \tag{2.16}$$

This equation describes the time evaluation of the distribution function of a Brownian particle and it is an equation of motion for that particle. Now we will derive Fokker-Planck equation by using Langevin equation and starting with Liouville equation [12] which describes the conservation of probability

$$\frac{\partial}{\partial t}w(v,t) + \frac{\partial}{\partial v}\left[\dot{v}w(v,t)\right] = 0. \tag{2.17}$$

This equation corresponds to the continuity equation and it is given in the velocity space. Second term of this equation ,which is the multiplication of time derivative of velocity, gives flow of the probability. The derivative of the velocity can be obtained from the Langevin equation Eq. (2.4) and when this is replaced in the Eq. (2.17) derivative of the distribution obtained as

$$\frac{\partial}{\partial t}w(v,t) = -\Omega(v,t)w(v,t) \tag{2.18}$$

where $\Omega(v,t) = -\frac{\partial}{\partial v}[-\beta v + \frac{1}{m}R(t)]$. Integrating Eq. (2.18) over t between t and $t+\Delta t$ the probability at time $t+\Delta t$ is obtained as

$$\begin{aligned} w(v,t+\Delta t) &= w(v,t) + \int_t^{t+\Delta t} dt_1 \Omega(v,t_1)w(v,t_1) \\ &= \left[1 + \int_t^{t+\Delta t} dt_1 \Omega(v,t_1) \right. \\ &\quad \left. + \int_t^{t+\Delta t} dt_1 \int_t^{t_1} dt_2 \Omega(v,t_1)\Omega(v,t_2) + \ldots\right] w(v,t). \end{aligned} \tag{2.19}$$

This equation contains random force. If its average is taken using the properties Eq. (2.5) and (2.7) we obtain

$$\begin{aligned}\frac{w(v,t+\Delta t)-w(v,t)}{\Delta t} &= \frac{\partial}{\partial v}\beta v w(v,t)+\frac{1}{2}\frac{\partial}{\partial v}\beta v w(v,t)\Delta t \\ &\quad +\frac{1}{2}\frac{q_k}{m^2}\frac{\partial^2}{\partial v^2}w(v,t)+O(\Delta t) \qquad (2.20)\end{aligned}$$

and in the $\lim \Delta t \to 0$

$$\frac{\partial}{\partial t}w(v,t) = -\frac{\partial}{\partial v}\left[\beta v+\frac{1}{2}\frac{q_k}{m^2}\frac{\partial}{\partial v}\right]w(v,t) \qquad (2.21)$$

where q_k is given in Eq. (2.14). With this property Fokker-Planck equation is obtained from the Langevin equation as Eq. (2.16). This means that they are equivalent equations. However their treatments are different. Argument of Fokker-Planck equation is distribution function. On the other hand in the Langevin equation, deterministic equation is used with a random force.

As the next step we consider Brownian motion in a potential. Again by starting with Liouville equation and using Langevin equation Eq. (2.15) we will obtain Kramers equation. This time Liouville equation contains one more term due to the position dependence of the potential and it is given by

$$\frac{\partial}{\partial t}w(p,q,t) = -\frac{\partial}{\partial p}\left[\dot{p}w(p,q,t)\right]-\frac{\partial}{\partial q}\left[\dot{q}w(p,q,t)\right] \qquad (2.22)$$

and putting momentum from Eq. (2.15) to Eq. (2.22) and by integrating it over t, we can find distribution function at time $t+\Delta t$ as

$$\begin{aligned}w(p,q,t+\Delta t) &= w(p,q,t)+\int_t^{t+\Delta t} dt_1 \tilde{\Omega}(p,q,t_1)w(p,q,t_1) \\ &= \left[1+\int_t^{t+\Delta t} dt_1\tilde{\Omega}(p,q,t_1)\right. \qquad (2.23) \\ &\quad \left.+\int_t^{t+\Delta t} dt_1\int_t^{t_1} dt_2\tilde{\Omega}(p,q,t_1)\tilde{\Omega}(p,q,t_2)+\ldots\right]w(p,q,t)\end{aligned}$$

where

$$\tilde{\Omega}(p,q,t) = -\frac{\partial}{\partial v}\left[-\frac{\partial V}{\partial q} - \gamma p + \Gamma(t)\right] - \frac{\partial}{\partial q}\frac{p}{m} \tag{2.24}$$

and similarly taking its average Kramers equation is obtained as

$$\frac{\partial}{\partial t}w(p,q,t) = \left[-\frac{\partial}{\partial q}\frac{p}{m} + \frac{\partial}{\partial p}\frac{\partial V}{\partial q} + \frac{\partial}{\partial p}\left(\beta p + m\beta t\frac{\partial}{\partial p}\right)\right] w(p,q,t). \tag{2.25}$$

This equation can be applied to Brownian systems which contains potential and it was first derived by Kramers and applied to the decay rate of nuclear fission.

2.3 Solution of Langevin Equation

In this section solution of the Langevin equation will be obtained. As noted before it has an stochastic force which rapidly changes, so it has no derivative. Hence this equation can not be solved by the Runge-Kutta method [9] because this method assumes that the equation contains terms with defined derivatives. Then this equation should be solved by other method. We will use iteration method [14]. To solve Langevin equation iteratively we will start with rewriting this equation as

$$\begin{aligned} \frac{dp}{dt} &= h(p,q) + g\Gamma(t) \\ \frac{dq}{dt} &= \frac{1}{m}p \end{aligned} \tag{2.26}$$

where

$$h(p,q) = -\frac{\partial U}{\partial q} - \frac{\tilde{\gamma}}{m}p \tag{2.27}$$

$$g = \sqrt{\tilde{\gamma}kT} \tag{2.28}$$

$$\tilde{\gamma} = m\gamma. \tag{2.29}$$

By integrating Eq. (2.26) over t between t and $t + \Delta t$, the details of which are given in Appendix A, we obtain

$$\begin{aligned} p(t+\tau) - p(t) &= \tau h + \frac{1}{2}\tau^2 \left(\frac{\partial h}{\partial q}\frac{p}{m} + \frac{\partial h}{\partial p} h \right) \\ &+ \frac{1}{6}\tau^3 \frac{\partial^2 h}{\partial q^2}\left(\frac{p}{m}\right)^2 + \frac{\partial h}{\partial p}\left(\frac{\partial h}{\partial q}\frac{p}{m} + \frac{\partial h}{\partial p} \right) + \frac{h}{m}\frac{\partial h}{\partial q} + \dots \\ &+ g\tilde{\Gamma_1}(t) + \frac{\partial h}{\partial p} g\tilde{\Gamma_2}(t) + \left(\frac{\partial^2 h}{\partial p^2} + \frac{1}{m}\frac{\partial h}{\partial q} \right) g\tilde{\Gamma_3}(t) + \dots \end{aligned} \tag{2.30}$$

$$\begin{aligned} q(t+\tau) - q(t) &= \tau \frac{p}{m} + \frac{1}{2}\tau^2 \frac{h}{m} + \frac{1}{6}\tau^3 \frac{1}{m}\left(\frac{\partial h}{\partial q}\frac{p}{m} + \frac{\partial h}{\partial p} h \right) + \dots \\ &+ \frac{g}{m}\tilde{\Gamma_2}(t) + \frac{g}{m}\tilde{\Gamma_3}(t) + \dots \end{aligned} \tag{2.31}$$

where

$$\begin{aligned} \tilde{\Gamma_1}(t) &= \int_t^{t+\tau} dt' \Gamma(t') \\ &= \sqrt{\tau} w_1(t) \end{aligned} \tag{2.32}$$

$$\begin{aligned} \tilde{\Gamma_2}(t) &= \int_0^{\tau} d\tau' \int_t^{t+\tau'} dt' \Gamma(t') \\ &= \tau^{3/2}\left[\frac{1}{2} w_1(t) + \frac{1}{2\sqrt{3}} w_2(t) \right] \end{aligned} \tag{2.33}$$

$$\begin{aligned} \tilde{\Gamma_3}(t) &= \int_0^{\tau} d\tau' \int_0^{\tau'} d\tau'' \int_t^{t+\tau'} dt' \Gamma(t') \\ &= \tau^{5/2}\left[\frac{1}{6} w_1(t) + \frac{1}{3\sqrt{5}} w_3(t) \right]. \end{aligned} \tag{2.34}$$

