STOCHASTIC APPROACH TO FUSION DYNAMICS

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ABSTRACT

STOCHASTIC APPROACH TO FUSION DYNAMICS

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This doctoral study consists of two parts. In the first part, the quantum statistical effects on the formation process of the heavy ion fusion reactions have been investigated by using the c-number quantum Langevin equation approach. It has been shown that the quantum effects enhance the over-passing probability at low temperatures. In the second part, we have developed a simulation technique for the quantum noises which can be approximated by two-term exponential colored noise.

Keywords: stochastic nuclear collective dynamics, heavy ion fusion reactions, super heavy elements, Langevin equation, Fokker-Planck equation, dissipative quantum systems, simulation techniques of colored noises

ÖZ

FÜZYON DİNAMİĞİNE STOKASTİK YAKLAŞIM

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Bu doktora çalışması iki kısımdan oluşmaktadır. İlk kısımda, ağır çekirdek füzyon reaksiyonlarının formasyon sürecine kuantum istatistiksel etkileri, c-sayı kuantum Langevin denklemi kullanılarak araştırılmıştır. Düşük sıcaklıklarda kuantum etkilerinin engel üzerinden geçme olasılığını artırdığı gösterilmiştir. İkinci kısımda da iki terimli üstel renkli gürültü cinsinden ifade edilebilen kuantum gürültüler için bir simülasyon tekniği geliştirilmiştir.

Anahtar Kelimeler: stokastik çekirdek toplu dinamiği, ağır iyonların füzyon etkileşmeleri, süper ağır elementler, Langevin denklemi, Fokker-Planck denklemi, yitimli kuantum sistemler, renkli gürültünün simülasyon teknikleri

To My Parents

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TABLE OF CONTENTS

ABSTRACT iv

ÖZ v

DEDICATION vi

ACKNOWLEDGMENTS vi

TABLE OF CONTENTS viii

LIST OF FIGURES x

CHAPTER

1 INTRODUCTION 1

2 FORMULATION OF DISSIPATIVE DYNAMICAL SYSTEMS . 6

2.1 Fokker-Planck Equation 6

2.2 Langevin Equation 7

2.3 Equivalence of Langevin and Fokker-Planck Equations . . 11

2.4 Generalized Langevin Equation 12

2.5 Derivation of the Generalized Langevin Equation from a Microscopic Model 13

2.6 Quantum Langevin Equation 20

3 HEAVY-ION FUSION REACTIONS 27

3.1 Motivation: Superheavy Elements 27

3.2 The Reaction Mechanism 30

4 QUANTUM STATISTICAL EFFECTS ON THE HEAVY-ION FUSION REACTIONS 35
4.1 The Propagator Approach 37
4.2 Quantum Fokker-Planck Approach 39
4.3 Quantum Langevin Approach 43
4.3.1 Analysis of the Langevin Equation 53
4.3.2 Quantum Effects on Diffusion Along Conditional Saddle Towards Fusion 58
5 NUMERICAL INTEGRATION METHODS FOR STOCHASTIC DIFFERENTIAL EQUATIONS 62
5.1 Iteration Method 63
5.2 Stochastic Runge-Kutta Method 66
5.3 Spectral Method 70
5.4 Integration Method 72
5.5 Integration Method for two-term exponentially correlated colored noise 75
5.5.1 Motivation 75
5.5.2 The Method 77
5.5.3 Test and Application of the Correlated Algorithm 84
6 CONCLUSION 92
REFERENCES 94
APPENDICES 98
A THE SOLUTION OF THE LANGEVIN EQUATION 98
B THE AUTOCORRELATION FUNCTION OF THE NOISE . . . 102
VITA 104

LIST OF FIGURES

3.1 Schematic view of the reaction mechanism of the fusion process of the heavy ions. 32

4.1 The correlation function is plotted versus time for $\Delta = 15$ MeV. . 53

4.2 The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV. 56

4.3 The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV. 57

4.4 The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV and T=1.0 MeV. The cases with and without friction are compared. 58

4.5 The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV and T=1.0 MeV. The cases with and without friction are compared. 59

4.6 The formation probability is plotted versus initial kinetic energy minus barrier height. The result of classical diffusion approach is compared with that of quantum diffusion approach for $\Delta = 15$ MeV. 60

5.1 Four examples of the correlation function, Eq.(5.55) with $D_1 D_2 < 0$ are indicated. Two of the examples are unphysical due to violation of one of the conditions, Eqs.(5.95,5.96,5.97). 84

5.2 The comparison of the exact correlation function with simulated ones (dashed line with 10^3 initial values and dotted line with 10^4 initial values). 86

5.3 The comparison of the exact average of p with simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations). 87

5.4 The comparison of the exact variance of p and simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations). 88

5.5 The passing probability over the barrier is plotted versus the initial kinetic energy in arbitrary units. The analytical and numerical results (dashed line) are shown for the correlation $\chi(t) = 7e^{-4|t|} - 3e^{-2|t|}$. The computations are done with the time step, $\Delta t = 10^{-2}$ and 10^4 realizations. 91

CHAPTER 1

INTRODUCTION

The nuclear collective phenomenon was born with the discovery of the nuclear fission and the first influential description of the nuclear fission mechanism has come with the work of Bohr and Wheeler in 1939 [1]. They derived an expression for the fission rate adopting a purely statistical approach. One year later in 1940, Kramers in his seminal work proposed a dissipative model for nuclear fission and chemical reactions [2]. He has solved the Fokker-Planck equation for the density in the collective phase space, considering the collective dynamics of the nuclear reactions to be equivalent to that of a Brownian motion in a heat bath of nucleonic degrees of freedom and obtained an escape rate over the quasistationary fission barrier for large and small friction limits. In the subsequent forty years, the idea of Kramers has not gained much recognition in the community studying nuclear reaction theories due to the relative success of the more simple Bohr-Wheeler model and the insufficiency of the available experimental data to distinguish between Bohr-Wheeler and Kramers models. The experiments carried out in 80's revealed the fact that the fission of nuclei is a slower process

than the predicted time scales of the transition state model of Bohr and Wheeler [3]. This discrepancy lead Grange and his collaborators to follow Kramers' idea and investigate the effects of nuclear dissipation on the fission time scales [4]. They solved numerically the two-dimensional Fokker-Planck equation for the distribution function in phase space of the collective fissioning coordinate and the conjugate momentum assuming a constant friction and constant fission barrier. They found the fission rate as a function of time by calculating the probability current over the saddle point. The importance of the transients on the dynamics of the system, that is the time interval from the beginning of the induced fission process to the attainment of quasistationary flow over the barrier, has been indicated. They showed that the friction as well as the transients introduce a reduction on the fission probability which was consistent with the experimental results.

The dissipative nature of the nuclear collective dynamics is well established now and has been applied successfully to various studies on nuclear collective processes such as the heavy ion fusion reactions. It was found that the fusion reaction of heavy ions is a highly dissipative phenomenon with a low probability. Due to this low probability, the fusion reaction of the heavy ions leading to the synthesis of superheavy elements is a theoretical and experimental challenge. The theoretical formulations are obtained by splitting the reaction mechanism into two stages and treating them independently. In the approach stage, the

respective nuclei overcome the Coulomb barrier and a sticking configuration is formed. In the second formation stage, an amalgamated pear shaped dinuclear structure evolves over the conditional saddle to form a compound mononucleus. This stage is the least understood because of its complexity. The reason for dividing the fusion reaction into two stages is the difference of time scales and the necessity to use different sets of dynamical collective variables.

The synthesis of the superheavy elements is the main motivation for the enormous efforts devoted to enlighten the reaction mechanism of the heavy nuclei. Most of the studies are performed by employing a classical diffusive approach to the fusion reaction ignoring the quantum effects. However, Strutinski has shown that the stability of the superheavy elements is maintained by shell correction energies [5] and since the shell structure is destroyed at high excitation energies, superheavy nuclei should be synthesized at reasonably low excitation energies corresponding to low nuclear temperatures of the order of $0.5 - 1$ MeV. Consequently, quantum statistical effects are expected to play an important role on the fusion dynamics. The quantum statistical effects on the least studied formation phase of the fusion reaction can be investigated by considering the quantum transport equations for the diffusion process of a single collective variable over a parabolic potential barrier. In order to obtain a compound nucleus with a low excitation, the initial kinetic energy of collective system at the beginning of the

formation phase should be close to the conditional potential barrier which justifies the quadratic form assumption for the barrier. Within such a model, it has been shown that the quantum effects increase the over-passing probability at low nuclear temperatures as a result of enhancements in the variances caused by the quantum fluctuations of the nucleonic degrees of freedom [6, 7, 8].

The quantum diffusion of the collective variables can be formulated by using either the Fokker-Planck approach which is based on the evolution of the density matrix or the Langevin approach which is based on the evolution of the dynamical variables themselves. Both approaches are equivalent, however, Langevin description has certain advantages in practical applications. In realistic applications, the potential is complicated and hence only numerical calculations can be considered. Solving numerically the Langevin equation, which is a first order stochastic differential equation, is easier than the Fokker-Planck equation, which is a deterministic second order partial differential equation. The only difficulty with the Langevin approach is the simulation of the stochastic forces. There are some fast and accurate simulation methods for classical noises, but there is a lack of such methods for the more complicated quantum noises. Since the quantum noises with the Drude profile can be expressed as a sum of exponentials. A simulation technique for quantum noises which can be expressed by or fitted to a sum of two exponentials has been developed [9].

In the next chapter, we discuss the Fokker-Planck and Langevin formalisms

of the dissipative systems. The derivation of the classical as well as quantum Langevin equations are given. The properties of the stochastic forces are explained. In Chapter 3, we present the heavy-ion fusion reactions in connection with the synthesis of superheavy elements. The three stages of the reaction mechanism are reviewed. In Chapter 4, in order to illustrate the effects of the quantum statistical fluctuations, we present different approaches describing the intermediate stage of the heavy-ion fusion reactions at low nuclear temperatures. In Chapter 5, the simulation techniques of the stochastic forces appearing in the Langevin equations as well as the integration of the stochastic differential equations are discussed. Finally, we give conclusions in Chapter 6.

CHAPTER 2

FORMULATION OF DISSIPATIVE DYNAMICAL SYSTEMS

The formulations of dissipative systems with a special emphasis on the Langevin approach are discussed below. The basic considerations here will provide the essential ingredients for the next chapters.

2.1 Fokker-Planck Equation

The dissipative approach of Kramers has been later extended to all collective nuclear processes after the discovery of the nuclear dissipation for heavy nuclei. To this extent, an analogy between the Brownian motion which is the most basic dissipative model and the nuclear dynamics was established. A collective nuclear process is represented by one or a few collective variables representing some gross features of the process. For instance, in the case of a nucleus undergoing fission, shape parameters describing the surface of the nucleus or the distance between the center of masses of respective fission fragments can be used as a collective variable with a corresponding conjugate momentum. The equation of motion for the distribution function of the collective variable is given by the Fokker-Planck

equation

$$\frac{\partial}{\partial t}W(v,t) = \frac{\partial}{\partial v}\left(\beta v + \frac{\beta k_B T}{m}\frac{\partial}{\partial v}\right)W(v,t), \tag{2.1}$$

where β is the reduced friction coefficient which is a measure of the coupling strength between the collective and nucleonic degrees of freedom. m, T and k_B are the mass parameter of collective system, the temperature of the nucleonic heat bath, and the Boltzmann constant, respectively. $W(v,t)$ is the probability that the system has velocity between v and $v+dv$ at time t. In case of an external potential the corresponding Fokker-Planck equation is called Kramers equation and given by

$$\frac{\partial}{\partial t}W(q,p,t) = \left\{-\frac{\partial}{\partial q}\frac{p}{m} + \frac{\partial}{\partial p}\left(\frac{\partial U}{\partial q} + \beta p\right) + m\beta k_B T\frac{\partial^2}{\partial p^2}\right\}W(q,p,t), \tag{2.2}$$

where U is the external potential, q and p are the conjugate position and momentum variables, respectively. The mean value of any physical quantity can be calculated by integration as

$$\langle f(q(t),p(t))\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(q,p)W(q,p,t)\,dq\,dp, \tag{2.3}$$

where $\langle ...\rangle$ represents the mean over the distribution.

2.2 Langevin Equation

An equivalent formulation of dissipative systems can be achieved by using the Langevin approach where one deals with the phase space trajectories themselves

rather than their distribution function. The equation of motion is given by

$$\frac{dp}{dt} = -\frac{\partial U}{\partial q} - \beta p + R(t), \tag{2.4}$$

$$\frac{dq}{dt} = \frac{p}{m}, \tag{2.5}$$

and called Langevin equation. The first term on the right hand side of Eq.(2.4) is the external force, whereas the other two terms are the Stokes' law friction term, $-\beta p$, with the reduced friction coefficient β and the stochastic force $R(t)$ describing the fluctuations of the observables. These last two terms as will be explained in Section 2.5 arise due to the coupling of the collective degrees of freedom to the heat bath. The slowly varying friction term $-\beta p$ describes the average effect of the heat bath on the collective modes and the stochastic term $R(t)$ describes the rapid fluctuations around that average. The random force $R(t)$ arises due to the instantaneous collisions of the Brownian particle with the heat bath particles and does not have an explicit time dependence since the characteristic time (or observation time) for collective variables is always larger than collision time. The properties of the stochastic force can be deduced by using the solution of the Langevin equation (2.4) for a free Brownian motion,

$$p(t) = p(0)e^{-\beta t} + \int_0^t e^{-\beta(t-t')} R(t')dt'. \tag{2.6}$$

The first term describes the exponential decay of the initial momentum $p(0)$ over a relaxation time $1/\beta$, hence the larger the friction the faster the decay, so that the energy of the Brownian particle is more quickly transferred into the intrinsic

(heat bath) degrees of freedom. The mean of the second term and hence mean of the random force must be zero,

$$\langle R(t)\rangle = 0, \tag{2.7}$$

since the mean momentum must follow the classical trajectory of a damped system without fluctuations and it must become zero when the thermal equilibrium is reached, $\langle p(t \to \infty)\rangle = 0$. The mean $\langle ...\rangle$ indicates an ensemble averaging over all the realizations of the stochastic force $R(t)$. The mean square momentum reads

$$\langle p^2(t)\rangle = p^2(0)e^{-2\beta t} + \int_0^t dt' e^{-\beta(t-t')} \int_0^t dt'' e^{-\beta(t-t'')} \langle R(t')R(t'')\rangle, \tag{2.8}$$

which is expected to obey the equipartition theorem at the thermal equilibrium

$$\frac{\langle p^2(t \to \infty)\rangle}{2m} = \frac{1}{2} k_B T. \tag{2.9}$$

In order to satisfy this condition, it can be easily shown by substitution that the autocorrelation of the random force must be given by

$$\begin{aligned} \langle R(t)R(t')\rangle &= 2D\delta(t-t') \\ &= 2m\beta k_B T \delta(t-t'), \end{aligned} \tag{2.10}$$

where D is the diffusion coefficient and $\delta(t)$ is the Dirac delta function. The Eq.(2.10) is called fluctuation-dissipation theorem since it connects the thermal fluctuation $R(t)$ with the dissipation factor β via the diffusion coefficient D. This

result is not much surprising since the origin of both effects is the same; the collisions of the heat bath particles with the Brownian particle. The theorem also states that the dissipation is always associated with fluctuations. One can discard the fluctuations only when the mass of the Brownian particle is much larger than that of the constituents of the heat bath [10]. The thermal noise $R(t)$ is function of the initial values of the heat bath degrees of freedom (see Section 2.5) which form an ensemble with Maxwellian distribution, hence $R(t)$ is a mean zero Gaussian noise with an autocorrelation given by Eq.(2.10).

The Langevin equation as well as the Fokker-Planck equation are not exact equations of motion for the Brownian particle in a sense that they are not valid for infinitesimally small times, that is they do not take into account the collisions themselves. These collisions are treated in a course grained manner over a time step Δt which should necessarily be larger than the characteristic collision time of the heat bath particles with the Brownian particle and smaller than the relaxation time of the Brownian motion itself. This fact is best illustrated by the random walk formalism of the Brownian motion where the Brownian particle is considered to perform displacements in a form of series of steps of equal length and random directions. For details refer to [11].

2.3 Equivalence of Langevin and Fokker-Planck Equations

The Fokker-Planck and Langevin equations are two different formulations of the stochastic processes with the same physical content. Their equivalence can be demonstrated by using the continuity equation,

$$\frac{\partial}{\partial t}W(q,p,t) + \frac{\partial}{\partial q}\left(\dot{q}W(q,p,t)\right) + \frac{\partial}{\partial p}\left(\dot{p}W(q,p,t)\right) = 0, \tag{2.11}$$

for the distribution function $W(q,p,t)$. Substituting the Langevin equation (2.4) for $\dot{p}$ and Eq.(2.5) for $\dot{q}$ into Eq.(2.11) and integrating within the interval $(t, t+\Delta t)$ where Δt is larger than the characteristic time of the intrinsic degrees of freedom and smaller than the relaxation time of the collective variables, one obtains

$$\begin{aligned} W(q,p,t+\Delta t) - W(q,p,t) &= \int_t^{t+\Delta t} dt_1 \Omega(q,p,t_1) W(q,p,t_1) \\ &= \int_t^{t+\Delta t} dt_1 \Omega(q,p,t_1) W(q,p,t) \\ &\quad + \int_t^{t+\Delta t} dt_1 \Omega(q,p,t_1) \int_t^{t_1} dt_2 \Omega(q,p,t_2) W(q,p,t_2) \\ &= \int_t^{t+\Delta t} dt_1 \Omega(q,p,t_1) W(q,p,t) \\ &\quad + \int_t^{t+\Delta t} dt_1 \Omega(q,p,t_1) \int_t^{t_1} dt_2 \Omega(q,p,t_2) W(q,p,t) \\ &\quad + ..., \end{aligned} \tag{2.12}$$

where

$$\Omega(q,p,t) = -\frac{p}{m}\frac{\partial}{\partial q} + \frac{\partial}{\partial p}\left(\frac{\partial U}{\partial q} + \beta p - R(t)\right). \tag{2.13}$$

Taking the ensemble average of Eq.(2.12) over all realizations of $R(t)$, one obtains

$$\frac{W(q,p,t+\Delta t)-W(q,p,t)}{\Delta t} = \left\{-\frac{\partial}{\partial q}\frac{p}{m}+\frac{\partial}{\partial p}\left(\frac{\partial U}{\partial q}+\beta p\right)\right\}W(q,p,t) + m\beta k_B T\frac{\partial^2}{\partial p^2}W(q,p,t)+O(\Delta t), \quad (2.14)$$

so that when $\Delta t \to 0$ this reduces to Kramers equation (2.2). In obtaining the last result the following statistical properties of the operator Ω are used;

$$\langle\Omega(q,p,t)\rangle = -\frac{p}{m}\frac{\partial}{\partial q}+\frac{\partial}{\partial p}\left(\frac{\partial U}{\partial q}+\beta p\right), \quad (2.15)$$

and

$$\langle\Omega(q,p,t_1)\Omega(q,p,t_2)\rangle = 2D\delta(t_1-t_2)\frac{\partial^2}{\partial p^2}+f(q,p), \quad (2.16)$$

where $f(q,p)$ stands for the time independent terms that have no contribution to the final result.

2.4 Generalized Langevin Equation

The Langevin equation (2.4) is Markovian which means that the system has no memory and there is no correlation between the stochastic forces at different times which is dictated by the Dirac delta function in Eq.(2.10). This form of the Langevin equation is restrictive and only valid for systems where a clear separation between relaxation time of the collective variable and characteristic time of the heat bath degrees of freedom is possible, making the Markovian limit a good approximation. For instance for the ordinary Brownian motion

of the pollen particle in a fluid, the difference between the time scale of the Brownian particle and the time scale of the heat bath is very large. On the other hand, in many mesoscopic systems such as nuclei, these two time scales are close to each other. Then the Markovian Langevin equation (2.4) becomes a poor approximation which needs to be replaced with the generalized Langevin equation to allow for finite memory and a correlation between stochastic forces at different times. The generalized Langevin equation is given by

$$\frac{dp}{dt} = -\frac{\partial U}{\partial q} - \int_{t_0}^{t} \chi(t-t')p(t')dt' + R(t), \tag{2.17}$$

with $\dot{q} = p/m$ where $\chi(t)$ is the friction-memory kernel. In general, the lower limit of the integral is $-\infty$ so that the memory effects of the remote past are also included, but it is possible to replace $-\infty$ with an arbitrary finite initial time $t_0 < t$ by redefining the stochastic force $R(t)$ [12]. The second moment of the zero mean stochastic force now reads

$$\langle R(t)R(t')\rangle = mk_BT\chi(|t-t'|), \tag{2.18}$$

which is the generalized form of the fluctuation-dissipation theorem.