The details of the second part of this calculation are shown in Appendix B. In this equation $\Gamma(t)$ satisfies

$$\begin{aligned} < \Gamma(t) > &= 0 \\ < \Gamma(t_1)\Gamma(t_2) > &= 2\delta(t_1 - t_2) \end{aligned} \tag{2.35}$$

and $w(t)$ is an Gaussian random number with properties

$$< w > = 0$$

$$< w^2 > \;=\; 2. \tag{2.36}$$

2.4 Derivation of Kramers Decay Rate for Fission

To derive the decay rate we should find probability flow over the barrier j_s and total probability inside the well n_A since decay rate is given by [12, 15]

$$r_K = \frac{j_s}{n_A}. \tag{2.37}$$

To find j_s and n_A we need the quasistationary solution of the Kramers equation Eq. (2.25) and the form of the solution is [12]

$$w(p,q) = W(p,q) \exp\left[-\frac{p^2/2m + U(q)}{T}\right]. \tag{2.38}$$

The potential for the dust particle is

$$U(q) = B_f - \frac{1}{2} m w'^2 (q - q_s)^2 \tag{2.39}$$

where B_f is the barrier height. We obtain $W(p,q)$ from the integration of the distribution function around the saddle point as

$$W(p,q) = N \int_{-\infty}^{u} du' e^{-\frac{\alpha-\gamma}{2m\gamma T} u'^2} \tag{2.40}$$

where

$$u \;=\; p - \alpha(q - q_s) \tag{2.41}$$

$$\alpha \;=\; \frac{\gamma + \sqrt{\gamma^2 + 4m^2 w'^2}}{2} \tag{2.42}$$

and N is the normalization constant. Kramers quasistationary solution is then obtained as

$$w(p,q) = N \int_{-\infty}^{u} du' e^{-\frac{\alpha-\gamma}{2m\gamma T} u'^2} \tag{2.43}$$

Using this we obtain the probability inside the pocket as

$$w_A(p,q) = N\sqrt{2m\gamma\alpha - \gamma}e^{-\frac{p^2/(2m)+U(q)}{T}} \tag{2.44}$$

and using this expression the total probability n_A around A can be calculated as

$$\begin{aligned} n_A &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dpdqw_A(p,q) \\ &= N\sqrt{\frac{2\pi m\gamma T}{\alpha-\gamma}}\frac{2\pi T}{w} \end{aligned} \tag{2.45}$$

with the approximation

$$U(q) \simeq \frac{1}{2}mw^2q^2 \tag{2.46}$$

around A which is minimum of the potential and using quassistationary solution probability flow can be calculated as

$$\begin{aligned} j_s &= \int_{-\infty}^{\infty} dp\frac{p}{m}w(p,q)|_{q=q_s} \\ &= NT\sqrt{\frac{2\pi m\gamma T}{\alpha}}e^{-B_f/T}. \end{aligned} \tag{2.47}$$

Then we obtain the Kramers decay rate as

$$r_k = \frac{w}{2\pi}\left[\sqrt{\tilde{\beta}^2+1} - \tilde{\beta}\right]e^{-B_f/T} \tag{2.48}$$

where

$$\tilde{\beta} = \frac{\beta}{2w'} = \frac{1}{2w'}\frac{\gamma}{m}. \tag{2.49}$$

CHAPTER 3

CALCULATIONS

In this chapter, we give the results of calculations. Firstly we give comparison for the elongation coordinate and corresponding momentum in the free potential case between the results of simulation and analytic calculations. Then we give decay rate results for simulation and Kramers solution. Lastly we give passing probability results for simulation and analytic solution.

3.1 Elongation Coordinate and Corresponding Momentum Calculations

For comparison, we obtain analytic solution of the Langevin equation for free potential case. These calculations are given in Appendix C. The average of p^2 is found as

$$< p^2 >= m \cdot kT \left[1 - e^{-2\frac{\tilde{\gamma}}{m} \cdot t}\right] + p_0^2 e^{-2\frac{\tilde{\gamma}}{m} \cdot t}. \tag{3.1}$$

This solution will be compared with the one obtained by simulation. To simulate Langevin equation we need gaussian random numbers since Langevin force is a random force, and its this property is shown in Fig. 3.1. By using this random force we will find elongation coordinate and corresponding momentum and then we will perform its ensemble average. Comparison of the results of Eq.

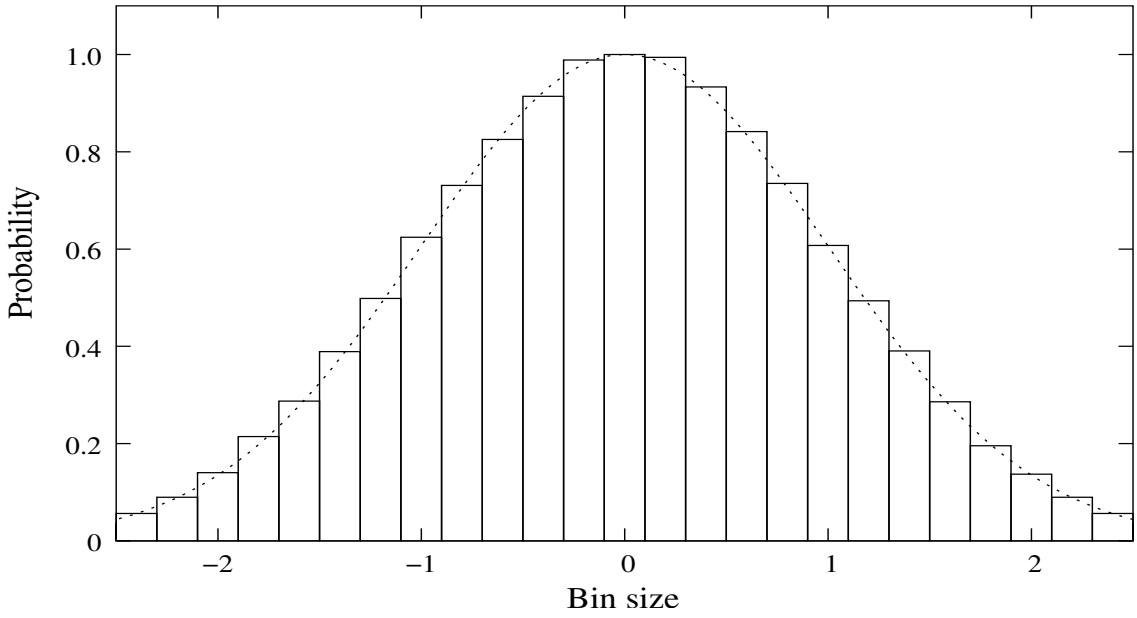

Figure 3.1: *An example Gaussian random number.* In this figure dotted line shows Gaussian distribution. Boxes are drawn by using output of the random number generator for 100000 random numbers.

(3.1) with simulated ones is shown in Fig. 3.2 for p^2.

Now we will solve Langevin equation for the elongation coordinate. The average of $(q-q_0)^2$ for the potential free case is found as

$$< (q-q_0)^2 >= \frac{p_0^2 - 3mkT}{\tilde{\gamma}^2} + \frac{2kT}{\tilde{\gamma}} \cdot t + 2\frac{2mkT - p_0^2}{\tilde{\gamma}^2} \cdot e^{-\frac{\tilde{\gamma}}{m} \cdot t} + \frac{p_0^2 - mkT}{\tilde{\gamma}^2} e^{-2\frac{\tilde{\gamma}}{m} \cdot t}. \quad (3.2)$$

Comparison of the results of Eq. (3.2) with simulated ones is shown in Fig. 3.3 for $(q-q_0)^2$.

These calculations are made for two different initial conditions for $p = 0$ and $p = 2p_{eq}$. Here in fact the results of the simulation for $< p^2 >$ and $< (q-q_0)^2 >$ are obtained simultaneously since the main reason of the change in the position is corresponding momentum and it changes randomly due to the Langevin force. In other words they are coupled equations and they can not be solved separately.

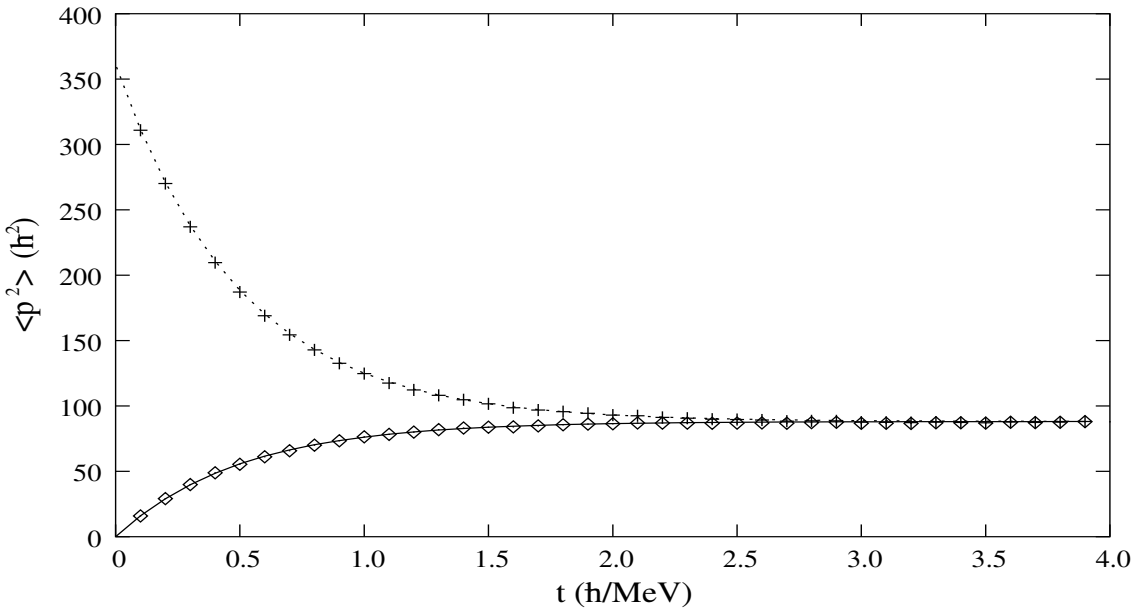

Figure 3.2: $< p^2 >$ *versus time graph.* This figure shows changes in $< p^2 >$ with respect to time for a free Brownian particle. The curve at the bottom is drawn by using analytic solution of $< p^2 >$ for $p_0 = 0$ and the $\diamond$ points show results of simulation. The dotted curve is the analytic solution of $< p^2 >$ for $p_0 = 2p_{eq}$, and the + points show results of simulation. For the simulation 100000 sample are used.

3.2 Decay Rate Calculation

In this section ^{205}At decay rate calculations are given. For the ^{205}At potential is given as [14]

$$V(q,p) = \begin{cases} 37.46(q-1)^2 & 0 < q < 1.27 \\ 8.0 - 18.73(q-1.8)^2 & 1.27 < q. \end{cases} \tag{3.3}$$

This potential is shown in Fig. 1.5. Here $B_f = 8$ MeV and $B = 1.8$. Initial distribution is given by [14]

$$d(q,p) = \begin{cases} N \exp -\frac{[\frac{p^2}{2B} + V(q)]}{kT} & q \leq 1.8 \\ d(q = 1.8) & 1.8 < q \end{cases} \tag{3.4}$$

where N is normalization constant and it is shown in Fig 3.4. Here collective

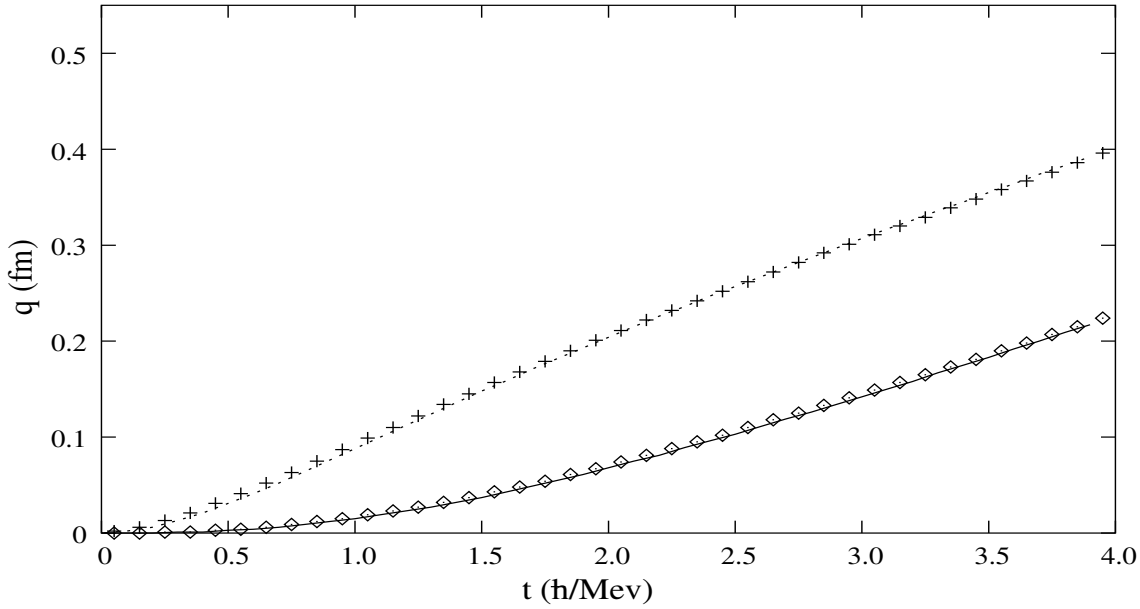

Figure 3.3: $< (q - q_0)^2 >$ *versus time graph.* This figure shows changes in $< (q - q_0)^2 >$ with respect to time for a free Brownian particle. The curve at the bottom is drawn by using analytic solution of $< (q - q_0)^2 >$ for $p_0 = 0$ and the $\diamond$ points show results of simulation. Similarly the dotted curve is the analytic solution of $< (q - q_0)^2 >$ for $p_0 = 2p_{eq}$, and the $+$ points show results of simulation. For the simulation 100000 sample are used.