2.5 Derivation of the Generalized Langevin Equation from a Microscopic Model

The goal in any sciences inspecting transport phenomena of complex systems is to start from a microscopic theory, derive the transport equations for the collective modes and solve these equations as general as possible. There are many models

for the Hamiltonians of the total system which lead to Langevin equations [13]. The most widely encountered model is regarding the heat bath as an assembly of harmonic oscillators at thermal equilibrium coupled bilinearly to the collective position. The idea was introduced by Magalinskij [14] for the classical systems and later extended to quantum systems by Senitzky [15], Ford et. al. [13], and Ullersma [16]. But the model is generally named after Caldeira and Leggett who made a detailed explanation of the model [17]. The classical Hamiltonian of the total system is given by

$$H = \frac{P^2}{2M} + U(Q) + \sum_i \left[\frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 \left(q_i - \frac{c_i}{m_i \omega_i^2} Q \right)^2 \right], \tag{2.19}$$

where (Q, P) and (q_i, p_i) are the phase space variables of the collective motion and the ith oscillator in the heat bath, respectively. M is the mass of the Brownian particle (or effective mass of the collective variable). m_i and ω_i are the mass and frequency of the ith oscillator. The coupling strength of the collective position Q with the position q_i of the ith oscillator is indicated by c_i. The solutions for the collective system has been derived by Zwanzig for the Hamiltonian above. He used a direct elimination technique to obtain the solution of the collective system [18]. The equations of motion for the collective system read

$$\begin{aligned} \frac{dQ}{dt} &= \frac{P}{M}, \\ \frac{dP}{dt} &= -\frac{\partial U}{\partial Q} + \sum_i c_i \left(q_i - \frac{c_i}{m_i \omega_i^2} Q \right), \end{aligned} \tag{2.20}$$

and for the bath degrees of freedom they are

$$\begin{aligned} \frac{dq_i}{dt} &= \frac{p_i}{m_i}, \\ \frac{dp_i}{dt} &= -m_i\omega_i^2\left(q_i - \frac{c_i}{m_i\omega_i^2}Q\right). \end{aligned} \tag{2.21}$$

The latter coupled equations can be easily solved either by writing these coupled equations in a matrix form and diagonalizing the corresponding drift matrix or by using the Green's functions method. The result is

$$\begin{aligned} q_i(t) &= \frac{c_i}{m_i\omega_i^2}Q(t) - \int_{t_0}^{t}\frac{c_i}{m_i\omega_i^2}\cos\omega_i(t-t')\frac{dQ(t')}{dt'}dt' \\ &\quad + \left[q_i(t_0) - \frac{c_i}{m_i\omega_i^2}Q(t_0)\right]\cos\omega_i(t-t_0) + \frac{p_i(t_0)}{m_i\omega_i}\sin\omega_i(t-t_0). \end{aligned} \tag{2.22}$$

Substituting Eq.(2.22) into Eq.(2.20) we get the equation,

$$\frac{dP}{dt} = -\frac{\partial U}{\partial Q} - \int_{t_0}^{t}\chi(t-t')P(t')dt' + R^{(0)}(t) + M\chi(t-t_0)Q(t_0), \tag{2.23}$$

where the friction-memory kernel is

$$\chi(t) = \Theta(t)\frac{1}{M}\sum_i \frac{c_i^2}{m_i\omega_i^2}\cos\omega_i t, \tag{2.24}$$

with $\Theta(t)$ being the Heaviside step function preserving the causality. The stochastic force reads

$$R^{(0)}(t) = \sum_i c_i\left[q_i(t_0)\cos\omega_i(t-t_0) + \frac{p_i(t_0)}{m_i\omega_i}\sin\omega_i(t-t_0)\right]. \tag{2.25}$$

At first glance the last equation looks like a deterministic expression, however the heat bath degrees of freedom constitute the irrelevant part of the dynamics

and their initial values are forming a Gaussian equilibrium ensemble with the distribution function given by

$$\rho_B^{(0)} = Z^{-1} \exp\left\{-\frac{1}{k_B T}\sum_i \left[\frac{p_i^2(0)}{2m_i} + \frac{1}{2}m_i\omega_i^2 q_i^2(0)\right]\right\}. \tag{2.26}$$

Hence when the Eq.(2.25) is averaged over the distribution Eq.(2.26), it acquires the usual statistical properties given by Eq.(2.7) and Eq.(2.18). The stochastic differential equation (2.23) without the last term would be the generalized Langevin equation. This transient slippage $M\chi(t-t_0)Q(t_0)$ can be eliminated by adding it into the random force $R^{(0)}$ and redefining the reservoir density Eq.(2.26) as

$$\rho_B = Z^{-1} \exp\left\{-\frac{1}{k_B T}\sum_i \left[\frac{p_i^2(0)}{2m_i} + \frac{1}{2}m_i\omega_i^2 \left(q_i(0) - \frac{c_i}{m_i\omega_i^2}Q(0)\right)^2\right]\right\}, \tag{2.27}$$

so that the stationary statistical properties given by Eq.(2.7) and Eq.(2.18) are preserved with the new stochastic force [13, 17, 19],

$$R(t) = \sum_i c_i \left[\left(q_i(t_0) - \frac{c_i}{m_i\omega_i^2}Q(t_0)\right)\cos\omega_i(t-t_0) + \frac{p_i(t_0)}{m_i\omega_i}\sin\omega_i(t-t_0)\right]. \tag{2.28}$$

The generalized Langevin equation now reads

$$\frac{dP}{dt} = -\frac{\partial U}{\partial Q} - \int_{t_0}^{t}\chi(t-t')P(t')dt' + R(t), \tag{2.29}$$

with memory kernel and random force given by Eq.(2.24) and Eq.(2.28), respectively.

There are some properties of the Caldeira-Leggett model that affect the

validity and applicability of the generalized Langevin equation. First one is the consideration of the number of harmonic oscillators forming the heat bath and the second one is regarding the form of memory kernel that should be modified for practical applications. Consider a system coupled to only one or a few harmonic oscillators within Caldeira-Leggett model. The energy will be feeded back and forth between the system and the harmonic oscillators over a short time interval called the Poincaré recurrence time. Here, short means that this time scale is comparable to any relevant time scale of the system. Then, Langevin approach loses its validity since the system is reversible. For systems coupled to more than a few dozens of harmonic oscillators the Poincaré recurrence time becomes so large that it can practically be considered as infinity when compared to any relevant collective time scale. Hence, the collective system becomes irreversible and the Langevin approach acquires validity. On the other hand, even though the derived generalized Langevin equation (2.29) is exact, the memory kernel Eq.(2.24) is impractical to use since it is a superposition of many cosines with unknown coupling strengths c_i and the frequencies ω_i. One can at best go to the continuum limit, hence the friction-memory kernel Eq.(2.24) becomes [19]

$$\chi(t) = \Theta(t)\frac{2}{\pi}\int_0^\infty \Gamma(\omega)\cos(\omega t)d\omega, \tag{2.30}$$

where $\Gamma(\omega) = J(\omega)/M\omega$ with $J(\omega)$ being the spectral density of the environmental coupling. Comparing Eq.(2.24) and Eq.(2.30), the exact value of $\Gamma(\omega)$

reads $\Gamma(\omega) = \frac{\pi}{2M}\sum_i \frac{c_i^2}{m_i\omega_i^2}\delta(\omega-\omega_i)$, which should be replaced by a proper continuous function. The form of Eq.(2.30) suggests that the density $\Gamma(\omega)$ is related to the Fourier transform of the memory function $\chi(t)$. Taking the inverse Fourier transform of the Eq.(2.30) we have

$$\begin{aligned}\Gamma(\omega) &= \int_0^\infty \chi(t)\cos(\omega t)dt \\ &= \tilde{\chi}'(\omega),\end{aligned} \tag{2.31}$$

where prime stands for the real part of the Fourier transformed memory function $\tilde{\chi}(\omega) = \int_{-\infty}^{\infty}\chi(t)\exp(i\omega t)dt$. This result states that it is the real part of the Fourier transform of the memory function that introduces the memory effect and dissipation and it is enough to introduce either the spectral density or the memory function in order to be able to solve generalized Langevin equation. The two most frequently encountered continuum choices of the memory kernel are the exponential and Gaussian memory functions. The exponential one has the following form

$$\chi(t) = \Theta(t)\frac{\beta}{\tau}e^{-\frac{t}{\tau}}, \tag{2.32}$$

where β is the reduced friction coefficient and τ is the relaxation time of the collective system. The corresponding density has a Lorentzian (Drude) profile,

$$\Gamma(\omega) = \frac{J(\omega)}{M\omega} = \frac{\beta}{1+(\omega\tau)^2}. \tag{2.33}$$

The Gaussian memory kernel is given by

$$\chi(t) = \Theta(t)\frac{2}{\sqrt{\pi}}\frac{\beta}{\tau}e^{-\frac{t^2}{\tau^2}}, \tag{2.34}$$

with the corresponding density,

$$\Gamma(\omega) = \frac{J(\omega)}{M\omega} = \beta e^{-\frac{\omega^2\tau^2}{4}}. \tag{2.35}$$

Note that when we let the memory time vanish with the limit $\tau \to 0$ (Markovian limit), both memories Eq.(2.32) and Eq.(2.34) reduce to the Dirac delta form and hence the Stokes' friction is recovered as expected. In the same limit, the densities Eq.(2.33) and Eq.(2.35) become constant hence the corresponding spectral densities $J(\omega)$ become linear in ω. Some other properties of the friction-memory kernels are discussed in Section 5.5.

We should stress that there are some other Hamiltonians from which the generalized Langevin equation can be obtained such as the generalized Caldeira-Leggett model where a bilinear coupling between all the system and reservoir degrees of freedom is allowed [20]. Another model leading to the generalized Langevin equation is the Rubin model where the heat bath is again considered to be consisted of harmonic oscillators but coupled to one another in a chain form [19, 21]. All these Hamiltonians lead to the same generalized Langevin equation with slight changes in the memory kernel.

The considerations up to here are classical and in the following section we explain the extension of the classical dissipative dynamics to quantum domain.

2.6 Quantum Langevin Equation

Since dissipation is an effective macroscopic or mesoscopic concept, the analysis of the dissipative systems within quantum dynamics has not been considered during the development of quantum physics which was accepted to apply only to microscopic systems. There appeared some physical applications such as the radiation field of a cavity which called for a quantum dissipative treatment and hence boosted such theoretical investigations. The first quantum formulations of the dissipative systems were carried out by Caldirola [22] and Kanai [23] who used a time dependent Hamiltonian for a damped harmonic oscillator,

$$\hat{H}(t) = \frac{\hat{P}^2}{2m} e^{-\beta t} + \frac{1}{2} m\omega^2 \hat{q}^2 e^{\beta t}, \tag{2.36}$$

where $\hat{P} = m\dot{\hat{q}}e^{\beta t}$ is the canonical momentum satisfying $[\hat{q}, \hat{P}] = i\hbar$ and hence

$$[\hat{q}, \dot{\hat{q}}] = i\hbar e^{-\beta t}/m. \tag{2.37}$$

The Hamiltonian Eq.(2.36) of this model gives the following equation of motion for the damped harmonic oscillator

$$\ddot{\hat{q}} + \beta\dot{\hat{q}} + \omega^2\hat{q} = 0, \tag{2.38}$$

and allows to adopt the standard method of quantization but the uncertainty relation cannot be satisfied as seen from Eq.(2.37) [15, 24, 25]. Dekker [26] used a Hamiltonian of complex canonical variables together with a canonical quantization to obtain the master equation for the Wigner distribution. But there are

stochastic terms introduced in the equations of position and momentum which contradicts the classical notion. Another approach is to change the method of quantization or to use nonlinear models. Kostin [27] and Yasue [28] introduced a nonlinear Schrödinger equation to deal with quantum dissipation, but it turned out that the superposition principle cannot be handled with this model [19]. Some progress has been achieved to explain and cure these discrepancies and even their equivalence has been shown to some extent, but that was performed by changing the form of the continuity equation which is questionable [29]. Furthermore, these models do not take into account properly the effect of the environment as can be seen form the lack of a stochastic term in the Eq.(2.38). For the classical systems, the zero temperature limit of the heat-bath leads to an equation without a random noise but that is not realistic since as temperature falls down the quantum effects become stronger. Hence, at zero temperature there are still fluctuations which are purely quantal.

Apart from all the previous models, the most consistent and widely accepted approach to quantum dissipation is to treat the system and an environment as parts of a conservative global system, the so called system-reservoir model. The quantization of the isolated global Hamiltonian is performed in usual way avoiding any ad hoc assumptions. At this stage one can either work with the Schrödinger picture where the dynamics is governed by master equation for the density matrix or Heisenberg picture where the quantum Langevin equation for the reduced

operators is used. The difficulty faced in both pictures is the reduction of the equations of motion for the global system into the ones for the relevant part and finding solutions of these equations. Generally the solutions can be obtained only with some assumptions.

The quantum analog of classical generalized Langevin equation (2.29) has the same form,

$$\frac{d\hat{P}}{dt} = -\left.\frac{\partial U}{\partial Q}\right|_{Q=\hat{Q}} - \int_{t_0}^{t} \chi(t-t')\hat{P}(t')dt' + \hat{R}(t), \tag{2.39}$$

and can be derived using the same but this time operator valued Hamiltonian Eq.(2.19) for a quantum system coupled to a heat bath of quantum oscillators. Mori derived the quantum Langevin equation (2.39) by using the projection formalism [30]. The memory function $\chi(t)$ is again given by Eq.(2.24) and the stochastic force $\hat{R}(t)$ has the same form with Eq.(2.28),

$$\hat{R}(t) = \sum_i c_i \left[\left(\hat{q}_i(t_0) - \frac{c_i}{m_i\omega_i^2}\hat{Q}(t_0)\right)\cos\omega_i(t-t_0) + \frac{\hat{p}_i(t_0)}{m_i\omega_i}\sin\omega_i(t-t_0)\right]. \tag{2.40}$$

It is apparent that the different time commutation relation of the stationary noise operator $\hat{R}(t)$ is non-zero. The correlation functions satisfy the following properties,

$$\begin{aligned}
\langle\hat{R}(0)\hat{R}(t)\rangle &= Tr\left\{\hat{R}(0)\hat{R}(t)e^{-\hat{H}_B/k_BT}\right\} \\
&= Tr\left\{\hat{R}(0)e^{-\hat{H}_B/k_BT}e^{-i(i\hbar/k_BT)\hat{H}_B/\hbar}\hat{R}(t)e^{i(i\hbar/k_BT)\hat{H}_B/\hbar}\right\} \\
&= Tr\left\{\hat{R}(0)e^{-\hat{H}_B/k_BT}\hat{R}(t-i\hbar/k_BT)\right\} \\
&= \langle\hat{R}(t-i\hbar/k_BT)\hat{R}(0)\rangle
\end{aligned} \tag{2.41}$$

and

$$\begin{aligned}\langle\hat{R}(0)\hat{R}(t)\rangle^{*} &= Tr\left\{\left(\hat{R}(0)\hat{R}(t)e^{-\hat{H}_B/k_BT}\right)^{\dagger}\right\} \\ &= Tr\left\{e^{-\hat{H}_B/k_BT}\hat{R}(t)\hat{R}(0)\right\} \\ &= \langle\hat{R}(t)\hat{R}(0)\rangle, \end{aligned} \tag{2.42}$$

where $\hat{H}_B$ is the the Hamiltonian of the bath (reservoir) and the symbols $*$ and $\dagger$ denote the complex and Hermitian conjugations, respectively. It is possible to define the symmetrized correlation function of the random force as [19],

$$S(t) = \frac{1}{2}\left[C^{+}(t) + C^{-}(t)\right], \tag{2.43}$$

and the antisymmetrized correlation function as,

$$A(t) = \frac{1}{2i}\left[C^{+}(t) - C^{-}(t)\right], \tag{2.44}$$

where

$$C^{+}(t) = \langle\hat{R}(t)\hat{R}(0)\rangle - \langle\hat{R}^2(0)\rangle, \tag{2.45}$$

$$C^{-}(t) = \langle\hat{R}(0)\hat{R}(t)\rangle - \langle\hat{R}^2(0)\rangle. \tag{2.46}$$

Using the property Eq.(2.41), a general relation between the Fourier transforms $\tilde{S}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}S(t)dt$ and $\tilde{A}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}A(t)dt$ can be found as follows,

$$\begin{aligned}\tilde{S}(\omega) &= \frac{1}{2}\int_{-\infty}^{\infty} e^{i\omega t}\left[C^{+}(t) + C^{-}(t)\right]dt \\ &= \frac{1}{2}\left[1 + \exp\left(-\frac{\hbar\omega}{k_BT}\right)\right]\tilde{C}^{+}(\omega)\end{aligned}$$

$$
\begin{aligned}
&= i\frac{1+\exp\left(-\frac{\hbar\omega}{k_BT}\right)}{1-\exp\left(-\frac{\hbar\omega}{k_BT}\right)}\tilde{A}(\omega) \\
&= i\coth\left[\frac{\hbar\omega}{2k_BT}\right]\tilde{A}(\omega). \qquad (2.47)
\end{aligned}
$$

The last result is obtained by using the property $\tilde{C}^{-}(\omega) = e^{-\hbar\omega/k_BT}\tilde{C}^{+}(\omega)$. Since the antisymmetric correlation function is odd and it is the derivative of the memory function, $A(t) = M\frac{\hbar}{2}\frac{d}{dt}\chi(t)$, we have

$$
\begin{aligned}
\tilde{A}(\omega) &= 2i\int_0^\infty A(t)\sin(\omega t)dt \\
&= -iM\hbar\omega\tilde{\chi}'(\omega), \qquad (2.48)
\end{aligned}
$$

where $\tilde{\chi}'(\omega)$ is the real part of the Fourier transform of the memory function. Substituting Eq.(2.48) into Eq.(2.47), wet the quantum fluctuation-dissipation theorem in the Fourier space,

$$
\tilde{S}_Q(\omega) = M\hbar\omega\coth\left[\frac{\hbar\omega}{2k_BT}\right]\tilde{\chi}'(\omega), \qquad (2.49)
$$

which applies to any system with a thermal and quantum noise. The classical limit, $\hbar\omega \ll 2k_BT$, gives the expected value

$$
\tilde{S}_C(\omega) = 2Mk_BT\tilde{\chi}'(\omega). \qquad (2.50)
$$

The quantum (Q) and classical (C) correlation functions in the time domain are given by

$$
S_{Q,C}(t-t') = \langle R(t)R(t')\rangle = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\tilde{S}_{Q,C}(\omega), \qquad (2.51)
$$

The plot of the quantum correlation function $\langle R(t)R(0)\rangle$ can be seen in Figure 4.1. It is observed that as temperature increases the classical limit is recovered and as the temperature falls down the quantum coherence increase so that at zero temperature there is still a finite fluctuation, the so called zero point fluctuation.

The extra term $\frac{\hbar\omega}{2}\coth\left[\frac{\hbar\omega}{2k_BT}\right]$ that appears in the quantum correlation function is indeed the mean energy of a quantum oscillator of frequency ω. It is possible to comment further by rewriting the mean energy as follows,

$$\frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)=\frac{\hbar\omega}{2}+\frac{\hbar\omega}{\exp(\hbar\omega/k_BT)-1}. \tag{2.52}$$

The first term on the right hand side of Eq.(2.52) is the ground state energy of the oscillator where as the second term is the Planck distribution. Both terms have quantum mechanical origin. The Eq.(2.52) can also be considered as a frequency dependent effective temperature. This effective temperature is divergent at the high frequency limit $\omega\to\infty$ due to the ground state energy which means that in order to obtain a finite value a proper cut-off must be introduced. One way is to replace the limits of the frequency integral with a finite cut-off parameter and another is to allow for finite memories which will play the role of a cut-off function since the real part of the Fourier transform of the memory function $\tilde{\chi}'(\omega)$ appears in the spectral density Eq.(2.49).

The correlation function Eq.(2.49) has been obtained for the first time by Nyquist [31] but without the first term in Eq.(2.52). Later, the spectral density

has been corrected by Callen and Welton [32]. In both of these studies the voltage fluctuations of a resistor in a circuit has been considered as a physical system.

By using the Ehrenfest theorem, the quantum Langevin equation (2.39) can be expressed in terms of c-number (semiclassical) quantities as

$$\frac{dP}{dt} = -\frac{\partial U}{\partial Q} - \int_{t_0}^{t} \chi(t-t')P(t')dt' + R(t) + F(t), \tag{2.53}$$

where $R(t)$ is a mean zero quantum noise with the spectral distribution Eq.(2.49). There are two differences between the quantum c-number Langevin equation (2.53) and the classical generalized Langevin equation (2.29). One is the correlation functions of the stochastic forces and the other one is the extra term, $F(t)$, appearing in the quantum Langevin equation (2.53). This extra term,

$$F(t) = U'\left(\{\hat{Q}\}\right) - \left\{\hat{U}'(\hat{Q})\right\}, \tag{2.54}$$

is the quantum dispersion of the force $U' = \partial U/\partial Q$ [33]. $F(t)$ is due to the quantum nature of systems with non-linear external forces U'. It is clear that for linear external forces, the force dispersion $F(t)$ vanishes. $\{...\}$ represents the expectation value.

CHAPTER 3

HEAVY-ION FUSION REACTIONS

The heavy-ion reactions are one of the major subjects of study in nuclear physics today. The understanding of the collision dynamics of the nuclei provides very fruitful information about the nuclear structure and the properties of nuclei. Below, we explain the motivation and reaction mechanism of the fusion reactions of heavy nuclei.

3.1 Motivation: Superheavy Elements

Since the times of Mendeleev who formed the periodic table, many new elements have been added to the periodic table including the noble and radioactive elements. The discoveries of elements found on earth went on until the Uranium which has an atomic number $Z = 92$. The elements heavier than Uranium have been produced artificially and except Neptunium $Z = 93$ and Plutonium $Z = 94$ none of them exist naturally on Earth due to their short half lives compared to that of the Earth. These heavy elements are all radioactive and called transuranic elements. The discovery of the shell structure within nucleus has

invoked the possibility to produce even heavier elements called superheavy elements (SHE). The closed shells give extra stability to the nuclear structure with the corresponding neutron or proton numbers called magic numbers. The magic proton number next to $Z = 82$ is $Z = 114, Z = 120$ or $Z = 126$, depending on the model employed, while the magic neutron number next to $N = 126$ is predicted to be $N = 184$ [34]. The existence of doubly closed shell structure in the superheavy regime introduced the terminology "island of stability" which is the predicted region of superheavy elements with half-lives longer by several orders of magnitude than the neighboring isotopes or elements. The half-life of an ordinary superheavy nuclei before disintegrating into smaller parts is of order of nanoseconds whereas in the island of stability the half-life of a superheavy nuclei is predicted to be of orders of seconds or minutes. This predicted long half-life is the main motivation for the studies devoted to synthesizing the superheavy elements. Once synthesized, the long-lived superheavy elements will be a good test for the nuclear structure models.

The production of the heavy elements is performed by two methods. The first one is the neutron capture method where long-lived massive isotopes are bombarded with an intense beam of neutrons. Some of those neutrons are captured and through beta decay are transformed to protons. This method allows production of elements up to Fermium (Fm) Z=100 and heavier nuclei cannot be produced since they decay before they have enough time to capture another

neutron [35]. The second method is the fusion reaction of heavy ions which is the only mechanism by which the superheavy nuclei can be synthesized and therefore is very important. The heaviest actinides are fused with light elements from B to O and the resulting compound nucleus has an excitation energy about 40-50 MeV. This is know as actinide-based or hot fusion reactions which allowed the production of elements up to Seaborgium (Sg) Z=106. The trouble in this method is that the collision of two nuclei leaves the compound nucleus in a highly excited state which means that it is more likely the compound nucleus undergoes fission. Furthermore, the shell structure is destroyed at high excitations. In the cold fusion reactions, closed-shell nuclei like ^{208}Pb and ^{209}Bi are fused with medium-weight neutron-rich isotopes as ^{54}Cr to ^{74}Zn leading to less excited (10-20 MeV) configurations. The elements from Z=107 to Z=112 has been synthesized by this approach [36]. Since a less asymmetric combination of target and projectile nuclei are used, the Coulomb repulsion is larger and hence the formation of a compound nucleus in cold fusion reactions is more difficult than the one in the hot fusion reactions. Another limitation of this approach is that a small number of neutrons are contained in the produced compound nucleus which decreases the stability. In order to produce nuclei with larger number of neutrons, a rare neutron rich isotope of Calcium ^{48}Ca is used as a projectile and neutron rich isotopes of actinides are used as targets. The synthesis of $Z = 116$ and $Z = 118$ nuclei has been reported by Lawrence Berkeley National Laboratory (LBNL) scientists [37]

but the results still await a conformation by the other experimental facilities.