mass of the elongation is given by $B_c = m_0 = \frac{A^{5/3}}{160}$ $[\frac{\hbar^2}{MeV}]$ and friction coefficient $\tilde{\gamma} = m_0$ $[\hbar]$. Using this initial conditions and parameters to find elongation coordinate and corresponding momentum, iteration method is followed. After finding these at each iteration step, number of compound nuclei is calculated and decay rate is found by using

$$r(t) = -\frac{1}{P_{CN}} \frac{dP_{CN}}{dt} \tag{3.5}$$

where P_{CN} is total number of compound nucleus at each iteration step. The result of the simulation is given in the Fig. 3.5. The result is compared with the

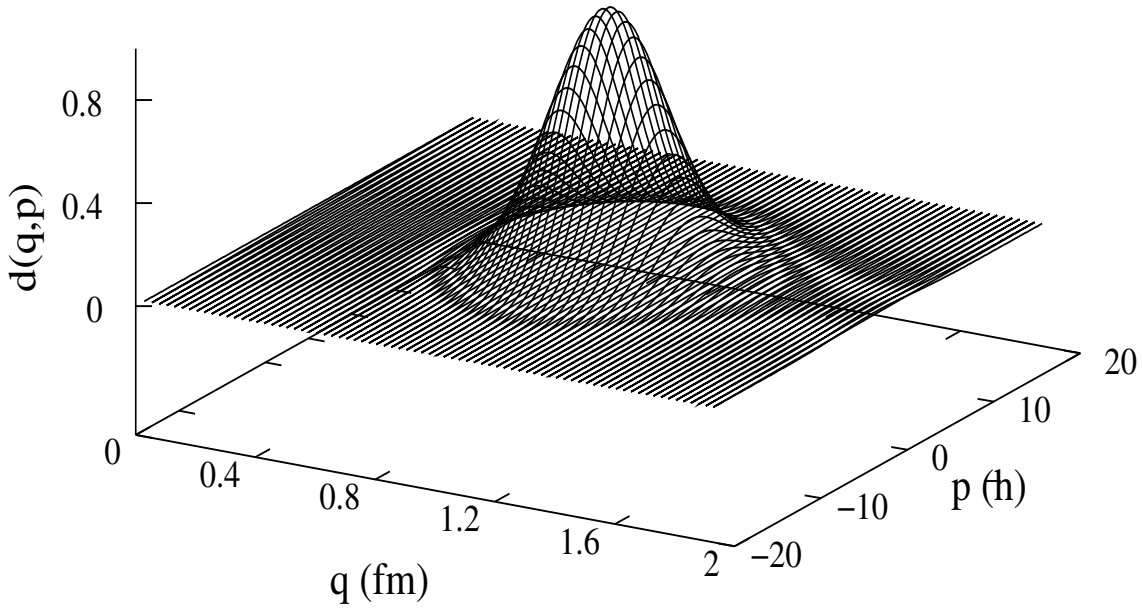

Figure 3.4: *Initial distribution.* This figure shows initial distribution with respect to elongation coordinate and corresponding momentum. In this distribution if we take corresponding momentum as zero mean of elongation coordinate occur at 1 and if we take elongation coordinate as 1 mean of corresponding momentum occur at zero.

result of Kramers decay rate formula

$$r_k = \frac{\hbar w}{2\pi\hbar w'}\left(\sqrt{(\hbar w')^2 + \left(\frac{\tilde{\gamma}}{2B_c}\right)^2} - \frac{\tilde{\gamma}}{2B_c}\right) e^{-\frac{V_s}{kT}} \tag{3.6}$$

where

$$\hbar w = \hbar\sqrt{\left|\frac{\partial^2 V}{\partial q^2}\right|_{q=1}/B_c} \tag{3.7}$$

$$\hbar w' = \hbar\sqrt{\left|\frac{\partial^2 V}{\partial q^2}\right|_{q=1.8}/B_c}, \tag{3.8}$$

V_s is the barrier height and $kT = \sqrt{E^*/a}$. The excitation energy E* is taken to be 80 MeV and level density parameter a to be A/10. The given Kramers equation is valid only for $\frac{\tilde{\gamma}}{B} > \frac{\hbar w kT}{V_s}$.

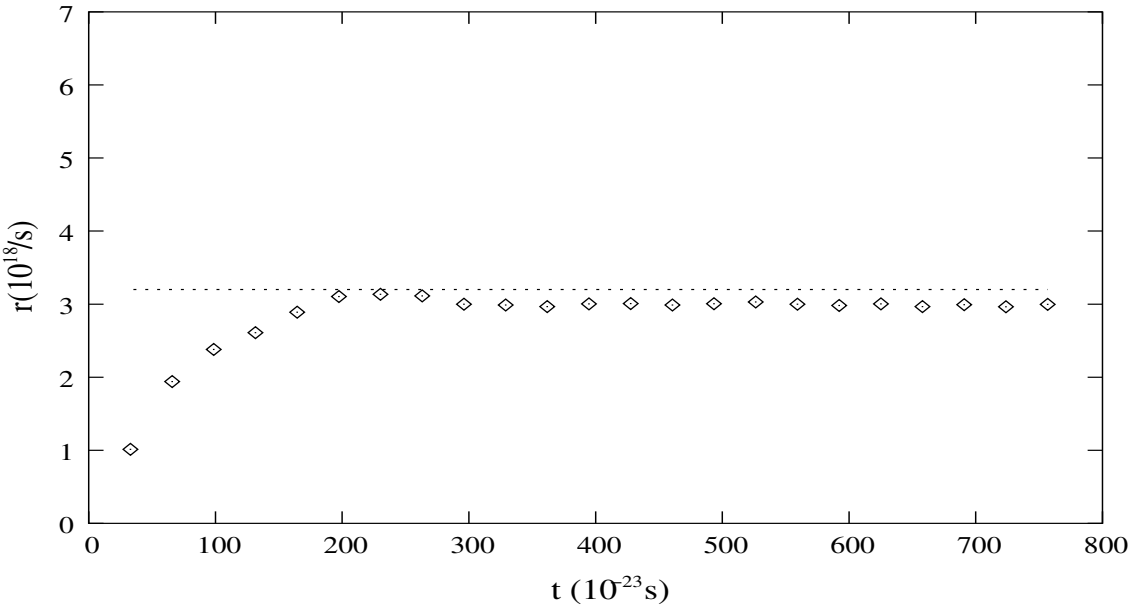

Figure 3.5: *Decay rate calculation.* This figure shows change in the decay rate with respect to time. In the figure dashed line shows the result of decay rate calculation by using Kramers formula. The $\diamond$ points show simulation results performed using Langevin approach.

3.3 Formation Probability Calculation for Fusion

Langevin equation can also be applied to calculate the fusion probability. As expressed before there are two parts of fusion probability. In this paper we calculate only one part of it which refers to the passing probability over the barrier. Here we take barrier as an inverted parabola. We find an analytic solution and results of analytic solution and the solution obtained by simulation are compared. To find analytic solution we start with the eigencoordinates, which read with $p_1 = \dot{q_1}$

$$X = \frac{\beta_1' + \beta_1}{2} q_1 + p_1$$
$$Y = \frac{\beta_1 - \beta_1'}{2} q_1 + p_1 \tag{3.9}$$

where β_1 is the friction coefficent and $\beta_1' = \sqrt{\beta_1^2 + 4w_1^2}$ with $\hbar w_1 = 1$ MeV. Then the Euler type variables are defined as

$$\begin{aligned} x &= Xe^{-at} - X_0 \\ &= \sqrt{2T\beta_1/m_1}\int_0^t d\tau e^{-a\tau} v_1(\tau) \\ y &= Ye^{-bt} - Y_0 \\ &= \sqrt{2T\beta_1/m_1}\int_0^t d\tau e^{-b\tau} v_1(\tau) \end{aligned} \tag{3.10}$$

where $a = (\beta_1' - \beta_1)/2$ and $b = -(\beta_1' + \beta_1)/2$. Here Euler type variables are Gaussian random variables and have the properties[16]

$$\begin{aligned} < x^2(t) > &= \frac{T\beta_1}{am_1}(1 - e^{-2at}) \\ < y^2(t) > &= \frac{T\beta_1}{bm_1}(1 - e^{-2bt}) \\ < x(t)y(t) > &= \frac{2T\beta_1}{(a+b)m_1}(1 - e^{-(a+b)t}). \end{aligned} \tag{3.11}$$

For the evaluation of passing probability over the barrier there should be Gaussian distribution function as

$$W(q_1, t; q_{10}, p_{10}) = \frac{1}{\sqrt{2\pi}\sigma_{q_1}(t)} \exp - \frac{[q_1 - < q_1(t) >]^2}{2\sigma_{q_1}^2(t)}. \tag{3.12}$$

From the eigencoordinates equation one can get q as

$$q_1 = \frac{1}{\beta_1'}(xe^{at} - ye^{bt}) + \frac{1}{\beta_1'}(X_0 e^{at} - Y_0 e^{bt}). \tag{3.13}$$

In this equation the first part corresponds to the diffusion and second part corresponds to the average trajectory of the Brownian particle. By using Eq. (3.13) $< q_1 >$ and $\sigma_{q_1}^2(t)$ obtained as

$$< q_1(t) >= q_{10} e^{\beta_1 t/2} \left[\cosh \frac{\beta_1' t}{2} + \frac{\beta_1}{\beta_1'} \sinh \frac{\beta_1' t}{2}\right] + \frac{2p_{10}}{\beta_1'} e^{-\beta_1 t/2} \sinh \frac{\beta_1' t}{2} \tag{3.14}$$

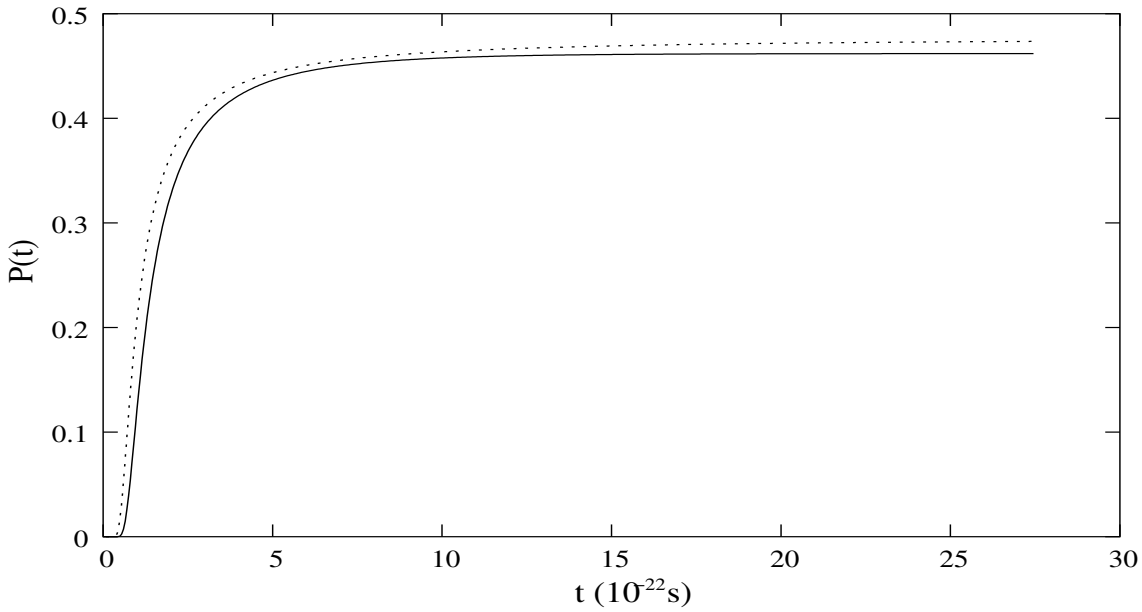

Figure 3.6: *Passing probability for the fusion.* This figure represents formation probability of the fusion process. The full curve is the analytic solution and the dashed curve shows the results of simulation.

and

$$\begin{aligned}\sigma^2_{q_1}(t) &= < q_1^2 > - < q_1 >^2 \\ &= -\frac{T}{m_1 w_1^2} 1 - e^{-\beta_1 t} \left[\frac{2\beta_1^2}{\beta_1'^2} \sinh^2(\frac{\beta_1' t}{2}) + \frac{\beta_1}{\beta_1'} \sinh(\beta_1' t) + 1 \right]. \quad (3.15)\end{aligned}$$

Using these equations one can easily obtain passing probability over the barrier as

$$\begin{aligned}P(t; q_{10}, p_{10}) &= \int_0^{+\infty} W(q_1, t; q_{10}, p_{10}) dq_1 \\ &= \frac{1}{2} erfc \left(-\frac{< q_1(t) >}{\sqrt{2}\sigma_{q_1}(t)} \right) \quad (3.16)\end{aligned}$$

The results of analytic solution and simulation are given in Fig. 3.6.

CHAPTER 4

CONCLUSION

In this thesis we have tried to apply Langevin approach, which was originally proposed to explain the Brownian motion, to nuclear dissipative dynamics by choosing observable variables, elongation coordinate and corresponding momentum. As a check point of these calculations we compare the results of simulation with the results of analytic solution. In Fig. 3.2 and Fig. 3.3, we see that the results are very close to each other for free potential case. This means that Langevin approach is a self-consistent approach. Also in Fig. 3.2 we see that for two different initial values of corresponding momentum, at large times $< p^2 >$ reaches a constant value, which is equal to the equilibrium solution $p_{eq} = \sqrt{m \cdot kT}$. In other words if a small enough particle, which is bigger than the particles or molecules of the medium, enters in a fluid medium, in the equilibrium it has some momentum. The ensemble average of this momentum can be found by using equipartition law. As a result of this momentum there should be change in the position of this dust particle in the equilibrium. This change is shown in Fig. 3.3 and we see that it increases with time as expected.

As a next step we calculated the decay rate for fission in this model. The results in Fig. 3.5 are obtained by using two different methods. One of them is

Kramers decay rate calculation and the other is calculated with the simulation technique by using Langevin approach. There is a small difference between them. This difference raises due to not considering asymmetries in the mother nucleus during its fluctuations and taking friction as a constant value.

Lastly we calculated formation probability in the fusion process. Results are shown in Fig. 3.6. There is a small difference between the result of analytic solution and simulation. Again friction and mass asymmetry is a problem. As noted before this is not a realistic calculation. For a realistic calculation one may obtain better results using more realistic parameters in the simulation. Also there are some better and more realistic calculations [17, 18].