Synthesis of superheavy elements is a long-standing and important subject in nuclear physics. It is a challenge both experimentally and theoretically because of the low production probabilities due to the so called fusion hindrance which states that even when the initial center of mass energy is of the same order with the Coulomb barrier the over-passing probability is not 1/2 but much less and to get higher probability an extra energy is required, the so called extra-push energy. The fusion hindrance is an experimental observation and occurs for the condition $Z_p.Z_t > 1600$ where Z_p and Z_t are the projectile and the target atomic numbers, respectively [38]. The existence of the fusion hindrance is due to the strong friction between the fusing nuclei where most of the initial kinetic energy is dissipated into intrinsic (nucleonic) degrees of freedom and due to the fact that the conditional saddle is inside the fusion barrier hence the system should further progress over the conditional saddle to form the compound nucleus.

3.2 The Reaction Mechanism

Enormous experimental effort was used to synthesize the superheavy elements by means of heavy ion fusion reactions but mostly in empirical way since a complete theoretical explanation of the complex dynamics of the heavy ion fusion reactions is not found yet. Since the production cross section of the superheavy

elements is of picobarn level, it is important to develop a more substantial theoretical model of the reaction mechanism and provide predictions about the optimum entrance channels which lead to the synthesis of superheavy elements.

In order to formulate the reaction, one needs to parameterize the evolution of the system in terms of some suitable collective variables. The heavy ion fusion reaction similar to fission reaction is a diffusion process. The reaction is highly dissipative with the associated fluctuations of the dynamical collective variables. Hence, it is possible to draw direct analogy between Brownian motion and heavy ion fusion reactions. The nucleonic degrees of freedom are forming the heat bath and the nuclear collective variables are treated as the ones of Brownian particle.

Now, it is a well established fact that the whole fusion reaction consists of three stages which are treated independently but connected via the conserved physical quantities such as total energy and total angular momentum [35, 39, 40, 41]. The first stage is the approaching phase where the respective nuclei are under the influence of Coulomb repulsion which can be represented by an effective potential barrier for the collective variable under consideration (see Figure 3.1). The mean distance between the center of masses of the nuclei (elongation) and the orbital angular momentum are the two collective variables of this stage. The nuclei can either pass over the Coulomb barrier or undergo the so called 'quasi-fission' where the nuclei do not touch and hence do not lose their identities. The quasi-fission

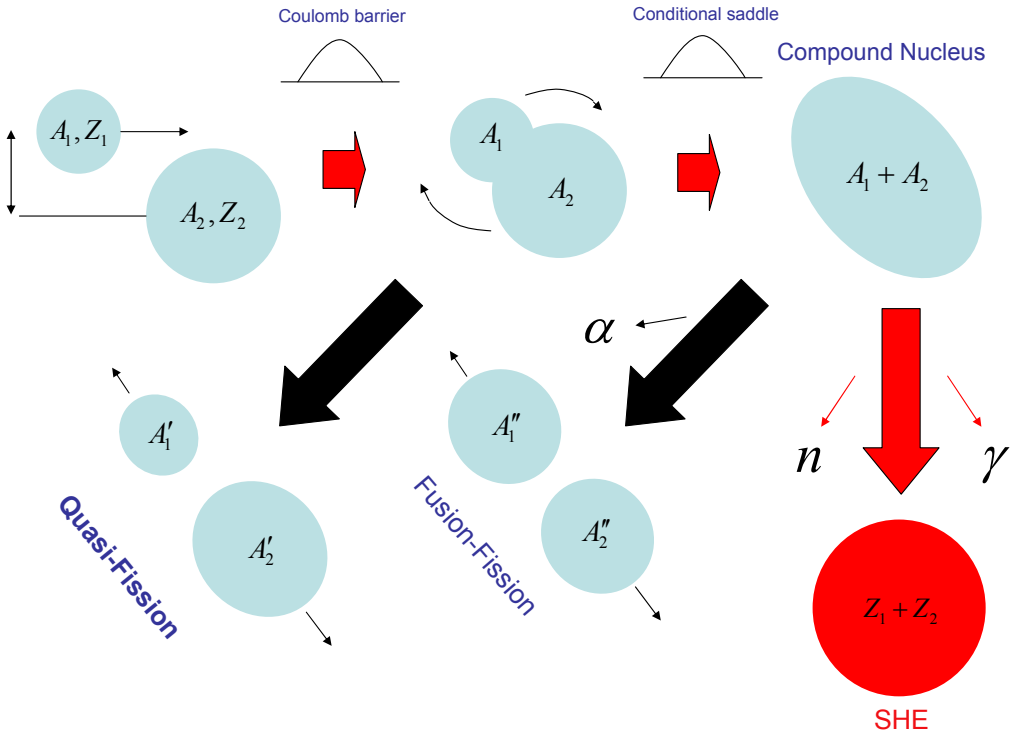

Figure 3.1: Schematic view of the reaction mechanism of the fusion process of the heavy ions.

does not occur for the fusion reactions of light nuclei because the conditional saddle is outside the Coulomb barrier and hence passing over the Coulomb barrier always results with a complete fusion. The intermediate stage called formation (or capture) phase starts when the nuclei touch until the formation of the compound mononucleus. The dynamics of the reaction is cast into a multidimensional space of shape parameters where next to the elongation parameter, the mass asymmetry parameter defined as $\alpha = (A_1 - A_2)/(A_1 + A_2)$, the deformation parameter and

necking parameter should be taken into account for a realistic treatment leading to the compound mononucleus. The pear shaped amalgamated nuclei diffuse over the conditional saddle to form the compound nucleus with a low probability P_{form} since most of the initial kinetic energy is dissipated. The dominant exit channel is the so called 'fusion-fission' with a probability $1 - P_{form}$. The last stage is the deexcitation or cooling of the compound nucleus via γ and light particle emission against the spontaneous fission to give the evaporation residue. This stage is well understood within the statistical decay of atomic nuclei. The division of the whole fusion reaction into three stages is justified by the different time scales of the stages and the fact that the evolution of the stages is governed by different dynamical collective variables.

The production cross section of a residue C formed through the reaction $A_1 + A_2 \rightarrow B \rightarrow C$ is given by [39, 41, 42]

$$\sigma_{ER} = \frac{\pi\hbar^2}{2\mu E_{c.m.}} \sum_{J=1}^{\infty} (2J+1) P^J_{fus}(A_1 + A_2 \rightarrow B; E_{c.m.}) P^J_{surv}(B \rightarrow C; E^*), \quad (3.1)$$

where

$$P^J_{fus}(A_1 + A_2 \rightarrow B; E_{c.m.}) = P^J_{stick}(E_{c.m.}) P^J_{form}(E_{c.m.}). \quad (3.2)$$

A_1 and A_2 represent the target and projectile nuclei and B denotes the compound nucleus, μ is the reduced mass of the nuclei, $E_{c.m.}$ is the initial center of mass energy, J is the angular momentum, E^* is the excitation energy of the compound nucleus, P_{fus} is the fusion probability which is a product of sticking probability

P_{stick} and formation probability P_{form}. The survival probability of the compound nucleus to form the evaporation residue (ER) by emission of γ rays and neutrons against the spontaneous fission or charged particle evaporation is denoted by P_{surv}. When the center of mass energy $E_{c.m.}$ is increased, the fusion probability will increase as well leading to a highly excited compound nucleus and hence the survival probability P_{surv} will decrease. Since the superheavy elements are stabilized by shell correction energies, they should be synthesized at low excitation energies. The initial kinetic energy is one of the parameters which can be tuned to minimize the excitation energy and optimize the residue cross section. The most suitable choices of the center of mass energy are the ones leaving the system at the near-barrier energies where the further evolution of the system from touching to compound nucleus formation is due to the thermal diffusion over the conditional saddle.

In the next chapter, we will consider the quantum statistical effects on the formation process of the reaction which is the least studied reaction stage.

CHAPTER 4

QUANTUM STATISTICAL EFFECTS ON THE HEAVY-ION FUSION REACTIONS

In most of the studies devoted to the nuclear heavy-ion fusion reactions, the evolution of the collective variables is treated as a classical diffusion process [43]. The intermediate stage of the reaction called the formation process is visualized as a diffusion over a conditional saddle where initially most of the collective energy is dissipated due to the fusion hindrance and the system is left at sub-barrier energies. Hence, the evolution of the system over the saddle from the touching configuration to the compound nucleus formation is realized by the thermal fluctuations. It is desirable to obtain a compound nucleus with low excitation since otherwise the compound nucleus cannot resist against fission or charged particle decays and therefore the synthesis of the superheavy elements cannot be achieved. The superheavy elements are stabilized by shell correction energy and hence they should be synthesized at low excitation energies, consequently the quantum effects are expected to play an important role [6, 7, 8].

For the systems with initial near-barrier energies which is the case for the formation stage of the heavy-ion fusion reactions leading to superheavy elements, it is possible to approximate the conditional saddle to a parabolic potential barrier. Then, assuming a constant inertia and constant friction for the collective system as well as a Gaussian distribution for the collective phase space variables, a simple expression for the passing probability over the parabolic potential barrier can be derived [44, 45]. The Gaussian distribution function of the phase space variables is given by

$$\begin{aligned} W(q,p) &= \frac{1}{2\pi\sqrt{\Delta}} \exp\left\{ -\frac{(q-\langle q(t)\rangle)^2\sigma_{pp} + (p-\langle p(t)\rangle)^2\sigma_{qq}}{2\Delta} \right. \\ &\qquad \left. + \frac{2(q-\langle q(t)\rangle)(p-\langle p(t)\rangle)\sigma_{qp}}{2\Delta} \right\}, \end{aligned} \tag{4.1}$$

where $\Delta = \sigma_{qq}\sigma_{pp} - \sigma_{qp}^2$. Integrating the last result over p gives the reduced distribution as

$$W'(q) = \frac{1}{\sqrt{2\pi\sigma_{qq}(t)}} \exp\left(-\frac{(q-\langle q(t)\rangle)^2}{2\sigma_{qq}(t)} \right). \tag{4.2}$$

For the usual initial value choice $q_0 < 0$, the over-passing probability is simply the probability that the system is found on the other side of the potential barrier, hence the probability reads

$$\begin{aligned} P(q_0,p_0,t) &= \int_0^\infty W'(q)dq \\ &= \frac{1}{2}\,\mathrm{Erfc}\left(-\frac{\langle q(t)\rangle}{\sqrt{2\sigma_{qq}(t)}} \right), \end{aligned} \tag{4.3}$$

where Erfc stands for the complimentary error function. It is interesting to observe that the last expression is given only by the mean position $\langle q(t)\rangle$ of the collective system and its variance $\sigma_{qq}(t)$. The argument of the error function in Eq.(4.3) acquires a finite value for the asymptotic time $t \to \infty$.

The over-passing probability has been found numerically and analytically for classical systems [44, 45, 46]. The extension of the classical diffusion of the nuclear collective variables over a parabolic barrier to include quantum effects within linear response theory has been considered in a number of papers with different approaches [6, 7, 8, 47]. In the following sections we review some of these studies where the over-passing probability has been calculated and we discuss our contribution in the last section.

4.1 The Propagator Approach

An explicit expression for the over-passing probability has been obtained by Bao and Boilley [6] by using the real-time path integral propagator approach. Here, we summerize their result. In their work, they have adopted the standard model where the collective system is coupled to infinite number of harmonic oscillators. Assuming a parabolic potential barrier of the form,

$$U(q) = -\frac{1}{2}M\Omega^2 q^2, \tag{4.4}$$

for the collective system and an initial state for the reduced density operator described by an initial position $q_0 < 0$ and average momentum $p_0 > 0$, they have

derived an expression for the reduced density function given by

$$\tilde{\rho}(q,t) = C \exp\left[-\frac{(q-\langle q(t)\rangle)^2}{2\sigma_q^2(t)}\right], \tag{4.5}$$

where C is a normalization constant and

$$\begin{aligned}\langle q(t)\rangle &= \exp\left(-\frac{\beta}{2}t\right)\left\{q_0\left[\frac{\beta}{\beta'}\sinh\left(\frac{1}{2}\beta' t\right)+\cosh\left(\frac{1}{2}\beta' t\right)\right]\right. \\ &\left.+\frac{2p_0}{M\beta'}\sinh\left(\frac{1}{2}\beta' t\right)\right\}, \end{aligned}\tag{4.6}$$

$$\begin{aligned}\sigma_q^2(t) &= \left[\frac{M\beta'\exp\left(\frac{\beta}{2}t\right)}{4\sinh\left(\frac{1}{2}\beta' t\right)}\right]^{-2}\left\{\frac{\hbar M\beta}{\pi}\int_0^{\omega_c}\frac{\omega\coth\left(\frac{\hbar\omega}{2k_BT}\right)}{a^2+\omega^2}d\omega+\sigma_{p_0}^2\right. \\ &\left.+\sigma_{q_0}^2M^2\left[\beta+\beta'\coth\left(\frac{1}{2}\beta' t\right)\right]^2\right\}, \end{aligned}\tag{4.7}$$

are the mean and variance of the collective position, respectively. In the last two equations M, $\sigma_{q_0}^2$ and $\sigma_{p_0}^2$ stand for the inertia of the collective system, initial variances of the position and momentum, respectively. $a = (\beta' - \beta)/2$ is the positive root of the secular equation $a^2 + \beta a - \Omega^2 = 0$ and $\beta' = (\beta^2 + 4\Omega^2)^{1/2}$ [46]. The mean position given by Eq.(4.6) is the same with the classical one as expected from the Ehrenfest theorem [46]. But the variance $\sigma_q^2(t)$ is different since it depends on the correlation function which carries the quantum effects (see Section 2.6).

The expressions derived here are Markovian i.e. no memory effects are included and in the Markovian approach a cut-off frequency ω_c is required to guarantee a finite value for the integral appearing in the Eq.(4.7). For $\omega_c \to \infty$, the

integral is logarithmically divergent. As discussed in the next sections, it is possible to obtain convergent variance $\sigma_q^2(t)$ by including the non-Markovian effects which will play the role of a cut-off function and the inverse of the memory time will be the cut-off parameter.

For long times, the over-passing probability Eq.(4.3) obtains the asymptotic value,

$$P(q_0, p_0, t \to \infty) = \frac{1}{2} \operatorname{Erfc}\left(\frac{\frac{1}{2}(\beta + \beta')q_0 + \frac{1}{M}p_0}{\Phi(\sigma_{q_0}^2, \sigma_{p_0}^2)} \right), \tag{4.8}$$

where

$$\Phi(\sigma_{q_0}^2, \sigma_{p_0}^2) = \left\{ \frac{2\hbar\beta}{M\pi} \int_0^{\omega_c} \frac{\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right)}{a^2 + \omega^2} d\omega + \frac{2}{M^2}\sigma_{p_0}^2 + \frac{(\beta + \beta')^2}{2}\sigma_{q_0}^2 \right\}^{1/2}. \tag{4.9}$$

4.2 Quantum Fokker-Planck Approach

A different approach based on a density matrix formalism leading to the non-Markovian Fokker-Planck equation for the collective degrees of freedom has been developed by Takigawa et. al. [7]. We largely follow their derivation. The starting point is the von Neumann equation for the time evolution of the density matrix of the global system,

$$i\hbar \frac{\partial}{\partial t}\hat{\rho}(t) = [\hat{H}, \hat{\rho}(t)], \tag{4.10}$$

where the Hamiltonian is assumed to have the form,

$$\hat{H} = \hat{H}_A + \hat{H}_B + \hat{V}_c(\hat{q}, \hat{x}), \tag{4.11}$$

with the Hamiltonian of the collective subspace A given by,

$$\hat{H}_A = \frac{\hat{p}^2}{2M} + \hat{U}(\hat{q}). \tag{4.12}$$

$\hat{U}(\hat{q})$ is the parabolic potential of the collective motion given by Eq.(4.4). H_B is the environment (bath) Hamiltonian and $\hat{V}_c(\hat{q}, \hat{x})$ is the coupling Hamiltonian. With the use of the Ehrenfest theorem, the c-number position $q(t)$ and momentum $p(t)$ variables can be introduced as

$$\begin{aligned} q(t) &= Tr(\hat{q}\hat{\rho}(t)), \\ p(t) &= Tr(\hat{p}\hat{\rho}(t)). \end{aligned} \tag{4.13}$$

It is convenient to work with the Galilei transformed quantities with vanishing average values, in order to deal only with the fluctuations around the average values. The Hamiltonian in the Galilei transformed picture is expanded up to the second order terms of the fluctuations. The coupled equations for the densities of the subspaces A and B are solved by using the perturbation method. Then, a von Neumann equation for the relevant density is obtained as

$$\begin{aligned} \frac{\partial}{\partial t}\hat{D}_A(t) &= \frac{1}{i\hbar}[\frac{\hat{p}^2}{2M} + \frac{1}{2}C\hat{q}^2, \hat{D}_A(t)] \\ &\quad -\frac{1}{\hbar^2}[\hat{q}, [\chi^{(+E)}(t)\hat{q} - \chi^{(+O)}(t)\hat{p}, \hat{D}_A(t)]] \\ &\quad -\frac{1}{2i\hbar}[\hat{q}, [\chi^{(-E)}(t)\hat{q} - \chi^{(-O)}(t)\hat{p}, \hat{D}_A(t)]_+], \end{aligned} \tag{4.14}$$

where

$$\chi^{(\pm E)}(t) = \int_{t_0}^{t} dt_1 \mathcal{C}(t, t_1)\chi^{(\pm)}(t, t_1), \tag{4.15}$$

$$\chi^{(\pm O)}(t) = \int_{t_0}^{t} dt_1 \mathcal{S}(t,t_1)\chi^{(\pm)}(t,t_1), \tag{4.16}$$

with

$$\mathcal{C}(t,t_1) = \cosh[\Omega(t-t_1)], \tag{4.17}$$

$$\mathcal{S}(t,t_1) = \frac{1}{M\Omega}\sinh[\Omega(t-t_1)], \tag{4.18}$$

and

$$\chi^{(-)}(t,t_1) = \frac{i}{\hbar} Tr_B([\hat{f}(t),\hat{f}(t_1)]\hat{D}_B(t_1)), \tag{4.19}$$

$$\chi^{(+)}(t,t_1) = \frac{1}{2} Tr_B([\hat{f}(t),\hat{f}(t_1)]_+\hat{D}_B(t_1)). \tag{4.20}$$

The fluctuating force operator $\hat{f}(t)$ is given by

$$\hat{f}(t) = \hat{u}_B^{\dagger}(t,t_0)\left\{\frac{\partial V_c(q(t),\hat{x})}{\partial q} - Tr\left[\frac{\partial V_c(q(t),\hat{x})}{\partial q}\hat{\rho}_G(t)\right]\right\}\hat{u}_B(t,t_0), \tag{4.21}$$

where $\hat{u}_B(t,t_0)$ is the time evolution operator for the subspace B and $\hat{\rho}_G(t)$ is the density operator in the Galilei transformed picture. The functions $\chi^{(-)}(t,t_1)$ and $\chi^{(+)}(t,t_1)$ are the response and correlation functions, respectively. The superscripts E and O in the Eq.(4.14) and Eq.(4.16) stand for even and odd. By taking the Wigner transform of the von-Neumann equation (4.14) as

$$D_{AW}(p,q,t) = \int_{-\infty}^{\infty} dr e^{-ipr/\hbar} < q + \frac{1}{2}r|\hat{D}_A(t)|q - \frac{1}{2}r > \tag{4.22}$$

the Fokker-Planck equation with the non-Markovain quantal transport coefficients is obtained,

$$\frac{\partial}{\partial t}D_{AW}(t) = \left\{-\frac{1}{M}p\frac{\partial}{\partial q} - M\Omega^2 q\frac{\partial}{\partial p} - \chi^{(-E)}q\frac{\partial}{\partial p} + \chi^{(-O)}\frac{\partial}{\partial p}p\right.$$

$$+ \chi^{(+O)}\frac{\partial^2}{\partial p\partial q} + \chi^{(+E)}\frac{\partial^2}{\partial p\partial p}\Bigg\} D_{AW}(p,q,t). \qquad (4.23)$$

Assuming a Gaussian form for the density $D_{AW}(t)$ as

$$D_{AW}(p,q,t) = \frac{1}{2\pi\Delta^{1/2}} \times \exp\left[-\frac{1}{2\Delta}\begin{pmatrix} q & p \end{pmatrix}\begin{pmatrix} \sigma_{qq} & \sigma_{qp} \\ \sigma_{qp} & \sigma_{pp} \end{pmatrix}^{-1}\begin{pmatrix} q \\ p \end{pmatrix}\right], \quad (4.24)$$

where $\Delta = \sigma_{qq}\sigma_{pp} - \sigma_{qp}^2$ and substituting Eq.(4.24) into Eq.(4.23), we get

$$\begin{aligned}
\frac{d}{dt}\sigma_{qq}(t) &= \frac{2}{M}\sigma_{qp}(t), \\
\frac{d}{dt}\sigma_{qp}(t) &= (M\Omega^2 + \chi^{(-E)})\sigma_{qq}(t) - \chi^{(-O)}\sigma_{qp}(t) + \frac{1}{M}\sigma_{pp}(t) + \chi^{(+O)}, \\
\frac{d}{dt}\sigma_{pp}(t) &= 2(M\Omega^2 + \chi^{(-E)})\sigma_{qp}(t) - 2\chi^{(-O)}\sigma_{pp}(t) + 2\chi^{(+E)}. \qquad (4.25)
\end{aligned}$$

In order to find the over-passing probability Eq.(4.3), the knowledge of the mean and the variance of the position is required. The average position is the same with the classical one and given by Eq.(4.6). On the other hand, the variance should be calculated from the coupled equations (4.25) which depend on the transport coefficients $\chi^{(\pm E)}$ and $\chi^{(\pm O)}$. By defining a spectral density as

$$J(t;\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} Tr_B(\hat{f}(t)\hat{f}(t_1)\hat{\rho}_B(t_1)), \qquad (4.26)$$

where $\tau = t - t_1$, it is possible to obtain the response and correlation functions as

$$\begin{aligned}
\chi^{(-)}(t,t_1) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega\tau}\frac{i}{\hbar}\left(1 - e^{-\beta(t)\hbar\omega}\right)J(t;\omega), \qquad (4.27) \\
\chi^{(+)}(t,t_1) &= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega\tau}\frac{1 + e^{-\beta(t)\hbar\omega}}{2}J(t;\omega), \qquad (4.28)
\end{aligned}$$

which are obtained by using Eq.(4.19) and Eq.(4.20) together with the property

$$J(t;\omega) = e^{\beta(t)\hbar\omega} J(t;-\omega). \tag{4.29}$$

The spectral function $J(t;\omega)$ reads

$$J(t;\omega) = 2\pi J(\omega)\,\frac{1}{1-e^{-\beta(t)\hbar\omega}} \qquad (\omega > 0) \tag{4.30}$$

where $J(\omega)$ is given by either Eq.(2.33) for Drude regularization (Lorentzian cut-off) or Eq.(2.35) for Gaussian cut-off. In obtaining the results Eqs.(4.27,4.28,4.30) a weak bilinear coupling of the collective system to the heat bath is assumed so that the linear response theory can be employed. It is also assumed that the density for the bath space is given by a canonical distribution, $\rho_B(t) \propto \exp\left[\beta(t)(F-\hat{h}_B)\right]$.