It is noted above that in the fluctuation dissipation theorem fluctuations and dissipation have same microscopic origin. Fluctuations show themselves in the Langevin equation as a stochastic force and dissipation shows itself as friction and the relation between them is found in Eq.(2.14) by using equipartition law. However this an only a relation, so we do not know them exactly. There are some reviews on the calculations of them from microscopic Hamiltonian [19, 20]. Also we considered a constant friction in our calculations which is an approximation. In fact it does not have a constant value because during the fluctuations shape of mother nucleus changes and this should effect the friction.

As a result of these calculations we can say that Langevin approach is a self-consistent approach and it can be applied to nuclear dissipative dynamics. By this approach we can calculate decay rates of different nuclei. Also this approach can be applied to dynamic systems where the dynamics of the system arises from

collisions of small particles. In fact there are some applications of this approach to current in an electrical circuit, electrical field in a laser and to other similar systems [13].

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APPENDIX A

ELONGATION COORDINATE AND CORRESPONDING MOMENTUM EQUATIONS

Here we will obtain two equations for elongation coordinate and corresponding momentum which will be used to simulate them. To find corresponding momentum at time $t+\tau$ we integrate momentum part of Langevin equation given in Eq. (2.15)

$$p(t+\tau) - p(t) = \int_t^{t+\tau} dt' h(p', q') + \int_t^{t+\tau} dt' g\Gamma(t') \tag{A.1}$$

where

$$h(p', q') = h(p, q) + \frac{\partial h}{\partial p}(p' - p) + \frac{\partial h}{\partial q}(q' - q) + \frac{1}{2}\frac{\partial^2 h}{\partial q^2}(q' - q)^2. \tag{A.2}$$

Here h, q, p, q' and p' denote $h(p, q)$, $q(t)$, $p(t)$, $q(t') = q(t+\tau)$ and $p(t') = p(t+\tau)$ respectively. In Eq. (A.1) we replace $h(p', q')$ with Eq. (A.2) and we obtain

$$\begin{aligned} p(t+\tau) - p(t) &= \int_t^{t+\tau} dt' \left[h(p, q) + \frac{\partial h}{\partial p}(p' - p) + \frac{\partial h}{\partial q}(q' - q) + \frac{1}{2}\frac{\partial^2 h}{\partial q^2}(q' - q)^2 \right] \\ &\quad + \int_t^{t+\tau} dt' g\Gamma(t'). \end{aligned} \tag{A.3}$$

Then by replacing $p' - p$ with Eq. (A.1) and using

$$q' - q = \frac{1}{m}\int_t^{t+t'} dt'' p(t'') \tag{A.4}$$

we rewrite Eq. (A.3) as

$$p(t+\tau)-p(t)=\int_t^{t+\tau}dt' \qquad \left[h(p,q)+\frac{\partial h}{\partial p}\int_t^{t+t'}dt''h(p'',q'')+\int_t^{t+t'}dt''g\Gamma(t'')\right.$$
$$\left.+\frac{\partial h}{\partial q}\frac{1}{m}\int_t^{t+t'}dt''p(t'')+\frac{1}{2}\frac{\partial^2 h}{\partial q^2}\left(\frac{1}{m}\int_t^{t+t'}dt''p(t'')\right)^2\right]$$
$$+\int_t^{t+\tau}dt'g\Gamma(t'). \tag{A.5}$$

Similarly by replacing $p(t')$ and $h(p',q')$ with Eq. (A.1) and Eq. (A.2) respectively we obtain

$$\begin{aligned}
p(t+\tau)-p(t) &= \int_t^{t+\tau}dt'h(p,q)+\frac{\partial h}{\partial p}\int_t^{t+\tau}dt'\int_t^{t+t'}dt''h(p,q)\\
&+\left(\frac{\partial h}{\partial p}\right)^2\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\int_t^{t+t''}dt'''[h(p,q)+\ldots]\\
&+\left(\frac{\partial h}{\partial p}\right)^2\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\int_t^{t+t''}dt'''\Gamma(t''')\\
&+\frac{1}{m}\frac{\partial h}{\partial q}\frac{\partial h}{\partial p}\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\int_t^{t+t''}dt'''[p+\ldots]\\
&+\frac{1}{2m^2}\frac{\partial^2 h}{\partial q^2}\frac{\partial h}{\partial p}\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\left[\int_t^{t+t''}dt'''(p+\ldots)\right]^2\\
&+\int_t^{t+\tau}dt'g\Gamma(t')+\frac{\partial h}{\partial q}\frac{1}{m}\int_t^{t+\tau}dt'\int_t^{t+t'}dt''p\\
&+\frac{\partial h}{\partial q}\frac{1}{m}\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\int_t^{t+t''}dt'''[h(q,p)+\ldots]\\
&+\frac{\partial h}{\partial p}g\int_t^{t+\tau}dt'\int_t^{t+t'}dt''\Gamma(t'')+\frac{1}{2m^2}\frac{\partial^2 h}{\partial q^2}\int_t^{t+\tau}dt'\left[\int_t^{t+t'}dt''p\right]^2\\
&+\ldots,
\end{aligned} \tag{A.6}$$

and finally by performing the integrations we arrive at

$$\begin{aligned}
p(t+\tau)-p(t) &= \tau h(p,q)+\frac{1}{2}\tau^2\left[\frac{\partial h}{\partial p}h(p,q)+\frac{\partial h}{\partial q}\frac{p}{m}\right]\\
&+\frac{1}{6}\tau^3\left[\frac{\partial h}{\partial p}\left(\frac{\partial h}{\partial p}h(p,q)+\frac{\partial h}{\partial q}\frac{p}{m}\right)+\frac{\partial h}{\partial q}\frac{1}{m}h(p,q)+\frac{\partial^2 h}{\partial q^2}\left(\frac{p}{m}\right)^2\right]+\ldots\\
&+g\tilde{\Gamma}_1(t)+\frac{\partial h}{\partial p}g\tilde{\Gamma}_2(t)+\left[\left(\frac{\partial h}{\partial p}\right)^2+\frac{\partial h}{\partial q}\frac{1}{m}\right]g\tilde{\Gamma}_3(t)+\ldots
\end{aligned} \tag{A.7}$$

where $\tilde{\Gamma}$'s are given in the formalism chapter and they are determined in the Appendix B. Now we will obtain an equation for the elongation coordinate similarly for potential free case. To do this firstly we perform integral of the second part of the Langevin equation

$$q(t+\tau) - q(t) = \frac{1}{m}\int_t^{t+\tau} dt' p(t') \tag{A.8}$$

and replacing $p(t')$ with Eq. (A.1) we obtain

$$q(t+\tau) - q(t) = \frac{1}{m}\int_t^{t+\tau} dt' \left[p + \int_t^{t+t'} dt'' h(p'', q'') + \int_t^{t+t'} dt'' g\Gamma(t'') \right]. \tag{A.9}$$

Similarly putting $h(p'', q'')$ from Eq. (A.2) gives

$$\begin{aligned} q(t+\tau) - q(t) = \frac{p}{m}\int_t^{t+\tau} dt' \quad &+ \quad \frac{1}{m}\int_t^{t+\tau} dt' \int_t^{t+t'} dt'' g\Gamma(t'') \\ + \frac{1}{m}\int_t^{t+\tau} \quad dt' \quad &\int_t^{t+t'} dt'' \left[h(p,q) + \frac{\partial h}{\partial p}(p''-p) \right. \\ &+ \quad \left. \frac{\partial h}{\partial q}(q''-q) + \frac{1}{2}\frac{\partial^2 h}{\partial q^2}(q''-q)^2 \right]. \end{aligned} \tag{A.10}$$

With further manipulation we obtain

$$\begin{aligned} q(t+\tau) - q(t) \quad = \quad & \frac{p}{m}\int_t^{t+\tau} dt' + \frac{1}{m}\int_t^{t+\tau} dt' \int_t^{t+t'} dt'' g\Gamma(t'') \\ & + \int_t^{t+\tau} dt' \int_t^{t+t'} dt'' \frac{h(p,q)}{m} \\ & + \frac{1}{m}\frac{\partial h}{\partial p}\int_t^{t+\tau} dt' \int_t^{t+t'} dt'' \int_t^{t+t''} dt''' [h(p,q) + \ldots] \\ & + \frac{g}{m}\frac{\partial h}{\partial p}\int_t^{t+\tau} dt' \int_t^{t+t'} dt'' \int_t^{t+t''} dt''' \Gamma(t''') \\ & + \frac{1}{m^2}\frac{\partial h}{\partial q}\int_t^{t+\tau} dt' \int_t^{t+t'} dt'' \int_t^{t+t''} dt''' [p + \ldots], \end{aligned} \tag{A.11}$$

and then finally by performing the integrations we arrive at

$$\begin{aligned} q(t+\tau) - q(t) \quad = \quad & \tau\frac{p}{m} + \frac{1}{2}\tau^2\frac{h(p,q)}{m} + \frac{1}{6}\tau^3\frac{1}{m}\left[\frac{\partial h}{\partial p}h(p,q) + \frac{\partial h}{\partial q}\frac{p}{m}\right] + \ldots \\ & + \frac{g}{m}\tilde{\Gamma}_2(t) + \frac{\partial h}{\partial p}\frac{g}{m}\tilde{\Gamma}_3(t) + \ldots. \end{aligned} \tag{A.12}$$

APPENDIX B

INTEGRALS OF RANDOM FORCE

Here we will find integrations of Γ in terms of w which is a Gaussian random number and properties of it are given in Eq. (2.36). Firstly we start with the definition

$$\tilde{\Gamma_1}(t) = \int_t^{t+\tau} dt' \Gamma(t') = \sqrt{\tau} w_1(t), \tag{B.1}$$

thus

$$\begin{aligned} < \tilde{\Gamma_1}(t)\tilde{\Gamma_1}(t) > &= \int_0^\tau d\tau' \int_0^\tau dt' < \Gamma(\tau')\Gamma(t') > \\ &= \int_0^\tau d\tau' \int_0^\tau dt' 2\delta(t'-\tau') \\ &= 2\tau. \end{aligned} \tag{B.2}$$

Now we will find $\tilde{\Gamma}_2(t)$ which is

$$\tilde{\Gamma_2}(t) = \int_0^\tau dt' \int_t^{t+t'} dt'' \Gamma(t''). \tag{B.3}$$

To find it in terms of w, we start with average of its square

$$\begin{aligned} < \tilde{\Gamma_2}(t)\tilde{\Gamma_2}(t) > &= \int_0^\tau d\tau' \int_t^{t+\tau} dt' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' < \Gamma(t')\Gamma(\xi') > \\ &= \int_0^\tau d\tau' \int_t^{t+\tau'} dt' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' 2\delta(t'-\xi') \\ &= \frac{2}{3}\tau^3 \end{aligned} \tag{B.4}$$

and we write $\tilde{\Gamma}_2(t)$ in term of w's as

$$\tilde{\Gamma_2}(t) = \tau^{3/2}\left[a_1 w_1(t) + a_2 w_2(t)\right] \tag{B.5}$$

and we take average of $\tilde{\Gamma_1}(t)\tilde{\Gamma_2}(t)$ by using integral and w representation to find a_1. We start with

$$\begin{aligned} < \tilde{\Gamma_1}(t)\tilde{\Gamma_2}(t) > &= < \left[\tau^{1/2} w_1(t)\right]\left[\tau^{3/2}(a_1 w_1(t) + a_2 w_2(t))\right] > \\ &= \tau^2 < a_1 w_1^2(t) + a_2 w_1(t) w_2(t) > \\ &= \tau^2 2a_1. \end{aligned} \tag{B.6}$$

Here average of multiplications of w_1 and w_2 gives zero since they are independent random variables and their averages are zero. Now we find

$$\begin{aligned} < \tilde{\Gamma_1}(t)\tilde{\Gamma_2}(t) > &= \int_0^\tau d\tau' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' < \Gamma(\tau')\Gamma(\xi') > \\ &= \int_0^\tau d\tau' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' 2\delta(\xi' - \tau') \\ &= \tau^2, \end{aligned} \tag{B.7}$$

then using results of Eq. (B.6) and Eq. (B.7) we find $2a_1 = 1$ and from this we obtain $a_1 = \frac{1}{2}$. We take average of $\tilde{\Gamma_2}(t)\tilde{\Gamma_2}(t)$ by using w representation to find a_2

$$\begin{aligned} < \tilde{\Gamma_2}(t)\tilde{\Gamma_2}(t) > &= < \left[\tau^{3/2}(a_1 w_1(t) + a_2 w_2(t))\right]\left[\tau^{3/2}(a_1 w_1(t) + a_2 w_2(t))\right] > \\ &= \tau^2 < a_1^2 w_1^2(t) + a_2^2 w_2^2(t) > \\ &= \tau^3 2(a_1^2 + a_2^2) \end{aligned} \tag{B.8}$$

then using results of Eq. (B.4) and Eq. (B.8) we find $2(a_1^2 + a_2^2) = \frac{2}{3}$ and from which we obtain $a_2 = \frac{1}{2\sqrt{3}}$. Finally we find $\tilde{\Gamma_2}$ as

$$\tilde{\Gamma_2}(t) = \tau^{3/2}\left[\frac{1}{2}w_1(t) + \frac{1}{2\sqrt{3}}w_2(t)\right]. \tag{B.9}$$

Similarly we will find $\tilde{\Gamma}_3(t)$ in terms w. Firstly we note that it is given as

$$\tilde{\Gamma_3}(t) = \int_0^\tau dt' \int_t^{t+t'} dt'' \int_t^{t+t''} dt'''\Gamma(t'''). \tag{B.10}$$

To find it in terms of w we start with

$$\begin{aligned} < \tilde{\Gamma_3}(t)\tilde{\Gamma_3}(t) > &= \int_0^\tau d\tau' \int_t^{t+\tau'} dt' \int_t^{t+t'} dt'' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \\ &\quad \int_t^{t+\xi'} d\xi'' < \Gamma(\xi'')\Gamma(t'') > \\ &= \int_0^\tau d\tau' \int_t^{t+\tau'} dt' \int_t^{t+t'} dt'' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \\ &\quad \int_t^{t+\xi'} d\xi'' 2\delta(\xi'' - t'') \\ &= \frac{1}{10}\tau^5 \end{aligned} \tag{B.11}$$

and we write $\tilde{\Gamma}_3(t)$ in term of w's

$$\tilde{\Gamma_3}(t) = \tau^{5/2}\left[b_1 w_1(t) + b_2 w_2(t) + b_3 w_3(t)\right]. \tag{B.12}$$