The correlation and response functions are obtained by substituting Eq.(4.27) and Eq.(4.28) into Eq.(4.15) and Eq.(4.16). Then, the variance $\sigma_{qq}(t)$ is evaluated by numerical integration of the coupled equations Eq.(4.25).

In this study it is shown that the over-passing probability is enhanced at low temperatures and recovers the classical value at high temperatures.

4.3 Quantum Langevin Approach

The inclusion of quantum statistical effects to the nuclear collective dynamics is achieved by using an approach based on Langevin formulation [8]. We closely follow our derivation in [8]. In this approach, we consider the same model for the

Hamiltonian Eq.(4.11),

$$\hat{H} = \hat{H}_{coll} + \hat{H}_0 + \hat{V}_{coup} \tag{4.31}$$

where $\hat{H}_{coll}$, $\hat{H}_0$ and $\hat{V}_{coup}$ represent the Hamiltonian of the collective variable, the Hamiltonian of the intrinsic nucleonic degrees of freedom, and the coupling potential of the collective variable with the intrinsic nucleonic degrees of freedom, respectively. For simplicity, we consider a harmonic form for the collective Hamiltonian $\hat{H}_{coll} = \hat{p}^2/2M \pm M\Omega^2\hat{q}^2/2$, where M is the mass parameter of the collective variable and $M\Omega^2$ denotes the magnitude of the curvature parameter of the potential, positive sign stands for a parabolic potential well and negative sign for a parabolic potential barrier. Furthermore, we assume that the coupling Hamiltonian has a linear form, $\hat{V}_{coup} = \hat{q}\hat{F}$. The classical equation of motion for the collective variable can be deduced by using the Heisenberg equations of motion:

$$\frac{d}{dt}q(t) = \frac{1}{i\hbar}\left([\hat{q}, \hat{H}]\right), \tag{4.32}$$

$$\frac{d}{dt}p(t) = \frac{1}{i\hbar}\left([\hat{p}, \hat{H}]\right), \tag{4.33}$$

where $(...) = Tr(...\hat{\rho})$ denotes an average over the intrinsic degrees of freedom, to give,

$$\frac{d}{dt}q(t) = \frac{1}{M}p(t) \qquad \text{and} \qquad \frac{d}{dt}p(t) \pm M\Omega^2 q(t) = -Tr(\hat{F}\hat{\rho})\,. \tag{4.34}$$

Here, the quantity on the right hand side of the second equation denotes the force of the intrinsic degrees of freedom on the collective motion. We consider the case

where the coupling $\hat{F}$ is a one-body operator. We then need only the single-particle density matrix $\hat{\rho}$ of the intrinsic degrees of freedom to calculate the force. As we discuss below, temporal evolution of the single-particle density matrix exhibits a stochastic behavior. As a result, the intrinsic force has a fluctuating part on the top of its average value. Here, we find it more convenient to calculate the fluctuating part of force, which is determined by the fluctuating part of the single-particle density matrix $\delta\hat{\rho}(t) = \hat{\rho}(t) - \bar{\hat{\rho}}(t)$, where the bar means taking ensemble average. Assuming the fluctuations are small, $\delta\hat{\rho}(t)$ is determined by a linearized transport equation [48] around the average $\bar{\hat{\rho}}(t)$,

$$i\hbar\frac{\partial}{\partial t}\delta\hat{\rho}(t) - [\bar{\hat{h}}(t), \delta\hat{\rho}(t)] - [\delta q(t)\hat{F}, \bar{\rho}(t)] = 0 \tag{4.35}$$

where $\bar{\hat{h}}(t) = \hat{h} + \bar{q}(t)\hat{F}$, $\hat{h}$ being the Hartree-Fock Hamiltonian of the separated nuclei and $\delta q(t) = q(t) - \bar{q}(t)$ denotes the fluctuation of the collective variable around its average value $\bar{q}(t)$. The ensemble average value of the density matrix is determined by,

$$i\hbar\frac{\partial}{\partial t}\bar{\hat{\rho}}(t) - [\bar{\hat{h}}(t), \bar{\hat{\rho}}(t)] = 0\,. \tag{4.36}$$

For simplicity of derivation, we neglect the collision term on the right hand side of Eq.(4.35) and Eq.(4.36) [43, 49, 50], however subsequently, we incorporate the damping width of single-particle states. Starting from an initial state $\delta\hat{\rho}(s)$ at some time s, the formal solution of Eq.(4.35) can be given as,

$$\delta\hat{\rho}(t) = -\frac{i}{\hbar}\int_s^t dt'\delta q(t')\left[\hat{G}(t,t')\hat{F}\hat{G}^\dagger(t,t'), \bar{\hat{\rho}}(t)\right] + \hat{G}(t,s)\delta\hat{\rho}(s)\hat{G}^\dagger(t,s) \tag{4.37}$$

where the first term describes the effects of the perturbation during the time interval $t-s$ with $\hat{G}(t,s) = \exp\left[-(i/\hbar)\int_s^t dt'\bar{\hat{h}}(t')\right] \approx \exp\left[-(i/\hbar)(t-s)\bar{\hat{h}}(t)\right]$ as the mean-field propagator, i.e. the propagator in the absence of thermal fluctuation, and the second term represent the propagation of the initial fluctuations $\delta\hat{\rho}(s)$ of the intrinsic degrees of freedom during the time interval from s to t. Here, the initial time s does not represent the remote past, but rather it is sufficiently close to the time t, so that the time interval is much shorter than the relaxation time of the intrinsic degrees of freedom $t-s \ll \tau_{rel}$. Hence, the neglect of correlations due to collision term is justified in the description of Eq.(4.37). In this case, the effect of correlations enters through the initial fluctuation term. Furthermore, we assume that the collective motion is sufficiently slow so that the intrinsic degrees of freedom is close to local equilibrium for each value of the collective variable. In order to evaluate the matrix elements of the fluctuating part of the density operator based on Eq.(4.37), we approximate the average density matrix in terms of the instantaneous single-particle wave functions as $\bar{\hat{\rho}}(t) \approx \sum |\phi_l(t)\rangle n_l \langle\phi_l(t)|$, where we neglect the off diagonal elements. In this expression, the instantaneous wave functions $\phi_l(t) = \phi_l[q(t)]$ are determined from $(\hat{h} + q\hat{F})|\phi_l(q)\rangle = \varepsilon_l(q)|\phi_l(q)\rangle$ for each value of the collective variable q, and $n_i = 1/\left[\exp\left[(\varepsilon_i - \varepsilon_F)/T\right] + 1\right]$ denotes the Fermi-Dirac occupation factor at a temperature T. Employing the instantaneous representation, the matrix elements of fluctuations can be expressed as,

$$\delta\rho_{ij}(t) = -\frac{i}{\hbar}\int_s^t dt'\delta q(t')G_{ij}(t,t')\langle i|\hat{F}|j\rangle(n_j - n_i) + G_{ij}(t,s)\delta\rho_{ij}(s) \qquad (4.38)$$

with $G_{ij}(t,s) = \exp[-i(t-s)(\varepsilon_i - \varepsilon_j)/\hbar]$. It is not possible to determine detailed structure of initial fluctuations of the intrinsic degrees of freedom. Therefore, it is plausible to assume that each matrix element of $\delta\hat{\rho}(s)$ is a Gaussian random quantity with zero mean $\overline{\langle i|\delta\hat{\rho}|j\rangle} = 0$. In accordance with the fluctuation-dissipation relation of the single-particle density matrix, we specify the second moment of $\delta\hat{\rho}(s)$ as,

$$\overline{\langle i|\delta\hat{\rho}|j\rangle\langle j'|\delta\hat{\rho}|i'\rangle} = \delta_{ii'}\delta_{jj'}\frac{1}{2}\left[n_i(1-n_j) + n_j(1-n_i)\right] . \tag{4.39}$$

In the special case of diagonal elements this formula gives the known result for fluctuations of occupation numbers, $\overline{\langle i|\delta\hat{\rho}|i\rangle\langle i|\delta\hat{\rho}|i\rangle} = n_i(1-n_i)$ [51]. Substituting Eq.(4.37) into the right hand side of Eq.(4.34), we find a generalized Langevin equation for the fluctuations of the collective variable,

$$\frac{d}{dt}\delta p(t) \pm M\Omega^2\delta q(t) = \int_s^t dt'\gamma(t-t')\delta q(t') + \xi(t) \tag{4.40}$$

where the memory kernel in the retarded force and the random force term are given by

$$\gamma(t-t') = \frac{i}{\hbar}\sum |\langle i|\hat{F}|j\rangle|^2 G_{ji}(t,t')\left[n_i(1-n_j) - n_j(1-n_i)\right] \tag{4.41}$$

and

$$\xi(t) = -\sum \langle i|\hat{F}|j\rangle G_{ji}(t,s)\langle j|\delta\hat{\rho}|i\rangle. \tag{4.42}$$

Using Eq.(4.39), the auto-correlation function of the random force can be

expressed as,

$$\begin{aligned}\overline{\xi(t)\xi(t')} &= \sum |\langle i|\hat{F}|j\rangle|^2 G_{ij}(t,t')\frac{1}{2}\left[n_i(1-n_j)+n_j(1-n_i)\right] \\ &= \sum \frac{|\langle i|\hat{F}|j\rangle|^2}{\hbar\omega_{ji}} G_{ij}(t,t')\frac{\hbar\omega_{ji}}{2}\coth\left(\frac{\hbar\omega_{ji}}{2T}\right) \\ &\qquad \times \left[n_i(1-n_j)-n_j(1-n_i)\right] , \end{aligned} \tag{4.43}$$

where $\hbar\omega_{ji} = \varepsilon_j - \varepsilon_i$ and the equation $n_j(1-n_i) = \exp(\hbar\omega_{ij}/T)n_i(1-n_j)$ has been used. Dissipation and fluctuation aspects of dynamics are closely connected to each other, the similarity of expressions for the correlation function and the memory kernel reflects this fact. If the decay time of the memory kernel is sufficiently short, we can explicitly incorporate the memory effect into the retarded force in Eq.(4.40). For evolution over a short time interval from t' to t, by neglecting the right hand side of Eq.(4.40), we find the following relation,

$$\delta q(t') \approx C(t-t')\delta q(t) - S(t-t')\delta p(t)\,. \tag{4.44}$$

For a parabolic potential well, propagators $C(t-t')$ and $S(t-t')$ are given by,

$$C(t-t') = \cos\Omega(t-t') \qquad \text{and} \qquad S(t-t') = \frac{1}{M\Omega}\sin\Omega(t-t')\,. \tag{4.45}$$

On the other hand, for a parabolic potential barrier, these propagators are given by,

$$C(t-t') = \cosh\Omega(t-t') \qquad \text{and} \qquad S(t-t') = \frac{1}{M\Omega}\sinh\Omega(t-t')\,. \tag{4.46}$$

The first term in Eq.(4.44) involving $\delta q(t)$ introduces a shift in the curvature parameter of the potential. Here, we neglect this effect and substitute the second

term on the right hand side of Eq.(4.44) into the right hand side of Eq.(4.40). Note that, since the fluctuations are linear, the same equation as Eq.(4.40), but without the last term on the right hand side, holds for the average evolution by replacing $\delta p(t)$ and $\delta q(t)$ with $\bar{p}(t)$ and $\bar{q}(t)$, respectively. Therefore, combining the average evolution with the fluctuations, we obtain a generalized Langevin equation for the actual variables, $p(t) = \bar{p}(t) + \delta p(t)$ and $q(t) = \bar{q}(t) + \delta q(t)$,

$$\frac{d}{dt}p(t) \pm M\Omega^2 q(t) = -\beta p(t) + \xi(t)\,. \tag{4.47}$$

Here, the reduced friction coefficient is given by,

$$\beta = \frac{i}{\hbar}\int_0^{t-s} d\tau \sum |\langle i|\hat{F}|j\rangle|^2 e^{-\frac{i}{\hbar}\tau(\varepsilon_j-\varepsilon_i)} n_i(1-n_j)S(\tau) + c.c.\,. \tag{4.48}$$

Substituting Eqs.(4.45) and (4.46) for $S(\tau)$, we find for the friction coefficient for a parabolic well,

$$\begin{aligned}\beta &= -\frac{1}{2iM\Omega}\sum |\langle i|\hat{F}|j\rangle|^2 \left[\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i-\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i-\hbar\Omega-i\eta}\right. \\ &\qquad \left. -\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i+\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i+\hbar\Omega-i\eta}\right] n_i(1-n_j) \\ &\quad + c.c.\end{aligned} \tag{4.49}$$

and for a parabolic barrier,

$$\begin{aligned}\beta &= +\frac{1}{2M\Omega}\sum |\langle i|\hat{F}|j\rangle|^2 \left[\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i-i\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i-i\hbar\Omega-i\eta}\right. \\ &\qquad \left. -\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i+i\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i+i\hbar\Omega-i\eta}\right] n_i(1-n_j) \\ &\quad + c.c.\,.\end{aligned} \tag{4.50}$$

In obtaining these results, we include the damping width η of the single-particle states into the propagator in Eq.(4.48) [52]. In further evaluation of the friction coefficients, we neglect the time-dependent terms in Eq.(4.49) and Eq.(4.50). The reason is the following: the dominant contributions to the friction coefficient arise from the coupling matrix element over an energy interval of the order of major shell spacing, $\varepsilon_j - \varepsilon_i = \Delta \approx 10$ MeV, which is much larger than typical values of collective frequency we consider here, $\hbar\Omega \approx 1.0$ MeV. If the single-particle spectrum is sufficiently dense, the summations over the single particle states can be converted to energy integrals. As a result, exponential factors in Eq.(4.49) and Eq.(4.50) damp out over a time interval of the order of $\tau_0 = \hbar/\Delta$. Furthermore, in particular for low frequency collective motion, $\hbar\Omega \leq \eta$, these exponential factors damp out even over a shorter time scale as a result of damping of the single-particle states. Therefore, for a sufficiently long time interval, $t - s \gg \tau_0$, neglecting time dependent terms, we have for a parabolic well,

$$\begin{aligned} \beta &= \sum |\langle i|\hat{F}|j\rangle|^2 \frac{1}{M\Omega} \left[\frac{\eta}{(\varepsilon_j - \varepsilon_i - \hbar\Omega)^2 + \eta^2} \right. \\ &\qquad \left. - \frac{\eta}{(\varepsilon_j - \varepsilon_i + \hbar\Omega)^2 + \eta^2} \right] n_i(1 - n_j) \end{aligned} \tag{4.51}$$

and for a parabolic barrier,

$$\begin{aligned} \beta &= \sum |\langle i|\hat{F}|j\rangle|^2 \frac{1}{M\Omega} \left[\frac{\varepsilon_j - \varepsilon_i}{(\varepsilon_j - \varepsilon_i)^2 + (\hbar\Omega - \eta)^2} \right. \\ &\qquad \left. - \frac{\varepsilon_j - \varepsilon_i}{(\varepsilon_j - \varepsilon_i)^2 + (\hbar\Omega + \eta)^2} \right] n_i(1 - n_j)\,. \end{aligned} \tag{4.52}$$

As seen from these results, for finite Ω, the friction coefficient has different expressions around a well and a barrier. However, in the limit $\Omega \to 0$, it can be easily seen that these expressions become identical, known as the one-body friction formula. We call this limiting value as the classical friction coefficient and denote as β_0. We introduce the Fourier transform of the correlation function of the random force [17],

$$\overline{\xi(t)\xi(t')} = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \frac{\hbar\omega}{2T} \coth \frac{\hbar\omega}{2T} \cdot 2D(\omega) \tag{4.53}$$

where,

$$\begin{aligned} D(\omega) &= T \sum |\langle i|\hat{F}|j\rangle|^2 \frac{1}{\omega} \left[\frac{\eta}{(\varepsilon_j - \varepsilon_i - \hbar\omega)^2 + \eta^2} \right. \\ &\qquad \left. - \frac{\eta}{(\varepsilon_j - \varepsilon_i + \hbar\omega)^2 + \eta^2} \right] n_i(1 - n_j)\,. \end{aligned} \tag{4.54}$$

At low frequencies, $D(\omega)$ is just $D(\omega \to 0) = D_0 = MT\beta_0$ the classical diffusion coefficient. On the other hand, the high frequency behavior is restricted by the magnitude of the coupling matrix elements. If the single particle spectrum is sufficiently dense, the magnitude of coupling matrix elements must decrease as a function of energy difference, mainly due to the mismatch of the overlap of the wave functions. We can represent this behavior by a Gaussian or a Lorentzian function $\langle i|\hat{F}|j\rangle^2 \propto \exp[-(\varepsilon_j - \varepsilon_i)^2/2\Delta^2]$ or $\propto 1/\left[1 + (\varepsilon_j - \varepsilon_i)^2/2\Delta^2\right]$. Furthermore, because of the Lorentzian factors in Eq.(4.54), we can replace the energy difference $\varepsilon_j - \varepsilon_i$ with the frequency $\hbar\omega$ and approximately describe frequency dependence of diffusion coefficient as $D(\omega) = D_0 \exp\left[-(\hbar\omega)^2/2\Delta^2\right]$, here we take

the Gaussian for the frequency spectrum. As a result, the correlation function Eq.(4.53) of the random force can be expressed as,

$$\overline{\xi(t)\xi(t')} = 2D_0 \cdot \chi(t-t') \tag{4.55}$$

where

$$\chi(t-t') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \frac{\hbar\omega}{2T} \coth\frac{\hbar\omega}{2T} \cdot \exp\left[-(\hbar\omega)^2/2\Delta^2\right] . \tag{4.56}$$

The correlation function is characterized by two different parameters, the cut-off energy and temperature. Figure 4.1 shows the correlation function versus time at different temperatures $T = 0.5$ MeV, 1.0 MeV and 5.0 MeV. The results presented in this work are not very sensitive to the cut-off energy over a range of values $\Delta = 10-20$ MeV. Therefore, in this figure and all other figures, we employ $\Delta = 15$ MeV for the cut-off energy. At relatively high temperature $\hbar\omega \ll 2T$, $(\hbar\omega/2T)\coth(\hbar\omega/2T) \approx 1$, and the correlation function reduces to its classical form,

$$\begin{aligned} \chi_0(t-t') &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \exp\left[-\frac{(\hbar\omega)^2}{2\Delta^2}\right] \\ &= \frac{1}{\sqrt{2\pi}\tau_0} \exp\left[-(t-t')^2/2\tau_0^2\right] . \end{aligned} \tag{4.57}$$

For sufficiently short decay time τ_0, it can be approximated by a delta function, $\chi_0(t-t') \to \delta(t-t')$, and as a result at high temperatures, the temporal evolution becomes Markovian and the random force $\xi(t)$ acts like a white noise. However, as seen from the Figure 4.1, in the quantal regime i.e. at low temperatures $\hbar\Omega \geq 2T$, we are faced with a stochastic evolution with a correlated noise [19, 53].

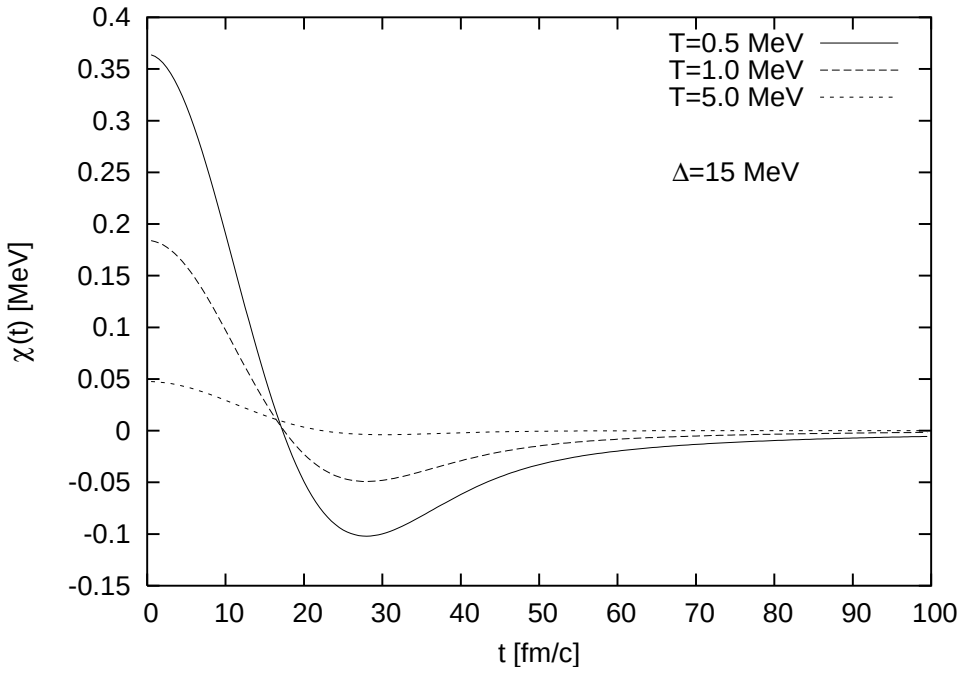

Figure 4.1: The correlation function is plotted versus time for $\Delta = 15$ MeV.

4.3.1 Analysis of the Langevin Equation

In order to obtain the joint probability distribution function $P(q, p, t)$ of the collective variable and its conjugate momentum (q, p) by numerical simulation of the Langevin equation, in general, we need to generate a sufficiently large ensemble of trajectories. Since, we have a correlated noise problem, we cannot use the standard methods [43, 46, 54] and we need to adopt suitable algorithms for numerical simulations. However, in the situation that we consider here, the solution of the Langevin equation (4.47) can be given analytically [10]. Since the equation is linear with a Gaussian random source, the probability distribution $P(q, p, t)$ of collective variables is also Gaussian, which is determined by the mean values $\overline{q}(t)$,

$\overline{p}(t)$ and the variances $\sigma_{qq}(t) = \overline{\delta q(t)\delta q(t)}$, $\sigma_{qp}(t) = \overline{\delta q(t)\delta p(t)}$, $\sigma_{pp}(t) = \overline{\delta p(t)\delta p(t)}$ of collective variables according to,

$$P(q,p,t) = \frac{1}{2\pi X}\exp\left\{-\frac{1}{2X^2}\left[(q-\overline{q})^2\tilde{\sigma}_{qq} + 2(q-\overline{q})(p-\overline{p})\tilde{\sigma}_{qp} + (p-\overline{p})^2\tilde{\sigma}_{pp}\right]\right\} \tag{4.58}$$

where $X^2 = \sigma_{qq}\sigma_{pp} - \sigma_{qp}^2$ and $\tilde{\sigma}_{ij}$ is the inverse of the 2×2 matrix (σ_{ij}) with elements $\sigma_{11} = \sigma_{qq}$, $\sigma_{12} = \sigma_{qp}$, $\sigma_{21} = \sigma_{pq}$ and $\sigma_{22} = \sigma_{pp}$. The mean values of collective variables $\overline{q}(t)$, $\overline{p}(t)$ are determined by the classical equations of motion,

$$\frac{d}{dt}\overline{q}(t) = \frac{1}{M}\overline{p}(t) \qquad \text{and} \qquad \frac{d}{dt}\overline{p}(t) \pm M\Omega^2\overline{q}(t) = -\beta\overline{p}(t)\,. \tag{4.59}$$

Equations for variances are deduced from the Langevin equations for the fluctuating quantities $\delta q(t) = q(t) - \overline{q}(t)$ and $\delta p(t) = p(t) - \overline{p}(t)$,

$$\frac{d}{dt}\delta q(t) = \frac{1}{M}\delta p(t) \qquad \text{and} \qquad \frac{d}{dt}\delta p(t) \pm M\Omega^2\delta q(t) = -\beta\delta p(t) + \xi(t)\,. \tag{4.60}$$

Multiplying both sides of these equations by $\delta q(t)$, $\delta p(t)$ and performing ensemble averaging, we find

$$\frac{d}{dt}\sigma_{qq}(t) = \frac{2}{M}\sigma_{qp}(t) \tag{4.61}$$

$$\frac{d}{dt}\sigma_{qp}(t) \pm M\Omega^2\sigma_{qq}(t) = \frac{1}{M}\sigma_{pp}(t) - \beta\sigma_{qp}(t) + D_{qp}(t) \tag{4.62}$$

$$\frac{d}{dt}\sigma_{pp}(t) \pm 2M\Omega^2\sigma_{qp}(t) = -2\beta\sigma_{pp}(t) + 2D_{pp}(t) \tag{4.63}$$

where $D_{pp}(t) = \overline{\delta p(t)\xi(t)}$ and $D_{qp}(t) = \overline{\delta q(t)\xi(t)}$ denotes the momentum and mixed diffusion coefficients, respectively. In order to evaluate diffusion coefficients, we need to calculate the dynamical fluctuations of collective variables in terms of the random force. This is carried out in Appendix A. Using the results for $\delta p(t) = \int_0^t dt' Q(t-t')\xi(t')$ and from Eq.(A.7) and Eq.(A.8), diffusion coefficients can be expressed in terms of the correlation function of the random force as,

$$D_{pp}(t) = \int_0^t dt' Q(t-t') \cdot \overline{\xi(t')\xi(t)} = 2D_0 \int_0^t ds\, Q(s) \cdot \chi(s) \tag{4.64}$$

and

$$D_{qp}(t) = \int_0^t dt' S(t-t') \cdot \overline{\xi(t')\xi(t)} = 2D_0 \int_0^t ds\, S(s) \cdot \chi(s)\,. \tag{4.65}$$

In these expressions, the initial time is taken to be zero for convenience, $t_0 = 0$, and the propagators $Q(s)$ and $S(s)$ associated with collective variables are given by Eq.(A.9) and Eq.(A.10) in Appendix A. At sufficiently high temperatures, correlation function $\chi(s)$ can be approximated by a delta function, and consequently, the momentum diffusion coefficient is time independent and takes its classical value, $D_{pp} = D_0$ and furthermore the mixed diffusion coefficient vanishes, $D_{qp} = 0$. The mixed diffusion coefficient is a genuine non-Markovian term, and it is absent in the Markovian limit. At low temperatures, due to the non-Markovian behavior of the correlation function, diffusion coefficients become time

dependent and their magnitude are strongly modified by the quantum statistical fluctuations. We, also, note that the modified frequency $\overline{\Omega} = \sqrt{\Omega^2 + (\beta/2)^2}$ enters in propagators $Q(s)$ and $S(s)$.

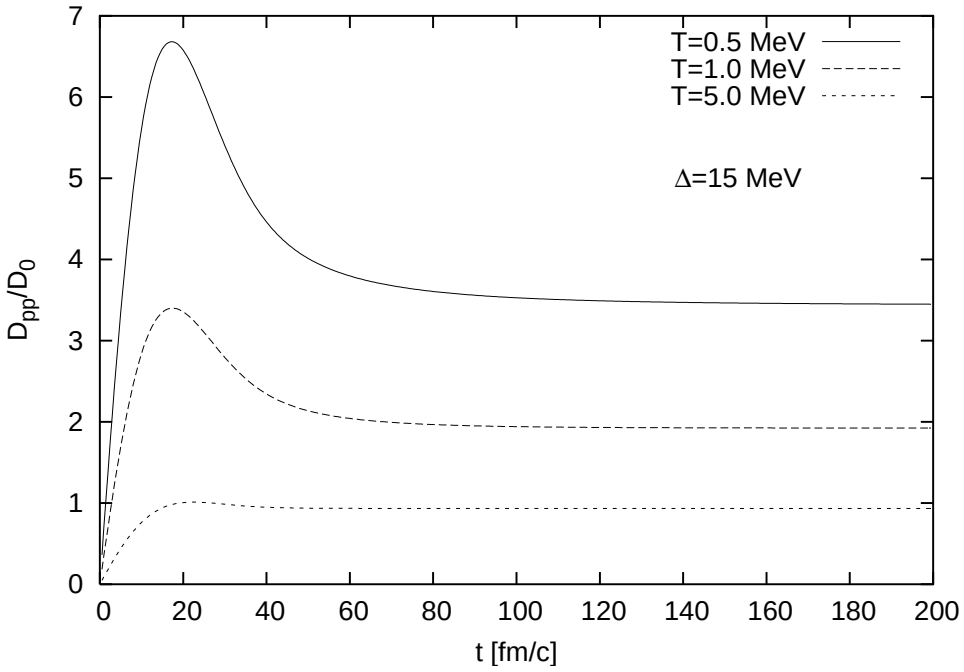

Figure 4.2: The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV.

The typical values of the frequency parameter $\hbar\Omega \approx 1.0$ MeV of the conditional saddle and the magnitude of the reduced friction coefficient $\hbar\beta/2 \approx 1.7$ MeV are comparable. As a result, the friction coefficient introduces a sizable modification of diffusion coefficients, which was not incorporated in the previous investigation [7]. Figures 4.2 and 4.3 show the diffusion coefficients in units of D_0, i.e., D_{pp}/D_0 and D_{qp}/D_0, as a function of time for different values of temperature, $T = 0.5$ MeV, $T = 1.0$ MeV and $T = 5.0$ MeV. In order to illustrate the effect of friction

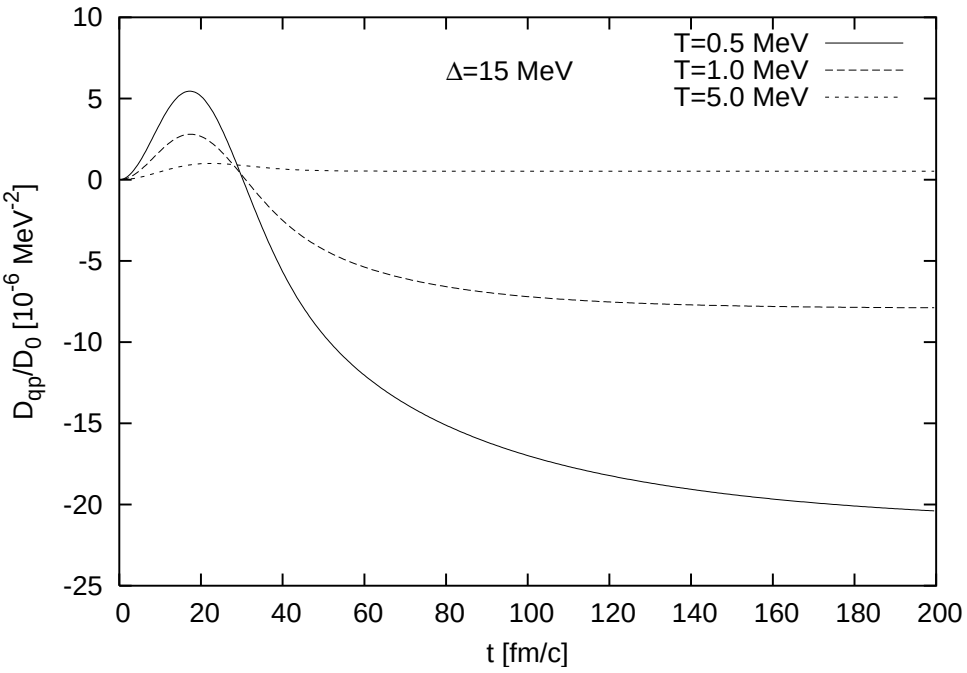

Figure 4.3: The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV.

on diffusion coefficients, we calculate diffusion coefficients by replacing $\overline{\Omega}$ with Ω in the propagators $Q(s)$ and $S(s)$. Figures 4.4 and 4.5 compare two different values of diffusion coefficients D_{pp}/D_0 and D_{qp}/D_0 calculated with $\overline{\Omega}$ and Ω as a function of time at temperature $T = 1.0$ MeV. The variances σ_{qq}, σ_{qp} and σ_{pp} can be determined by solving the coupled differential equations (4.61), (4.62) and (4.63). However, it is much easier to obtain these variances directly from the Langevin equation (4.47) with the help of one-sided Fourier transform [51], as shown in Appendix A.

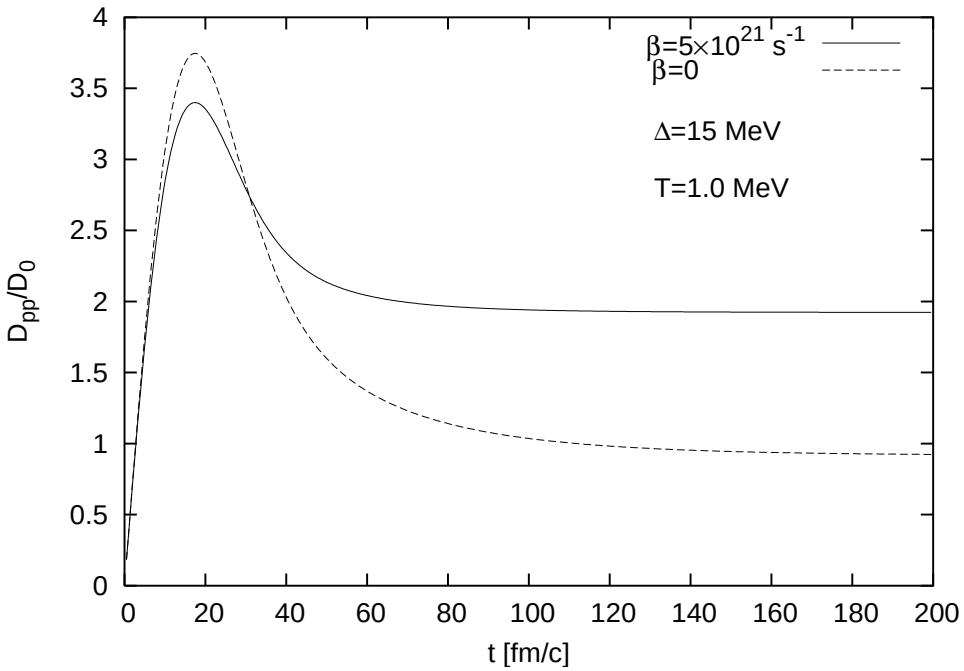

Figure 4.4: The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for Δ = 15 MeV and T=1.0 MeV. The cases with and without friction are compared.

4.3.2 Quantum Effects on Diffusion Along Conditional Saddle Towards Fusion

In this section, we apply the generalized Langevin approach to investigate the influence of quantum-statistical fluctuations on diffusion along the fusion barrier, i.e. the formation probability $P_f(t)$ of compound nucleus. When the conditional saddle, i.e. the inner fusion barrier, is approximately represented by an inverted parabola, the formation probability, i.e. the probability to cross the saddle point, can be calculated analytically in terms of distribution function of the elongation parameter q as [42, 44, 55],

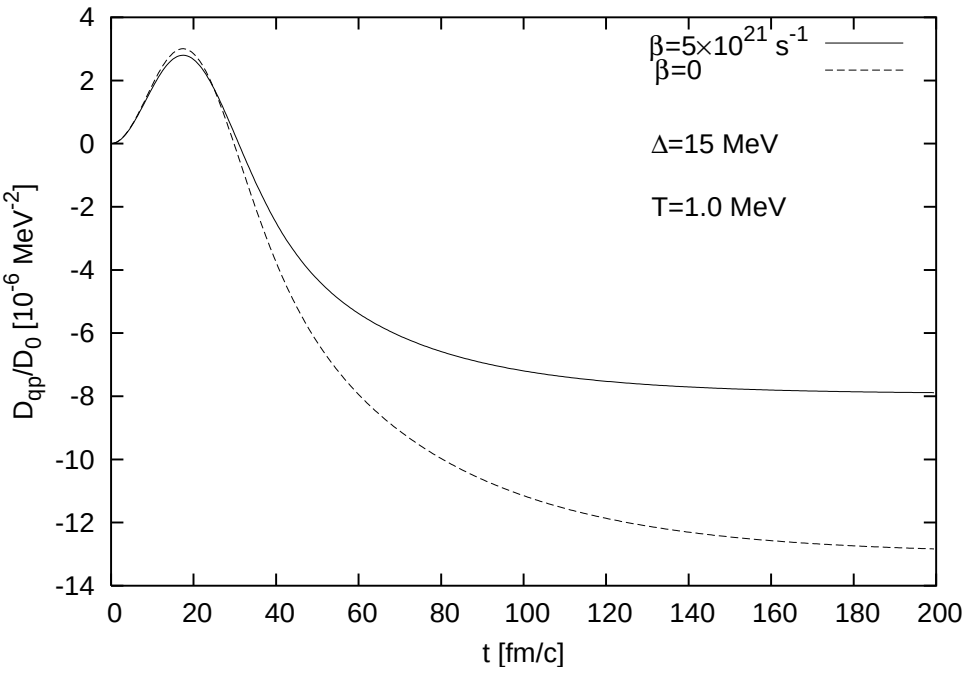

Figure 4.5: The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for Δ = 15 MeV and T=1.0 MeV. The cases with and without friction are compared.

$$P_f(t) = \int_0^\infty dq \frac{1}{\sqrt{2\pi\sigma_{qq}(t)}} \exp\left[-\frac{(q-\overline{q}(t))^2}{2\sigma_{qq}(t)}\right] = \frac{1}{2}\mathrm{erfc}\left(-\frac{\overline{q}(t)}{\sqrt{2\sigma_{qq}(t)}}\right). \quad (4.66)$$

Here, $\overline{q}(t)$ and $\sigma_{qq}(t)$ are the mean value and the variance of the elongation parameter, which are given by Eq.(A.12) and Eq.(A.13) in Appendix A. In these expressions, $(\overline{q}_0, \overline{p}_0)$ are the mean values of elongation parameter and its conjugate momentum, and $(\sigma_{q0}, \sigma_{p0})$ are the associated variances at the initial configuration. As it is stated already, during the approach phase of the collision, system overcome the Coulomb barrier and some of the initial kinetic energy is dissipated into internal excitations and a sticking configuration is formed. The quantities

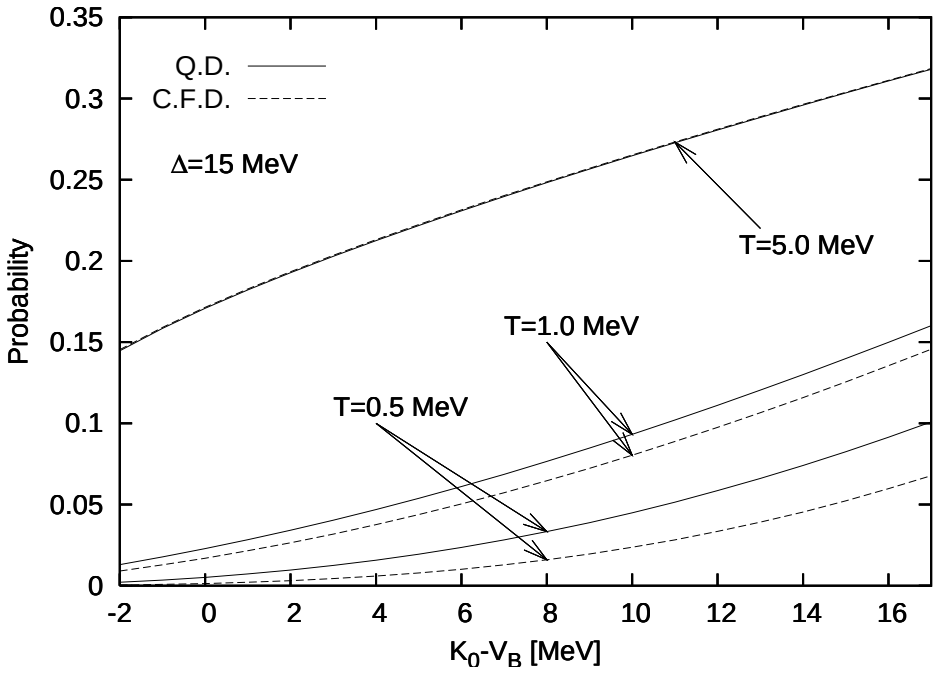

Figure 4.6: The formation probability is plotted versus initial kinetic energy minus barrier height. The result of classical diffusion approach is compared with that of quantum diffusion approach for $\Delta = 15$ MeV.

$(\overline{q}_0, \overline{p}_0)$ denote the average values of the elongation parameter and its momentum at the sticking configuration. In the second stage of the process, the shape of the system evolves from a sticking di-nuclear configuration towards formation of a spherical compound nucleus or re-separate again. The asymptotic value $P_f(t \to \infty)$ gives the transmission probability from a di-nuclear configuration to compound nucleus. In order to compare the results with our previous calculations [7], we consider collision of ^{48}Ca and ^{238}U nuclei and adopt the same value for the reduced friction coefficient and the curvature parameter of the conditional saddle to be $\beta = 5 \times 10^{21} s^{-1}$ and $\hbar\Omega = 1.0$ MeV. We choose the initial position

q_0 to make the height of the conditional saddle to be 4.0 MeV and neglect the dispersion, i.e. $(\sigma_{q0}, \sigma_{p0})$, in the initial configuration. In the classical limit, the variance $\sigma_{qq}(t)$ of the elongation parameter has an analytical expression given by Eq.(A.16), while in the quantum limit it is given by Eq.(A.20), and involves a one dimensional numerical integration over the frequency ω. Figure 4.6 shows the formation probability $P_f(t \to \infty)$ of compound nucleus as a function of the initial kinetic energy $K_0 = \overline{p}_0^2/2M$ relative to the fusion barrier V_B at temperatures $T = 0.5$ MeV, $T = 1.0$ MeV and $T = 5.0$ MeV. These results, which are not very sensitive to the cut-off factor Δ, are presented for $\Delta = 15$ MeV. Solid lines and dashed lines show the quantum and the classical calculations, respectively. At low temperatures, the quantum statistical fluctuations give rise to an enhancement of the formation probability, which is relevant to synthesis of superheavy elements by heavy-ion fusion reactions. The quantum enhancement is slightly less pronounced than that in the previous calculations [7]. The difference arises from the fact that in previous calculations the mixed diffusion coefficient D_{qp}, which is a genuine non-Markovian term, is neglected and the momentum diffusion coefficient D_{pp} is calculated with the unperturbed frequency Ω, rather than $\overline{\Omega}$.

CHAPTER 5

NUMERICAL INTEGRATION METHODS FOR STOCHASTIC DIFFERENTIAL EQUATIONS

In many physical applications one collective variable is not enough to treat the dynamics appropriately and the solution of the corresponding multi-variable Langevin or Fokker-Planck equation is required. Furthermore, the effective multi-variable potentials are nonlinear for many practical applications. Since the analytical solutions are possible for very special cases, one is urged to use numerical integration methods where the Langevin formulation is more advantageous than the Fokker-Planck formulation for a couple of reasons. The Fokker-Planck equation is a deterministic second order partial differential equation which is extremely difficult to solve even numerically for systems with a few collective degrees of freedom. On the other hand Langevin equation can be written as a set of coupled first order ordinary differential equations, a property which is very suitable for numerical analysis of multi-variable systems but the price to pay is that we must find a way of simulating the stochastic term. The numerical solution in Langevin

approach is obtained by simulating the stochastic force, performing the numerical integration many times with different realizations of the simulated force and finally averaging over these solutions. The simulation and integration are performed simultaneously in some of the integration methods, whereas a preparation of an array of simulated terms before the integration is required in some other methods.

In the following sections some major numerical simulation techniques of the stochastic differential equations will be reviewed and our contribution to the subject will be introduced in the last section.