We then take average of $\tilde{\Gamma_1}(t)\tilde{\Gamma_3}(t)$ by using integral and w representation to find b_1. We first calculate

$$\begin{aligned} < \tilde{\Gamma_1}(t)\tilde{\Gamma_3}(t) > &= < \left[\tau^{1/2}w_1(t)\right]\left[\tau^{5/2}(b_1 w_1(t) + b_2 w_2(t) + b_3 w_3(t))\right] > \\ &= \tau^3 < b_1 w_1^2(t) > \\ &= \tau^3 2b_1. \end{aligned} \tag{B.13}$$

We then find $< \tilde{\Gamma_1}(t)\tilde{\Gamma_3}(t) >$ by using integral representations as

$$\begin{aligned} < \tilde{\Gamma_1}(t)\tilde{\Gamma_3}(t) > &= \int_0^\tau d\tau' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \int_t^{t+\xi'} d\xi'' < \Gamma(\tau')\Gamma(\xi') > \\ &= \int_0^\tau d\tau' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \int_t^{t+\xi'} d\xi'' 2\delta(\xi'' - \tau') \\ &= \frac{1}{3}\tau^3. \end{aligned} \tag{B.14}$$

Then using results of Eq. (B.13) and Eq. (B14) we find $2b_1 = \frac{1}{3}$ or $b_1 = \frac{1}{6}$. We take average of $\tilde{\Gamma_2}(t)\tilde{\Gamma_3}(t)$ by using integral and w representation to find b_2. We start with

$$\begin{aligned} < \tilde{\Gamma_2}(t)\tilde{\Gamma_3}(t) > &= < \left[\tau^{3/2}(\frac{1}{2}w_1(t) + \frac{1}{2\sqrt{3}}w_2(t))\right] \\ &\quad \left[\tau^{5/2}(b_1 w_1(t) + b_2 w_2(t) + b_3 w_3(t))\right] > \\ &= \tau^4 < \frac{1}{2}b_1 w_1^2(t) + \frac{1}{2\sqrt{3}}b_2 w_2^2 > \\ &= \tau^4 \left(b_1 + \frac{b_2}{\sqrt{3}}\right). \end{aligned} \tag{B.15}$$

We also find

$$\begin{aligned} < \tilde{\Gamma_2}(t)\tilde{\Gamma_3}(t) > &= \int_0^\tau d\tau' \int_t^{t+\tau'} dt'' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \int_t^{t+\xi'} d\xi'' < \Gamma(t'')\Gamma(\xi'') > \\ &= \int_0^\tau d\tau' \int_t^{t+\tau'} dt'' \int_0^\tau d\xi \int_t^{t+\xi} d\xi' \int_t^{t+\xi'} d\xi'' 2\delta(\xi'' - t'') \\ &= \frac{1}{6}\tau^4. \end{aligned} \tag{B.16}$$

Then using results of Eq. (B.15) and Eq. (B.16) we find $(b_1 + \frac{b_2}{\sqrt{3}}) = \frac{1}{6}$ so $b_2 = 0$. We take average of $\tilde{\Gamma_2}(t)\tilde{\Gamma_3}(t)$ by using w representation to find b_3. We start with

$$\begin{aligned} < \tilde{\Gamma_3}(t)\tilde{\Gamma_3}(t) > &= < \left[\tau^{5/2}(b_1 w_1(t) + b_2 w_2(t) + b_3 w_3(t))\right] \\ &\quad \cdot \left[\tau^{5/2}(b_1 w_1(t) + b_2 w_2(t) + b_3 w_3(t))\right] > \end{aligned}$$

$$
\begin{aligned}
&= \tau^5 < b_1^2 w_1^2(t) + b_2^2 w_2^2(t) + b_3^2 w_3^2(t) > \\
&= \tau^5 2(b_1^2 + b_2^2 + b_3^2), \qquad \text{(B.17)}
\end{aligned}
$$

then using results of Eq. (B.11) and Eq. (B.17) we find $2(b_1^2 + b_2^2 + b_3^2) = \frac{1}{10}$ so we find $b_3 = \frac{1}{3\sqrt{5}}$. Finally we obtain

$$
\tilde{\Gamma_3}(t) = \tau^{5/2} \left[\frac{1}{6} w_1(t) + \frac{1}{3\sqrt{5}} w_3(t) \right]. \qquad \text{(B.18)}
$$

APPENDIX C

ANALYTIC SOLUTIONS OF $< p^2 >$ AND $< (q - q_0)^2 >$

Here we will find analytic solution of Langevin equation Eq. (2.15) for $< p^2 >$ and $< (q - q_0)^2 >$ for potential free case $V = 0$. Firstly momentum part of the Langevin equation Eq. (2.15) is multiplied with $e^{\frac{\tilde{\gamma}}{m}t}$ to solve it which results in

$$\frac{d}{dt}(pe^{\frac{\tilde{\gamma}}{m}t}) = g \cdot \Gamma(t) \tag{C.1}$$

and integrating this equation over t between 0 and t we obtain

$$p = \int_0^t dt' e^{-\frac{\tilde{\gamma}}{m}(t-t')} g\Gamma(t') + ce^{\frac{\tilde{\gamma}}{m}t}. \tag{C.2}$$

In this equation the last term comes from the integration. We can determine it by solving this equation at $t = 0$ and we obtain $c = p_0$ as it should be. Then, we take square of this equation and we arrive at

$$\begin{aligned} p^2 &= \int_0^t dt' \int_0^t dt'' e^{-\frac{\tilde{\gamma}}{m}(t-t')} e^{-\frac{\tilde{\gamma}}{m}(t-t'')} g^2 \Gamma(t')\Gamma(t'') \\ &\quad + 2\int_0^t dt' e^{-\frac{\tilde{\gamma}}{m}(t-t')} g\Gamma(t') p_0 e^{\frac{\tilde{\gamma}}{m}t} + p_0^2 e^{2\frac{\tilde{\gamma}}{m}t} \end{aligned} \tag{C.3}$$

and by using Eq. (2.35) we take average of Eq. (C.3) and we obtain

$$< p^2 >= m \cdot kT \left[1 - e^{-2\frac{\tilde{\gamma}}{m}t}\right] + p_0^2 e^{2\frac{\tilde{\gamma}}{m}t}. \tag{C.4}$$

To obtain analytic solution of $< (q - q_0)^2 >$ we use second part of Eq. (2.15) and if we integrate it over t as

$$q - q_0 = \frac{1}{m} \int_0^t dt' p \tag{C.5}$$

and using Eq. (C.2) we obtain

$$q - q_0 = \frac{p_0}{\tilde{\gamma}} \left[1 - e^{-\frac{\tilde{\gamma}}{m} t}\right] + \frac{1}{\tilde{\gamma}} \int_0^t dt' \left[1 - e^{-\frac{\tilde{\gamma}}{m}(t-t')}\right] g\Gamma(t') \tag{C.6}$$

and similarly we take square of this equation and using Eq. (2.35) we take average of this equation and finally we arrive at

$$< (q-q_0)^2 >= \frac{1}{\tilde{\gamma}^2} \left[p_0^2 - 3mkT + 2\tilde{\gamma}kTt + 2(2mkT - p_0^2)e^{-\frac{\tilde{\gamma}}{m}t} + (p_0^2 - mkT)e^{-2\frac{\tilde{\gamma}}{m}t}\right] \tag{C.7}$$