5.1 Iteration Method

The Langevin approach has been applied to nuclear fission process of heavy nuclei for the first time by Abe and coworkers [46]. They have introduced an iteration method (Euler method) to solve Langevin-type equations and then applied it to find the fission decay width of highly excited ^{205}At nuclei. In the derivation below, we closely follow their article [46].

Integrating the Langevin equations (2.4) and (2.5) from t to $t + \Delta t$, we get

$$p(t+\Delta t) = p(t) + \int_t^{t+\Delta t} F(q(t'))dt' - \beta \int_t^{t+\Delta t} p(t')dt' + \tilde{R}_1(t), \quad (5.1)$$

$$q(t+\Delta t) = q(t) + \frac{1}{m}\int_t^{t+\Delta t} p(t')dt', \quad (5.2)$$

with a first order solution

$$p(t+\Delta t) = (1-\Delta t\beta)p(t) + \Delta t F(q(t)) + \tilde{R}_1(t), \quad (5.3)$$

$$q(t+\Delta t) \;=\; q(t) + \Delta t \frac{1}{m} p(t), \tag{5.4}$$

where

$$\tilde{R}_1(t) = \int_t^{t+\Delta t} R(t')dt'. \tag{5.5}$$

For given initial values $q(0)$ and $p(0)$, the time evolution of the phase space variables q and p up to the time t can be calculated by dividing the time into small steps $\Delta t = t/N$. Then, all the dynamical quantities acquire discrete values such as $p(t_n)$, $q(t_n)$ and $\tilde{R}_1(t_n)$ where

$$t_n = n\Delta t, \tag{5.6}$$

with n being an integer. $\tilde{R}_1(t_n)$ is a Gaussian stochastic number since it is an integral of the Gaussian noise $R(t)$ over a short time interval Δt. The statistical properties of the stochastic numbers $\tilde{R}_1(t_n)$ can be deduced as

$$\langle \tilde{R}_1(t_n) \rangle = 0, \tag{5.7}$$

and

$$\langle \tilde{R}_1(t_n) \tilde{R}_1(t_{n'}) \rangle = 2m\beta k_B T \Delta t \delta_{nn'}, \tag{5.8}$$

by using the properties of $R(t)$ given by Eq.(2.7) and Eq.(2.10). The random numbers $\tilde{R}_1(t_n)$ can be simulated by using mean zero normalized Gaussian random numbers $\omega_1(t_n)$ satisfying

$$\langle \omega_1(t_n) \rangle \;=\; 0, \tag{5.9}$$

$$\langle \omega_1(t_n) \omega_1(t_{n'}) \rangle \;=\; \delta_{nn'}, \tag{5.10}$$

so that from Eq.(5.3) and Eq.(5.4) the first order solution of the Langevin equation reads

$$p(t_{n+1}) = (1 - \Delta t\beta)p(t_n) + \Delta t F(q(t_n)) + \sqrt{2m\beta k_B T \Delta t}\, \omega_1(t_n), \quad (5.11)$$

$$q(t_{n+1}) = q(t_n) + \Delta t \frac{1}{m} p(t_n). \quad (5.12)$$

Beginning from the initial conditions at t_0, the values of the phase space variables are calculated step by step by substituting the previous ones in Eq.(5.11) and Eq.(5.12) to obtain the next ones. This time iteration is repeated until the desired time evolution $t = N\Delta t$ is obtained. At each step a random number $\omega_1(t_n)$ with the suitable statistical properties is generated. This process produces one sample. Then, an ensemble of solutions is formed by repeating the sampling process many times over various realizations of the stochastic numbers $\omega_1(t_n)$. Averaging over these solutions, we obtain the moments of the phase space variables p and q such as the mean values $\langle p(t_N)\rangle$ and $\langle p(t_N)\rangle$ as well as the variances $\sigma_{pp}(t)$, $\sigma_{qq}(t)$ and $\sigma_{qp}(t)$.

The accuracy of the method can be enhanced by choosing a smaller time step Δt with the drawback that the integration process becomes more time consuming since the number of iterations is increased in order to reach the same final time of the system. Another way of increasing the accuracy is to use higher order approximations instead of the first order one that we explained. The proper value of the time step can be found by solving the Langevin equation with different

values of the time step and checking the convergence of the results. Then the largest value of the time step for which the desired convergence is achieved can be chosen.

Most of the high level programming languages have internal uniform random number generators. The pseudo random Gaussian numbers $\omega_1(t_n)$ are generated by using the Box-Muller algorithm which transforms a set of uniformly distributed random numbers into a set of normal (Gaussian) distributed random numbers [56].

5.2 Stochastic Runge-Kutta Method

An extension of the Runge-Kutta method to include the stochastic differential equations has been accomplished by Honeycutt [54]. She has developed the method for the white and Gaussian exponentially correlated noise. We closely follow her article in subsequent part.

For simplicity, only one-dimensional stochastic differential equation in the form,

$$\dot{x} = f(x) + R(t), \tag{5.13}$$

where the mean zero white noise $R(t)$ has the correlation Eq.(5.8), is considered. Using the iteration method explained in the previous section the second order

solution of Eq.(5.13) is obtained as

$$\begin{aligned}
x(t+\Delta t) &= x(t) + \int_t^{t+\Delta t} R(t')dt' + \int_t^{t+\Delta t} f(x')dt' \\
&= x(t) + \int_t^{t+\Delta t} R(t')dt' + \sum_{k=0}^{\infty} \frac{1}{k!} \frac{d^k f(x)}{dx^k} \int_t^{t+\Delta t} (x'-x)^k dt' \\
&= x(t) + \int_t^{t+\Delta t} R(t')dt' + \Delta t f(x) \\
&\quad + \sum_{k=1}^{\infty} \frac{1}{k!} \frac{d^k f(x)}{dx^k} \int_t^{t+\Delta t} \left[\int_t^{t'} R(t'')dt'' + (t'-t)f(x) \right. \\
&\qquad \left. + \sum_{j=1}^{\infty} \frac{1}{j!} \frac{d^j f(x)}{dx^j} \int_t^{t'} (x''-x)^j dt'' \right]^k dt' \\
&= x(t) + \Delta t f(x) + \frac{1}{2}\Delta t^2 f(x) \frac{df(x)}{dx} + \xi(t) + O(\Delta t^3), \qquad (5.14)
\end{aligned}$$

where the Taylor expansion of $f(x')$ about $x = x(t)$ is used, the the result for $x' - x$ with $x' = x(t')$ is substituted into itself and only the terms up to the order Δt^2 are kept. The stochastic portion of the equation is denoted by $\xi(t)$ and explicitly given by

$$\begin{aligned}
\xi(t) &= \int_t^{t+\Delta t} R(t')dt' + \frac{df(x)}{dx} \int_t^{t+\Delta t} dt' \int_t^{t'} dt'' R(t'') \\
&\quad + \frac{1}{2} \frac{d^2 f(x)}{dx^2} \int_t^{t+\Delta t} \left[\int_t^{t'} R(t'')dt'' \right]^2 dt'. \qquad (5.15)
\end{aligned}$$

The statistical properties of $\xi(t)$ read

$$\langle \xi(t) \rangle = \frac{1}{2} D \Delta t^2 \frac{d^2 f(x)}{dx^2}, \qquad (5.16)$$

$$\langle \xi^2(t) \rangle = 2D\Delta t + 2D\Delta t^2 \frac{df(x)}{dx}. \qquad (5.17)$$

The solution of deterministic differential equations of the form

$$\dot{x} = f(x), \qquad (5.18)$$

can be found by using the standard Runge-Kutta method. The second order approximation is given by

$$x(t+\Delta t) = x(t) + \frac{1}{2}\Delta t\,(F_1 + F_2)\,, \tag{5.19}$$

where

$$\begin{aligned} F_1 &= f(x), \\ F_2 &= f(x + \Delta t F_1). \end{aligned} \tag{5.20}$$

The stochastic noise included in any extension of Runge-Kutta method must satisfy the properties Eq.(5.16) and Eq.(5.17). The proper extension is given by

$$x(t+\Delta t) = x(t) + \frac{1}{2}\Delta t\,(F_1 + F_2) + \sqrt{2D\Delta t}\;\phi_1, \tag{5.21}$$

where

$$\begin{aligned} F_1 &= f(x(t) + \sqrt{2D\Delta t}\;\phi_2) \\ F_2 &= f(x(t) + \Delta t F_1 + \sqrt{2D\Delta t}\;\phi_3). \end{aligned} \tag{5.22}$$

ϕ_1, ϕ_2 and ϕ_3 are mean zero Gaussian random numbers and their correlation properties are going to be derived later. Substituting the expansions of F_1 and F_2 about $x(t)$ into Eq.(5.21) one obtains

$$x(t+\Delta t) = x(t) + \Delta t f(x) + \frac{1}{2}\Delta t^2 f(x)\frac{df(x)}{dx} + \xi'(t) + O(\Delta t^3), \tag{5.23}$$

where

$$\begin{aligned} \xi'(t) &= \sqrt{2D\Delta t}\;\phi_1 + \frac{1}{2}\Delta t\sqrt{2D\Delta t}\;\frac{df(x)}{dx}(\phi_2 + \phi_3) \\ &\quad + \frac{1}{2}D\Delta t^2\frac{d^2 f(x)}{dx^2}\left(\phi_2^2 + \phi_3^2\right). \end{aligned} \tag{5.24}$$

The statistical properties of the last equation are

$$\langle \xi'(t) \rangle = \frac{1}{2} D \Delta t^2 \frac{d^2 f(x)}{dx^2} \left(\langle \phi_2^2 \rangle + \langle \phi_3^2 \rangle \right), \tag{5.25}$$

$$\langle \xi'^2(t) \rangle = 2D\Delta t \langle \phi_1^2 \rangle + 2D\Delta t^2 \frac{df(x)}{dx} \langle \phi_1(\phi_2 + \phi_3) \rangle. \tag{5.26}$$

Comparing the properties of the stochastic term $\xi(t)$ derived from the iteration method Eq.(5.16) and Eq.(5.17) with that of $\xi'(t)$ derived from the Stochastic Runge-Kutta Eq.(5.25) and Eq.(5.26), we get three independent coupled equations,

$$\begin{aligned} \langle \phi_1^2 \rangle &= 1, \\ \langle \phi_1(\phi_2 + \phi_3) \rangle &= 1, \\ \langle \phi_2^2 \rangle + \langle \phi_3^2 \rangle &= 1, \end{aligned} \tag{5.27}$$

for the three stochastic variables which suggests that one variable ψ is enough to solve Eq.(5.27). For simplicity, the choice $\langle \psi \rangle = 0$ and $\langle \psi^2 \rangle = 1$ can be used. Then let $\phi_i = a_i \psi$ and substitute this into previous equation gives

$$\begin{aligned} a_1^2 &= 1, \\ a_1(a_2 + a_3) &= 1, \\ a_2^2 + a_3^2 &= 1. \end{aligned} \tag{5.28}$$

Choosing $a_2 = 0$ we get the final result:

$$x(t + \Delta t) = x(t) + \frac{1}{2} \Delta t \, (F_1 + F_2) + \sqrt{2D\Delta t} \, \psi, \tag{5.29}$$

where

$$\begin{aligned} F_1 &= f(x(t)), \\ F_2 &= f(x(t) + \Delta t F_1 + \sqrt{2D\Delta t}\ \psi). \end{aligned} \tag{5.30}$$

The stochastic Runge-Kutta method can be applied to exponentially correlated noises as well. Refer to [54] for details.

5.3 Spectral Method

A very powerful method for simulating stochastic terms has been developed as an application of the fast Fourier transformation [57, 58, 59]. Any noise having a correlation function whose Fourier transform exist, can be simulated by this method.

Consider the Fourier transform of the mean zero Gaussian random noise given by

$$\hat{R}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} R(t) dt. \tag{5.31}$$

The correlation of the mean zero noise $\hat{R}(\omega)$ reads

$$\langle \hat{R}(\omega)\hat{R}(\omega')\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-i\omega t - i\omega' t'} \langle R(t)R(t')\rangle dt dt'. \tag{5.32}$$

This integral can be solved by change of variables for stationary noises satisfying $\langle R(t)R(t')\rangle = \langle R(t-t')R(0)\rangle$ to give

$$\langle \hat{R}(\omega)\hat{R}(\omega')\rangle = 2\pi\delta(\omega+\omega')\hat{C}(\omega), \tag{5.33}$$

where $\hat{C}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} C(t) dt$ and $C(t) = \langle R(t)R(0)\rangle$ is the correlation function of the random force $R(t)$. The Eq.(5.33) is known as Wiener-Khintchine theorem which states that the correlation of the random noises in the frequency space is proportional to the Fourier transform of the correlation function. This important result is the starting point of the spectral method. By discretizing the time in $N = 2^n$ intervals of size Δt, the discrete Wiener-Khintchine theorem becomes

$$\langle \hat{R}(\omega_\mu)\hat{R}(\omega_\nu)\rangle = N\Delta t \hat{C}(\omega_\mu)\delta_{\mu+\nu,0}. \tag{5.34}$$

Then the noise in the frequency space can be constructed as

$$\hat{R}(\omega_\mu) = \sqrt{N\Delta t \hat{C}(\omega_\mu)}\alpha(\omega_\mu), \tag{5.35}$$

where $\hat{R}(\omega_0) = \hat{R}(\omega_N)$, $\omega_\mu = 2\pi\mu/N\Delta t$, and $\mu = 0, 1, 2, ..., N$. $\alpha(\omega_\mu) = \alpha_\mu$ are complex mean-zero Gaussian random numbers with the correlation

$$\langle \alpha_\mu \alpha_\nu \rangle = \delta_{\mu+\nu,0}, \tag{5.36}$$

and they satisfy $\alpha_\mu = \alpha^*_{-\mu}$. Let us write α in terms of its real and imaginary parts as $\alpha_\mu = a_\mu + ib_\mu$. Since α_0 is real, $\langle a_0^2\rangle = 1$ and $b_0 = 0$ and all other mean-zero random numbers have the correlation

$$\langle a_\mu^2\rangle = \langle b_\mu^2\rangle = \frac{1}{2}. \tag{5.37}$$

The random noises $\hat{R}(\omega_\mu)$ are put into an array and then inverse fast Fourier transform is used to obtain the noises $R(t_\mu)$ in time domain which satisfy the

desired correlation relation. The iteration method is used to integrate the deterministic part of the Langevin equation and for each step the random numbers generated by the spectral method are used. The implementation of the spectral method into the stochastic Runge-Kutta method has also been achieved [60]. The spectral method is different than the previous ones since it is used only to simulate the random noise.

Note that in this method a construction of the random noises is needed before they are used in the algorithm. The preparation of the random numbers is more time consuming than the previous methods since the Fourier transformation of the whole noise array is required next to the random number generation in the frequency space.

5.4 Integration Method

A very fast and accurate algorithm for the exponentially correlated colored noise has been developed by Fox and coworkers [61].

Consider the same stochastic differential equation Eq.(5.13) but with a colored noise satisfying the properties

$$\begin{aligned} \langle R(t) \rangle &= 0, \\ \langle R(t)R(t') \rangle &= D\lambda e^{-\lambda|t-t'|}, \end{aligned} \tag{5.38}$$

where D is the diffusion coefficient or more generally noise strength and $\lambda = \tau^{-1}$

is the inverse of the correlation time. The stochastic differential equation (5.13) with the exponential colored noise Eq.(5.38) can be transformed to a pair of equations

$$\frac{dx}{dt} = f(x) + \epsilon(t), \tag{5.39}$$

$$\frac{d\epsilon}{dt} = -\lambda\epsilon + \lambda g(t), \tag{5.40}$$

where the noise is white (delta correlated),

$$\begin{aligned} \langle g(t)\rangle &= 0, \\ \langle g(t)g(t')\rangle &= 2D\delta(t-t'). \end{aligned} \tag{5.41}$$

Formally integrating Eq.(5.40) we get

$$\epsilon(t) = \epsilon(0)e^{-\lambda t} + \lambda\int_0^t e^{-\lambda(t-t')}g(t')dt'. \tag{5.42}$$

with the mean values

$$\begin{aligned} \langle\epsilon(t)\rangle &= \epsilon(0)e^{-\lambda t}, \\ \langle\epsilon(t)\epsilon(t')\rangle &= D\lambda e^{-\lambda|t-t'|} + \left[\epsilon^2(0) - D\lambda\right]e^{-\lambda(t+t')}. \end{aligned} \tag{5.43}$$

Introducing a secondary averaging over the distribution of initial values $\epsilon(0)$,

$$W(\epsilon(0)) = \frac{1}{\sqrt{2\pi D\lambda}}\exp\left[-\frac{\epsilon^2(0)}{2D\lambda}\right], \tag{5.44}$$

we obtain the desired statistical properties which are

$$\begin{aligned} \{\langle\epsilon(t)\rangle\} &= 0, \\ \{\langle\epsilon(t)\epsilon(t')\rangle\} &= D\lambda e^{-\lambda|t-t'|}. \end{aligned} \tag{5.45}$$

The curly brackets indicate the secondary average.

The integral method is derived as follows. Rewrite Eq.(5.42) by replacing t with $t + \Delta t$ to obtain

$$\epsilon(t + \Delta t) = \epsilon(0)e^{-\lambda(t+\Delta t)} + \lambda \int_0^{t+\Delta t} e^{-\lambda(t+\Delta t-t')} g(t')dt'. \tag{5.46}$$

Comparing this equation with Eq.(5.42) we can write

$$\epsilon(t + \Delta t) = \epsilon(t)e^{-\lambda \Delta t} + h(t). \tag{5.47}$$

where

$$h(t) = \lambda \int_t^{t+\Delta t} e^{-\lambda(t+\Delta t-t')} g(t')dt', \tag{5.48}$$

is a mean zero Gaussian noise with the variance given by

$$\langle h^2(t) \rangle = D\lambda \left(1 - e^{-2\lambda \Delta t}\right). \tag{5.49}$$

Note that the Eq.(5.47) is exact in a sense that it includes all orders of Δt. Hence, this method is superior over the others with the drawback that it can be applied only to exponentially correlated noises.

The deterministic part of the Langevin-like equation (5.39) is integrated by using iteration method, for instance to the second order approximation, hence the final result reads

$$x(t + \Delta t) = x(t) + \Delta t f(x) + \frac{1}{2}\Delta t^2 f(x)\frac{df(x)}{dx} + \epsilon(t), \tag{5.50}$$

$$\epsilon(t + \Delta t) = \epsilon(t)e^{-\lambda \Delta t} + h(t). \tag{5.51}$$

Another advantage of this method is that for each iteration in time only two Gaussian random numbers, one for the initial value ϵ and another for h are needed regardless of the approximation order of the deterministic part. In the previous methods (Itertion and Stochastic Runge-Kutta methods), as the order of the approximation is increased, the needed number of generated random numbers per iteration in time is increased which in turn means that the computation time is increased as well.

5.5 Integration Method for two-term exponentially correlated colored noise

5.5.1 Motivation

As discussed in Chapter 4, the quantum effects on the collective modes of heavy-ion fusion reactions manifest themselves in the Gaussian c-number noise $R(t)$ with a correlation function given by [8, 19, 53],

$$\langle R(t)R(t')\rangle = Mk_BT\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}e^{-i\omega(t-t')}\frac{\hbar\omega}{2k_BT}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\Gamma(\omega), \qquad (5.52)$$

where $\Gamma(\omega) = J(\omega)/M\omega$ and $J(\omega)$ represents the spectral density of the intrinsic degrees of freedom. The most interesting feature of this correlation function (see Figure 4.1) is that it has a negative long time tail which is something particular to quantum systems. By choosing a Lorentzian profile Eq.(2.33) for the distribution of intrinsic degrees of freedom $\Gamma(\omega)$, the ω integration in Eq.(5.52) can be carried

out by using the residue theorem to give

$$\langle R(t)R(t')\rangle = Mk_BT\left\{\frac{\hbar}{2\tau k_BT}\cot\left(\frac{\hbar}{2\tau k_BT}\right)\frac{\beta}{\tau}e^{-\frac{1}{\tau}|t-t'|} + \sum_{n=1}^{\infty}\frac{2\beta\omega_n}{\omega_n^2\tau^2-1}e^{-\omega_n|t-t'|}\right\}, \tag{5.53}$$

where $\omega_n = 2k_BT\pi n/\hbar$ are the Matsubara frequencies. The correlation function is now expressed as a superposition of exponential terms with positive and negative coefficients.

In the previous section we have seen that the integration method is a very powerful method for simulating exponentially correlated noises. Since the quantum noise can be expressed as a sum of exponential terms, it is desirable to extend the method to include a noise with multi-exponential correlation. This method has already been proposed for superposition of exponential terms with positive coefficients [57, 59]. In order to perform a simulation of the quantum noises of the form given by Eq.(5.52) which has a negative part at the long time tail, we have to include exponential terms with negative coefficients as well. We have made a progress towards this direction by introducing a simulation technique for a two-term exponential form of the correlation function with a negative coefficient and we closely follow the derivation of [9] below.

5.5.2 The Method

We consider again the stochastic equation (5.13),

$$\dot{x} = f(x) + R(t). \tag{5.54}$$

where this time the mean-zero Gaussian random noise $R(t)$ has a correlation given by a linear combinations of two exponentials,

$$\langle R(t)R(t')\rangle = D_1\lambda_1 e^{-\lambda_1|t-t'|} + D_2\lambda_2 e^{-\lambda_2|t-t'|}. \tag{5.55}$$

Here, D_1 and D_2 are the respective noise strengths and λ_1^{-1} and λ_2^{-1} are the correlation times of respective terms. As an extension of the integral method, it is possible to develop an algorithm for numerical simulation of the exponentially correlated colored noise by replacing Eq.(5.54) by a set of three equations [59],

$$\dot{x} = f(x) + R(t), \tag{5.56}$$

$$\dot{R}_1(t) = -\lambda_1 R_1(t) + \lambda_1 g_1(t), \tag{5.57}$$

$$\dot{R}_2(t) = -\lambda_2 R_2(t) + \lambda_2 g_2(t). \tag{5.58}$$

where $R(t) = R_1(t) + R_2(t)$. In these equations, the stochastic sources g_1 and g_2 are mean-zero Gaussian white noises with second moments given by,

$$\langle g_1(t)g_1(t')\rangle = 2D_1'\delta(t-t'), \tag{5.59}$$

$$\langle g_2(t)g_2(t')\rangle = 2D_2'\delta(t-t'), \tag{5.60}$$

$$\langle g_1(t)g_2(t')\rangle = 2D_{12}'\delta(t-t'), \tag{5.61}$$

where D_1', D_2' and D_{12}' are parameters to be determined by the correlation function Eq.(5.55). When both coefficients D_1 and D_2 are positive, R_1 and R_2 behave as independent random numbers and therefore the mixed diffusion coefficient can be taken to be zero, $D_{12}' = 0$. On the other hand, when one of the coefficients, D_1 or D_2, is negative, the mixed diffusion coefficient D_{12}' must take a finite negative value.

As shown in Appendix B, solutions of Eq.(5.57) and Eq.(5.58) lead to the two-term exponentially correlated colored noise,

$$\{\langle R(t)\rangle\} = 0 \tag{5.62}$$

$$\{\langle R(t)R(t')\rangle\} = \left(\widetilde{D}_1 + \widetilde{D}_{12}\right) e^{-\lambda_1|t-t'|} + \left(\widetilde{D}_2 + \widetilde{D}_{12}\right) e^{-\lambda_2|t-t'|}, \tag{5.63}$$

where in addition to the ensemble averaging $< .. >$, an average $\{..\}$ over the initial $R(0)$ values must be carried out for the Gaussian distribution,

$$P(R(0)) = \frac{1}{2\pi\sqrt{\Delta}} \exp\left\{-\frac{1}{2\Delta}\left[R_1^2(0)\widetilde{D}_1 + 2R_1(0)R_2(0)\widetilde{D}_{12} + R_2^2(0)\widetilde{D}_2\right]\right\}, \tag{5.64}$$

where $\widetilde{D}_1 = D_1'\lambda_1$, $\widetilde{D}_2 = D_2'\lambda_2$, $\widetilde{D}_{12} = D_{12}'\frac{2\lambda_1\lambda_2}{\lambda_1+\lambda_2}$ and $\Delta = \widetilde{D}_1\widetilde{D}_2 - \widetilde{D}_{12}^{\,2}$.

Integrating Eq.(5.57) and Eq.(5.58) and using the results Eq.(B.1) and Eq.(B.2) we find the solutions of R_1 and R_2 as

$$R_1(t+\Delta t) = e^{-\lambda_1\Delta t}R_1(t) + h_1(t,\Delta t), \tag{5.65}$$

$$R_2(t+\Delta t) = e^{-\lambda_2\Delta t}R_2(t) + h_2(t,\Delta t), \tag{5.66}$$

where

$$h_1(t,\Delta t) = \lambda_1 \int_t^{t+\Delta t} e^{-\lambda_1(t+\Delta t-s)} g_1(s) ds, \tag{5.67}$$

$$h_2(t,\Delta t) = \lambda_2 \int_t^{t+\Delta t} e^{-\lambda_2(t+\Delta t-s)} g_2(s) ds. \tag{5.68}$$

The second moments of the mean zero h-functions are given by,

$$\langle h_1^2(t,\Delta t)\rangle = \widetilde{D}_1 \left(1 - e^{-2\lambda_1 \Delta t}\right), \tag{5.69}$$

$$\langle h_2^2(t,\Delta t)\rangle = \widetilde{D}_2 \left(1 - e^{-2\lambda_2 \Delta t}\right), \tag{5.70}$$

$$\langle h_1(t,\Delta t) h_2(t,\Delta t)\rangle = \widetilde{D}_{12} \left(1 - e^{-(\lambda_1+\lambda_2)\Delta t}\right). \tag{5.71}$$

Now that all the mean values of the noises are known, we can construct the correlated noises. The initial R values satisfying the distribution Eq.(5.64) can be simulated as

$$R_1(0) = C_{11}\,\omega_1, \tag{5.72}$$

$$R_2(0) = C_{21}\,\omega_1 + C_{22}\,\omega_2, \tag{5.73}$$

where ω_1 and ω_2 are Gaussian random numbers satisfying

$$\langle \omega_i \rangle = 0, \tag{5.74}$$

$$\langle \omega_i \omega_j \rangle = \delta_{ij}, \qquad i = 1,2 \quad j = 1,2. \tag{5.75}$$

Using the correlation properties of $R_1(0)$ and $R_2(0)$ given by Eqs.(B.11,B.12,B.13), the coefficients C_{11}, C_{21} and C_{22} are found as

$$C_{11} = \widetilde{D}_1^{1/2}, \tag{5.76}$$

$$C_{21} = \frac{\widetilde{D}_{12}}{\widetilde{D}_1^{1/2}}, \tag{5.77}$$

$$C_{22} = \left(\widetilde{D}_2 - C_{21}^2\right)^{1/2}. \tag{5.78}$$

The time evolution of R values given by Eq.(5.65) and Eq.(5.66) and satisfying Eqs.(5.69,5.70,5.71) can be simulated according to

$$R_1(t+\Delta t) = R_1(t)e^{-\lambda_1 \Delta t} + F_{11}\,\omega_3, \tag{5.79}$$

$$R_2(t+\Delta t) = R_2(t)e^{-\lambda_2 \Delta t} + F_{21}\,\omega_3 + F_{22}\,\omega_4, \tag{5.80}$$

In these expressions ω_3 and ω_4 are again uncorrelated Gaussian random numbers with zero mean and unit variances, and the coefficients are given by,

$$F_{11} = \left[\widetilde{D}_1\left(1 - e^{-2\lambda_1 \Delta t}\right)\right]^{1/2}, \tag{5.81}$$

$$F_{21} = \frac{\widetilde{D}_{12}}{\left[\widetilde{D}_1\left(1 - e^{-2\lambda_1 \Delta t}\right)\right]^{1/2}}\left(1 - e^{-(\lambda_1+\lambda_2)\Delta t}\right), \tag{5.82}$$

$$F_{22} = \left[\widetilde{D}_2\left(1 - e^{-2\lambda_2 \Delta t}\right) - F_{21}^2\right]^{1/2}. \tag{5.83}$$

The Eqs.(5.76,5.78,5.83) impose certain conditions on the magnitude of diffusion coefficients, which can be expressed as,

$$\widetilde{D}_1 > 0, \tag{5.84}$$

$$\widetilde{D}_2 > 0, \tag{5.85}$$

$$\frac{\widetilde{D}_{12}^2}{\widetilde{D}_1\widetilde{D}_2} < 1, \tag{5.86}$$

$$\frac{\widetilde{D}_{12}^2}{\widetilde{D}_1\widetilde{D}_2} < \frac{(1 - e^{-2\lambda_1 \Delta t})(1 - e^{-2\lambda_2 \Delta t})}{\left(1 - e^{-(\lambda_1+\lambda_2)\Delta t}\right)^2}. \tag{5.87}$$

The first two conditions are also necessary for the validity of the autocorrelation functions Eq.(5.59) and Eq.(5.60) at $t = t'$. Since the right hand side of Eq.(5.87) is less than one, we can discard the third condition Eq.(5.86). The right hand side of Eq.(5.87) is also rapidly decreasing function of the time step Δt and approaches its asymptotic value as

$$\lim_{\Delta t \to 0} \frac{(1 - e^{-2\lambda_1 \Delta t})(1 - e^{-2\lambda_2 \Delta t})}{\left(1 - e^{-(\lambda_1 + \lambda_2)\Delta t}\right)^2} = \frac{4\lambda_1 \lambda_2}{\left(\lambda_1 + \lambda_2\right)^2}, \tag{5.88}$$

which is a stronger condition. Finally, besides the conditions Eq.(5.84) and Eq.(5.85), we have

$$\frac{\widetilde{D}_{12}^2}{\widetilde{D}_1 \widetilde{D}_2} \leq \frac{4\lambda_1 \lambda_2}{\left(\lambda_1 + \lambda_2\right)^2}. \tag{5.89}$$

With these conditions in mind, we turn our attention in expressing the diffusion coefficients $\widetilde{D}_1$, $\widetilde{D}_2$ and $\widetilde{D}_{12}$ in terms of the given parameters D_1, D_2, λ_1 and λ_2. Equating the Eq.(5.55) to Eq.(5.63), we have

$$D_1 \lambda_1 = \widetilde{D}_1 + \widetilde{D}_{12}, \tag{5.90}$$

$$D_2 \lambda_2 = \widetilde{D}_2 + \widetilde{D}_{12}. \tag{5.91}$$

Here, we have two equations but three unknown parameters $\widetilde{D}_1$, $\widetilde{D}_2$ and $\widetilde{D}_{12}$ which means that one of these parameters is free and can be fixed in several ways. We choose to fix $\widetilde{D}_{12}$ by convention. Then using these two equations, the condition Eq.(5.89) can be written as

$$f(\widetilde{D}_{12}) = -\frac{\left(\lambda_1 - \lambda_2\right)^2}{4\lambda_1 \lambda_2} \widetilde{D}_{12}^2 - (D_1 \lambda_1 + D_2 \lambda_2) \widetilde{D}_{12} + D_1 \lambda_1 D_2 \lambda_2 \geq 0. \tag{5.92}$$

If both the parameters D_1 and D_2 are positive, the inequality above will always be valid for $\widetilde{D}_{12} = 0$. Hence the algorithm reduces to the superposition method [59]. If $D_1 D_2 < 0$, we have a more interesting case, in which the correlation function may have a negative portion, see Figure 5.1. Then the maximum of the function $f(\widetilde{D}_{12})$ is given by

$$f(\widetilde{D}_{12}^{(max)}) = \frac{\lambda_1 \lambda_2}{(\lambda_1 - \lambda_2)^2} (D_1 \lambda_1 + D_2 \lambda_2)^2 + D_1 \lambda_1 D_2 \lambda_2 \geq 0, \tag{5.93}$$

where

$$\widetilde{D}_{12}^{(max)} = -\frac{2\lambda_1 \lambda_2}{(\lambda_1 - \lambda_2)^2} (D_1 \lambda_1 + D_2 \lambda_2). \tag{5.94}$$

Once the inequality Eq.(5.93) is satisfied, we have at least one solution for $\widetilde{D}_{12}$, namely Eq.(5.94). The validity of correlation function Eq.(5.55) at $t = t'$ as well as the condition Eq.(5.93) impose certain restrictions on the given parameters as

$$D_1 + D_2 > 0, \tag{5.95}$$

$$D_1 \lambda_1 + D_2 \lambda_2 > 0, \tag{5.96}$$

$$D_1 \lambda_1^2 + D_2 \lambda_2^2 \geq 0. \tag{5.97}$$

Even though the conditions above seem to be restrictions only due to the algorithm, they are indeed also physical restrictions. For any multi-exponential correlation function of the form

$$\chi(|t - t'|) = \langle \epsilon(t) \epsilon(t') \rangle = \sum_i D_i \lambda_i e^{-\lambda_i |t - t'|} \tag{5.98}$$

there are three physical restrictions:

1. $\sum_i D_i\lambda_i > 0$. This is for the consistency of the correlation function at $t = t'$.

2. $\sum_i D_i > 0$. In the classical (Markovian) limit, that is all $\lambda_i \to \infty$, the correlation function reduces to the form $2\sum_i D_i\delta(t - t')$. And again for consistency in the classical limit one needs this condition.

3. $\sum_i D_i\lambda_i^2 \geq 0$. The time derivative of the correlation function at $t = t'$ must be negative or zero indicating the initial decrease of the correlation function. The equality case corresponds to Gaussian-like correlation functions where the roots of Eq.(5.92) are equal and given by Eq.(5.94).

The correlated algorithm incorporates these physical restrictions naturally. The three conditions above are also needed to guarantee a positive definite power spectrum of the noise [19]. The four possible shapes of the correlation function with two exponential terms satisfying the conditions $D_1D_2 < 0$ and Eq.(5.96) are shown in Figure 5.1 for four arbitrary examples. Two of the examples are unphysical due to violation of one of the conditions.

For a given correlation function in the form Eq.(5.55), which can be corresponding to a specific physical system or can be a fit of a correlation function, one must fix the value of $\widetilde{D}_{12}$ which in general can assume any value between the roots of Eq.(5.92). The numerical computations show that among these values the choice of $\widetilde{D}_{12}$ is not very affective, hence it is appropriate to fix it as in

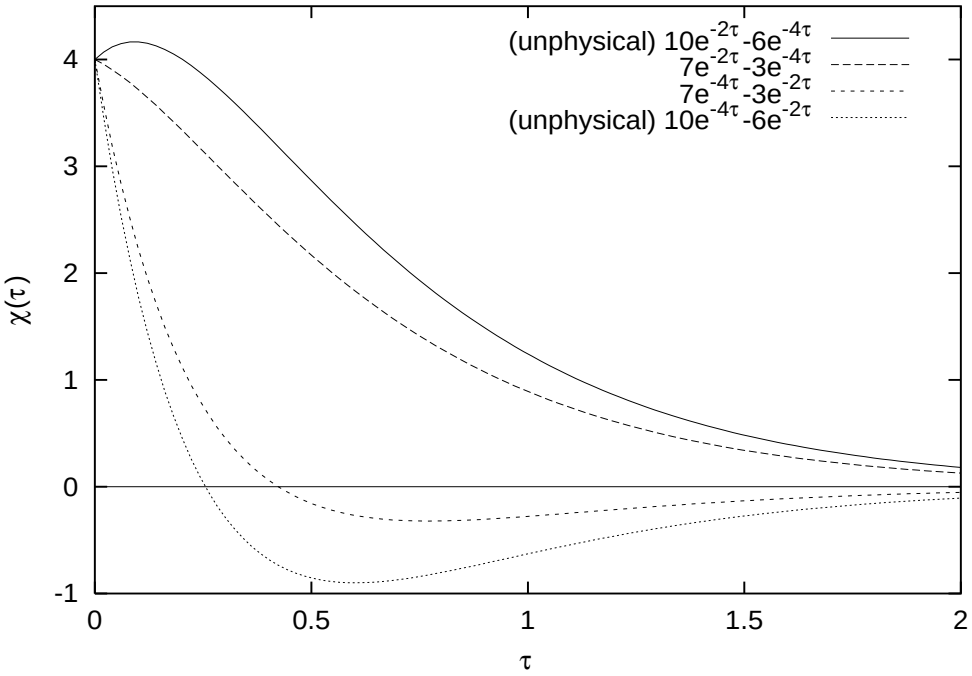

Figure 5.1: Four examples of the correlation function, Eq.(5.55) with $D_1 D_2 < 0$ are indicated. Two of the examples are unphysical due to violation of one of the conditions, Eqs.(5.95,5.96,5.97).

Eq.(5.94). Then, the simulation algorithm to the first order follows as,

$$x(t + \Delta t) \;=\; x(t) + [f(x) + R_1(t) + R_2(t)]\,\Delta t, \tag{5.99}$$

where $R_1(t + \Delta t)$ and $R_2(t + \Delta t)$ are given by Eq.(5.79) and Eq.(5.80) with the initial values determined by Eq.(5.72) and Eq.(5.73).

5.5.3 Test and Application of the Correlated Algorithm

In order to test the accuracy of the algorithm, we apply it to the free diffusing particle in momentum space with the two-term exponentially correlated noise where the analytical solution can be easily obtained. The corresponding simple

stochastic differential equation is given by

$$\dot{p} = R(t), \tag{5.100}$$

where $R(t)$ is a mean-zero Gaussian random number with the correlation Eq.(5.55). The average value of p does not change in time and remains equal to the initial value, $\langle p(t)\rangle = p(0)$, and the variance can be easily calculated to give,

$$\sigma_p^2(t) = -2\left[\frac{D_1}{\lambda_1}\left(1 - e^{-\lambda_1 t} - \lambda_1 t\right) + \frac{D_2}{\lambda_2}\left(1 - e^{-\lambda_2 t} - \lambda_2 t\right)\right]. \tag{5.101}$$

In the simulations, we consider a correlation function of the form

$$\chi(t) = \langle R(t+s)R(s)\rangle = 7e^{-4|t|} - 3e^{-2|t|}. \tag{5.102}$$

We fix the mixed diffusion coefficient as $\widetilde{D}_{12} = -16$, take the time step as $\Delta t = 10^{-2}$ and the sharp initial value $p(0) = 5$. Figure 5.2 shows a comparison of exact correlation function (solid line) with simulations (dashed line with 10^3 initial values and dotted line with 10^4 initial values). Figure 5.3 and Figure 5.4 show a comparison of the analytical results for the mean value and the variance of the variable p with simulations. Simulations carried out with 10^4 and 10^5 realizations are indicated by dashed lines and dotted lines respectively. As seen from the figures, already with 10^5 realization, the simulations provide a perfect agreement with the analytical results.

As a second application, let us consider a more realistic system where a particle undergoes a diffusion over a parabolic barrier, then the system can be described

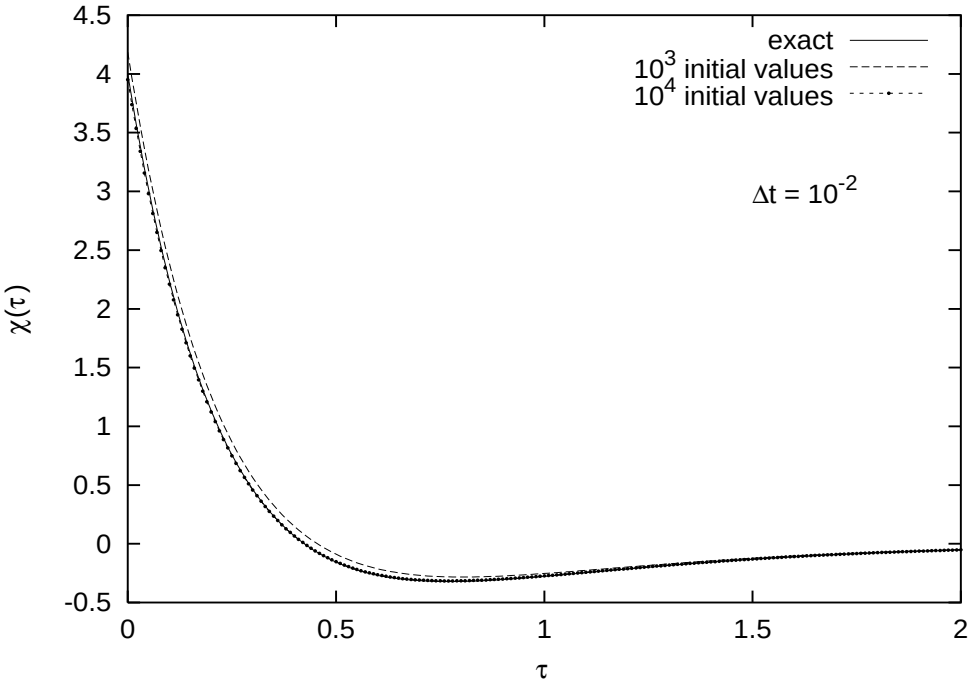

Figure 5.2: The comparison of the exact correlation function with simulated ones (dashed line with 10^3 initial values and dotted line with 10^4 initial values).

by the following Generalized Langevin Equation (GLE),

$$\dot{q}(t) = p(t), \tag{5.103}$$

$$\dot{p}(t) = -\frac{\partial V}{\partial q} - \int_0^t \chi(t-t')p(t')dt' + R(t), \tag{5.104}$$

where

$$\chi(t) = D_1\lambda_1 e^{-\lambda_1 t} + D_2\lambda_2 e^{-\lambda_2 t} \tag{5.105}$$

and the potential is

$$V(q) = \frac{1}{2}(q_0^2 - q^2(t)). \tag{5.106}$$

Here, we assume that the memory kernel has a two-term exponential form. And

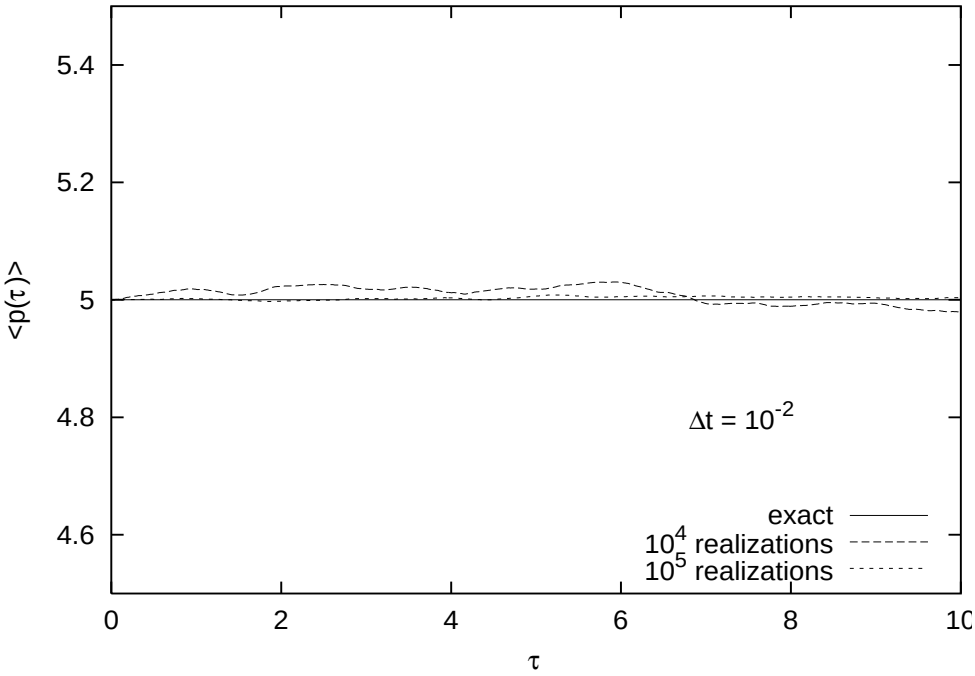

Figure 5.3: The comparison of the exact average of p with simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations).

from the fluctuation-dissipation theorem, we have

$$\langle R(t)\rangle = 0, \tag{5.107}$$

$$\langle R(t)R(t')\rangle = \chi(|t-t'|). \tag{5.108}$$

The mass of the particle as well as the temperature is chosen to be unity for convenience. Eq.(5.104) can be written as

$$\dot{p} = -\frac{\partial V}{\partial q} + \widetilde{R}_1 + \widetilde{R}_2, \tag{5.109}$$

$$\dot{\widetilde{R}}_1 = -\lambda_1 \widetilde{R}_1 - D_1\lambda_1 p + \lambda_1 g_1, \tag{5.110}$$

$$\dot{\widetilde{R}}_2 = -\lambda_2 \widetilde{R}_2 - D_2\lambda_2 p + \lambda_2 g_2, \tag{5.111}$$

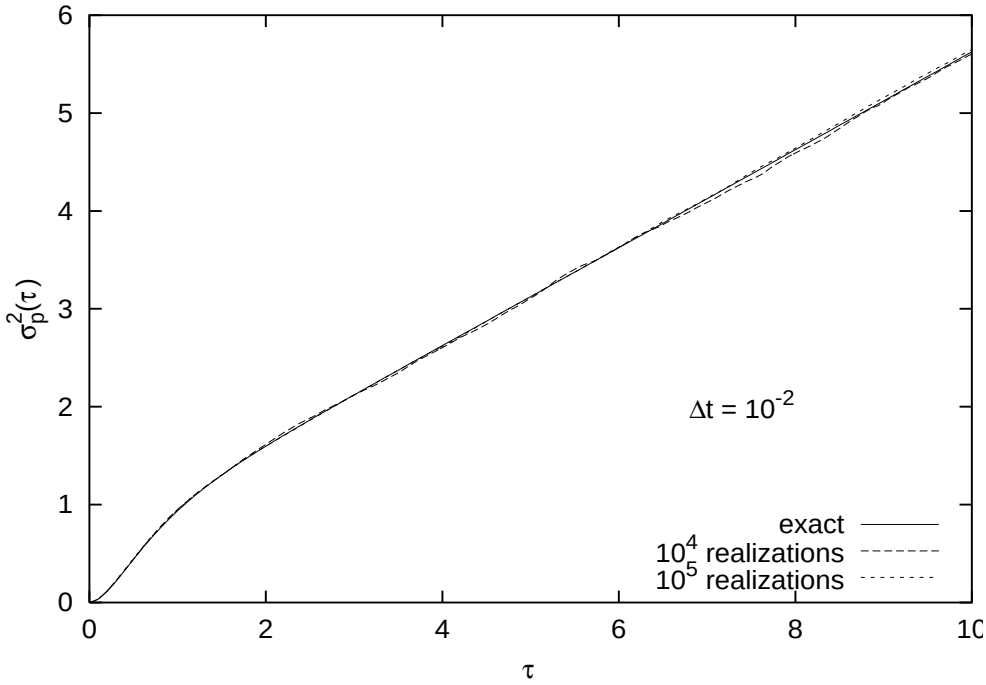

Figure 5.4: The comparison of the exact variance of p and simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations).

where g_1 and g_2 are the correlated white noises Eqs.(5.59,5.60,5.61) and

$$\widetilde{R}_1(t) = R_1(t) - D_1\lambda_1 \int_0^t e^{-\lambda_1(t-t')} p(t')dt', \tag{5.112}$$

$$\widetilde{R}_2(t) = R_2(t) - D_2\lambda_2 \int_0^t e^{-\lambda_2(t-t')} p(t')dt'. \tag{5.113}$$

Here R_1 and R_2 are given by Eq.(B.1) and Eq.(B.2). Note that the initial values of both $\widetilde{R}_i$ and R_i are the same (i=1,2). With this knowledge, the time evolution of the system to the first order follows as

$$q(t+\Delta t) = q(t) + p(t)\Delta t, \tag{5.114}$$

$$p(t+\Delta t) = p(t) + \left(-\frac{\partial V}{\partial q} + \widetilde{R}_1(t) + \widetilde{R}_2(t)\right)\Delta t, \tag{5.115}$$

$$\widetilde{R}_1(t+\Delta t) = \widetilde{R}_1(t)e^{-\lambda_1\Delta t} - D_1 p(t)\left(1 - e^{-\lambda_1\Delta t}\right) + F_{11}\,\omega_3, \tag{5.116}$$

$$\widetilde{R}_2(t+\Delta t) = \widetilde{R}_2(t)e^{-\lambda_2\Delta t} - D_2 p(t)\left(1-e^{-\lambda_2\Delta t}\right) + F_{21}\,\omega_3 + F_{22}\,\omega_4, \tag{5.117}$$

where the F functions are the ones given in Eqs.(5.81,5.82,5.83).

By extending the approach of [62] to two-term exponential correlation, it is possible to obtain analytical results for the mean values and variances. The analytical expression for passing probability over the parabolic is given by Eq.(4.3) [44, 45]

$$P(t,q_0,p_0) = \frac{1}{2}\,\mathrm{Erfc}\left(-\frac{\langle q(t)\rangle}{\sqrt{2}\sigma_q(t)}\right). \tag{5.118}$$

where $\langle q(t)\rangle$ and $\sigma_q^2(t)$ denotes the mean value and variance of the variable q. The analytical expressions for these quantities are given by,

$$\langle q(t)\rangle = R(t)q_0 + Q(t)p_0, \tag{5.119}$$

where

$$R(t) = \sum_{i=1}^{4}\left\{\frac{D_1\lambda_1(s+\lambda_2)+D_2\lambda_2(s_i+\lambda_1)}{\prod_{n\neq i}(s_i-s_n)} + \frac{s_i(s_i+\lambda_1)(s_i+\lambda_2)}{\prod_{n\neq i}(s_i-s_n)}\right\}e^{s_i t}, \tag{5.120}$$

$$Q(t) = \sum_{i=1}^{4}\frac{(s_i+\lambda_1)(s_i+\lambda_2)}{\prod_{n\neq i}(s_i-s_n)}e^{s_i t}, \tag{5.121}$$

and

$$\sigma_q^2(t) = \sum_{i,j=1}^{4}\frac{(s_i+\lambda_1)(s_i+\lambda_2)(s_j+\lambda_1)(s_j+\lambda_2)}{\prod_{n\neq i}(s_i-s_n)\prod_{m\neq j}(s_j-s_m)} \times\left[D_1\lambda_1 A_{ij}(t,\lambda_1)+D_2\lambda_2 A_{ij}(t,\lambda_2)\right] \tag{5.122}$$

where

$$
\begin{aligned}
A_{ij}(t,\lambda) &= \frac{1}{s_i+s_j}\left[\frac{1}{s_i+\lambda}+\frac{1}{s_j+\lambda}\right]e^{(s_i+s_j)t} \\
&\quad -\left[\frac{e^{(s_i-\lambda)t}}{(s_i-\lambda)(s_j+\lambda)}+\frac{e^{(s_j-\lambda)t}}{(s_i+\lambda)(s_j-\lambda)}\right] \\
&\quad +\frac{1}{s_i+s_j}\left[\frac{1}{s_i-\lambda}+\frac{1}{s_j-\lambda}\right].
\end{aligned} \tag{5.123}
$$

In these expressions $s_i\,(i=1,2,3,4)$, denote the roots of the secular equation

$$
\begin{aligned}
&s^4+(\lambda_1+\lambda_2)s^3+(\lambda_1\lambda_2+D_1\lambda_1+D_2\lambda_2-1)s^2 \\
&+\left[\lambda_1\lambda_2(D_1+D_2)-(\lambda_1+\lambda_2)\right]s-\lambda_1\lambda_2=0
\end{aligned} \tag{5.124}
$$

which is the denominator of the Laplace transform of $q(t)$ derived from the given GLE.

The passing probability over the parabolic barrier can be numerically calculated by generating sufficiently large number of events where Eqs.(5.114-5.117) are used for each event, counting the number of events for which the particle diffused over the barrier and dividing this number by the total number of events. On the other hand, the analytical result of the over-passing probability can be obtained by using Eq.(5.118) which, for large times, approaches an asymptotic value that can be written as a function of the initial kinetic energy $K=\frac{1}{2}p_0^2$ and the barrier height $B=\frac{1}{2}q_0^2$.

For the computations, we choose the correlation function as in Eq.(5.102) again and take sharp initial values for q and p as $q_0=-2$ and $p_0=(2K)^{1/2}$ where

K is the initial kinetic energy. The numerical computations (simulations) are obtained with the time step $\Delta t = 10^{-2}$, the mixed diffusion coefficient $\widetilde{D}_{12} = -16$ which is found from Eq.(5.94), 10^4 realizations of the algorithm and time iteration

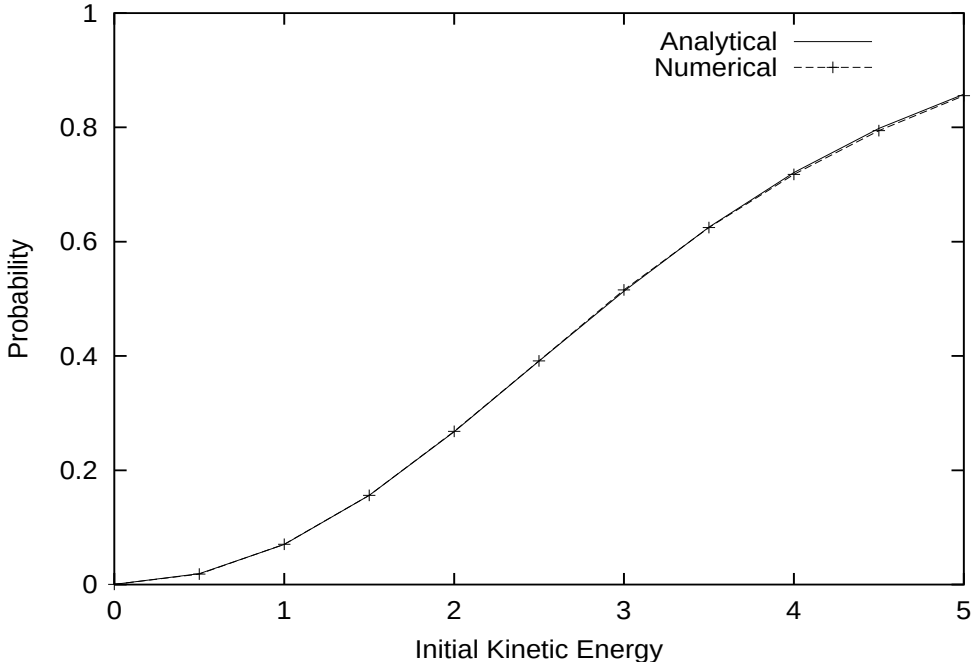

Figure 5.5: The passing probability over the barrier is plotted versus the initial kinetic energy in arbitrary units. The analytical and numerical results (dashed line) are shown for the correlation $\chi(t) = 7e^{-4|t|} - 3e^{-2|t|}$. The computations are done with the time step, $\Delta t = 10^{-2}$ and 10^4 realizations.

up to $t = 10$ which is enough for the probability to reach its asymptotic value. The numerical (dashed line) and analytical (solid line) results are shown in Figure 5.5 where the passing probability is plotted as a function of the initial kinetic energy. The results are in a good agreement with each other.

CHAPTER 6

CONCLUSION

The synthesis of the superheavy elements and hence the heavy ion fusion reactions are hotly debated and important subjects in nuclear physics. In most of the studies, the reaction mechanism of the fusing heavy nuclei is viewed as a classical diffusion process where the quantum statistical effects are ignored. Since the superheavy elements are stabilized by the shell correction energies, they should be synthesized at low excitation energies. Then, the quantum fluctuations are expected to play an important role on the dynamics.

In the first part of this study, a c-number quantum Langevin equation has been derived for the formation process of the heavy ion fusion reaction. A simple model where the fusion barrier is represented by an inverted parabola has been adopted. The memory effects has been incorporated into the transport coefficients and the correlation function of the stochastic force has been obtained in accordance with the quantum fluctuation-dissipation theorem. It is shown that the over-passing probability is enhanced at low temperatures when the quantum statistical effects are included [8].

The correlation function of the quantum noises exhibits a negative long time tail and when a Lorentzian cut-off is used it is possible to express the correlation function as a series of exponential terms with positive and negative coefficients. There is the superposition method for simulating the noises with correlation functions which contain many exponential terms. However, this method is restricted to the situations in which the correlation function of the noise is expressed as a sum of exponential terms with only positive coefficients. In the second part of the study, a simulation method for exponentially correlated colored noises is introduced as an extension of the superposition method to include negative terms as well [9].

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APPENDIX A

THE SOLUTION OF THE LANGEVIN EQUATION

In this Appendix, we analyze solutions of the Langevin Eq.(4.47) together with $dq/dt = p/M$ by employing one-sided Fourier transform [51]. After performing the Fourier transform, we obtain

$$-q_0 - i\omega q(\omega) = \frac{p(\omega)}{M}, \tag{A.1}$$

$$-p_0 - i\omega p(\omega) \pm M\Omega^2 q(\omega) = -\beta p(\omega) + \xi(\omega), \tag{A.2}$$

where (q_0, p_0) are the initial conditions, $q(\omega) = \int_0^\infty dt \exp(i\omega t) q(t)$ is the one-sided Fourier transform of the coordinate. The $p(\omega)$ and $\xi(\omega)$ are similarly defined. Solving for $q(\omega)$ and $p(\omega)$, we have

$$q(\omega) = iq_0 \frac{\omega + i\beta}{\omega^2 \mp \Omega^2 + i\omega\beta} - \frac{1}{M} \frac{p_0 + \xi(\omega)}{\omega^2 \mp \Omega^2 + i\omega\beta}, \tag{A.3}$$

$$p(\omega) = \frac{\pm M\Omega^2 q_0}{\omega^2 \mp \Omega^2 + i\omega\beta} + i\omega \frac{p_0 + \xi(\omega)}{\omega^2 \mp \Omega^2 + i\omega\beta}\,. \tag{A.4}$$

Time dependence of the collective variables are found by the inverse Fourier transformation,

$$q(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \exp(-i\omega t) q(\omega), \tag{A.5}$$

$$p(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \exp(-i\omega t) p(\omega)\,. \tag{A.6}$$

Integration over ω in these expressions can be carried out with the help of Cauchy theorem. Here, we give the results for a parabolic potential barrier,

$$q(t) = q_0 R(t) + p_0 S(t) + \int_0^t dt' S(t-t')\xi(t') \tag{A.7}$$

and

$$p(t) = q_0 \left(M\Omega\right)^2 S(t) + p_0 Q(t) + \int_0^t dt' Q(t-t')\xi(t') \tag{A.8}$$

where $Q(t)$, $S(t)$ and $R(t)$ are given by,

$$Q(t) = \exp\left(-\frac{\beta}{2}t\right)\left(\cosh\overline{\Omega}t - \frac{\beta}{2\overline{\Omega}}\sinh\overline{\Omega}t\right) \tag{A.9}$$

$$S(t) = \frac{1}{M\overline{\Omega}}\exp\left(-\frac{\beta}{2}t\right)\sinh\overline{\Omega}t \tag{A.10}$$

and

$$R(t) = \exp\left(-\frac{\beta}{2}t\right)\left(\cosh\overline{\Omega}t + \frac{\beta}{2\overline{\Omega}}\sinh\overline{\Omega}t\right) \tag{A.11}$$

where $\overline{\Omega} = \sqrt{\Omega^2 + (\beta/2)^2}$. The solutions can be given in a similar manner for a parabolic potential well. The mean values of collective variables are obtained by taking the ensemble average of Eq.(A.7) and Eq.(A.8),

$$\overline{q}(t) = \overline{q}_0 R(t) + \overline{p}_0 S(t) \qquad \text{and} \qquad \overline{p}(t) = \overline{q}_0 \left(M\Omega\right)^2 S(t) + \overline{p}_0 Q(t)\,. \tag{A.12}$$

The variances are given by,

$$\sigma_{qq}(t) = \sigma_{q0} R^2(t) + \sigma_{p0} S^2(t) + \int_0^t ds \int_0^t ds' S(s)S(s')2D_0\chi(s-s') \tag{A.13}$$

$$\sigma_{qp}(t) = \sigma_{q0}\left(M\Omega\right)^2 R(t)S(t) + \sigma_{p0}S(t)Q(t) + \int_0^t ds \int_0^t ds' S(s)Q(s')2D_0\chi(s-s') \quad \text{(A.14)}$$

and

$$\sigma_{pp}(t) = \sigma_{q0}\left(M\Omega\right)^4 S^2(t) + \sigma_{p0}Q^2(t) + \int_0^t ds \int_0^t ds' Q(s)Q(s')2D_0\chi(s-s')\,. \quad \text{(A.15)}$$

In these expressions, first two terms describe propagation of the initial fluctuations of the coordinate and momentum distributions σ_{q0}, σ_{p0} and the last term arises from dynamical fluctuations generated by the random force.

For calculation of the formation probability of compound nucleus, we need an explicit expression for variance $\sigma_{qq}(t)$ of the collective variable. In the Markovian limit, using the fact that the correlation function behaves like a delta function, $\chi(s-s') \to \delta(s-s')$, we obtain the known analytical result for the dynamical part of the $\sigma_{qq}(t)$ [44],

$$\begin{aligned}\sigma^{\chi}_{qq}(t) &= \int_0^t ds \int_0^t ds' S(s)S(s')2D_0\delta(s-s') \\ &= \frac{T}{M\Omega^2}e^{-\beta t}\left[\frac{\beta^2}{2\overline{\Omega}^2}(\sinh\overline{\Omega}t)^2 + \frac{\beta}{2\overline{\Omega}}(\sinh 2\overline{\Omega}t) - e^{+\beta t} + 1\right]. \quad \text{(A.16)}\end{aligned}$$

In the classical limit, the dynamical part of the $\sigma_{qp}(t)$ and $\sigma_{pp}(t)$ are similarly given by,

$$\begin{aligned}\sigma^{\chi}_{qp}(t) &= \int_0^t ds \int_0^t ds' S(s)Q(s')2D_0\delta(s-s') \\ &= \frac{\beta T}{\overline{\Omega}^2}e^{-\beta t}(\sinh\overline{\Omega}t)^2 \quad \text{(A.17)}\end{aligned}$$

and

$$\begin{aligned}\sigma_{pp}^{\chi}(t) &= \int_0^t ds \int_0^t ds' Q(s)Q(s')2D_0\delta(s-s') \\ &= \frac{MT\beta}{\overline{\Omega}} e^{-\beta t}\sinh\overline{\Omega}t\left[\cosh\overline{\Omega}t - \frac{\beta}{2\overline{\Omega}}\sinh\overline{\Omega}t\right] + MT\left(1-e^{-\beta t}\right). \quad \text{(A.18)}\end{aligned}$$

For quantal calculations, introducing the Fourier transform of the correlation function,

$$\chi(s-s') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(s-s')}\tilde{\chi}(\omega) \quad \text{(A.19)}$$

we can express the dynamical part of the variance in terms of a one-dimensional numerical integration over the frequency ω as,

$$\sigma_{qq}^{\chi}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left|\tilde{S}_t(\omega)\right|^2 \tilde{\chi}(\omega)2D_0 \quad \text{(A.20)}$$

where $\tilde{S}_t(\omega) = \int_0^t dsS(s)e^{-i\omega s}$. Dynamical parts of variances $\sigma_{qp}(t)$ and $\sigma_{pp}(t)$ can be evaluated in a similar manner to give,

$$\begin{aligned}\sigma_{qp}^{\chi}(t) &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{S}_t(\omega)\tilde{Q}_t^*(\omega)\tilde{\chi}(\omega)2D_0, \quad \text{(A.21)} \\ \sigma_{pp}^{\chi}(t) &= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left|\tilde{Q}_t(\omega)\right|^2 \tilde{\chi}(\omega)2D_0, \quad \text{(A.22)}\end{aligned}$$

where $\tilde{Q}_t(\omega) = \int_0^t dsQ(s)e^{-i\omega s}$.

APPENDIX B

THE AUTOCORRELATION FUNCTION OF THE NOISE

The solution of Eq.(5.57) and Eq.(5.58) are given by

$$R_1(t) = e^{-\lambda_1 t} R_1(0) + \lambda_1 \int_0^t e^{-\lambda_1 (t-s)} g_1(s) ds, \tag{B.1}$$

$$R_2(t) = e^{-\lambda_2 t} R_2(0) + \lambda_2 \int_0^t e^{-\lambda_2 (t-s)} g_2(s) ds. \tag{B.2}$$

Since $R(t) = R_1(t) + R_2(t)$, we have

$$\langle R(t) \rangle = e^{-\lambda_1 t} \langle R_1(0) \rangle + e^{-\lambda_2 t} \langle R_2(0) \rangle. \tag{B.3}$$

Let $R_1(0)$ and $R_2(0)$ be mean-zero Gaussian random numbers, then averaging over these random numbers we find

$$\{ \langle R(t) \rangle \} = 0. \tag{B.4}$$

By using the Eqs.(5.59,5.60,5.61), the correlations of R_1 and R_2 can be found as

$$\langle R_1(t) R_1(t') \rangle = \widetilde{D}_1 e^{-\lambda_1 |t-t'|} + \left[\langle R_1^2(0) \rangle - \widetilde{D}_1 \right] e^{-\lambda_1 (t+t')}, \tag{B.5}$$

$$\langle R_2(t) R_2(t') \rangle = \widetilde{D}_2 e^{-\lambda_2 |t-t'|} + \left[\langle R_2^2(0) \rangle - \widetilde{D}_2 \right] e^{-\lambda_2 (t+t')}, \tag{B.6}$$

$$\langle R_1(t) R_2(t') \rangle = \widetilde{D}_{12} e^{-\lambda_{12} |t-t'|} + \left[\langle R_1(0) R_2(0) \rangle - \widetilde{D}_{12} \right] e^{-(\lambda_1 t + \lambda_2 t')}, \tag{B.7}$$

where $\lambda_{12} = \lambda_1$ for $t > t'$ and $\lambda_{12} = \lambda_2$ for $t' > t$. Again averaging over the random numbers $R_1(0)$ and $R_2(0)$ we find

$$\{\langle R_1(t)R_1(t')\rangle\} = \widetilde{D}_1 e^{-\lambda_1|t-t'|}, \tag{B.8}$$

$$\{\langle R_2(t)R_2(t')\rangle\} = \widetilde{D}_2 e^{-\lambda_2|t-t'|}, \tag{B.9}$$

$$\{\langle R_1(t)R_2(t')\rangle\} = \widetilde{D}_{12} e^{-\lambda_{12}|t-t'|}, \tag{B.10}$$

once these random numbers satisfy the following equations

$$\{\langle R_1^2(0)\rangle\} = \widetilde{D}_1, \tag{B.11}$$

$$\{\langle R_2^2(0)\rangle\} = \widetilde{D}_2, \tag{B.12}$$

$$\{\langle R_1(0)R_2(0)\rangle\} = \widetilde{D}_{12}. \tag{B.13}$$

Now we have enough information to build the autocorrelation of $R(t)$ and it is found to be

$$\{\langle R(t)R(t')\rangle\} = \left(\widetilde{D}_1 + \widetilde{D}_{12}\right) e^{-\lambda_1|t-t'|} + \left(\widetilde{D}_2 + \widetilde{D}_{12}\right) e^{-\lambda_2|t-t'|}. \tag{B.14}$$

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