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QUANTUM STATISTICAL EFFECTS ON FUSION DYNAMICS OF HEAVY-IONS

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Abstract

In order to describe the fusion of two very heavy nuclei at near barrier energies, a generalized Langevin approach is proposed, which incorporates the quantum statistical fluctuations in accordance with the fluctuation and dissipation theorem. It is illustrated that the quantum statistical effects introduce an enhancement of the formation of compound nucleus, though the quantum enhancement is somewhat less pronounced as indicated in the previous calculations.

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I. INTRODUCTION

In recent years, there has been a great deal of interest in the synthesis of superheavy elements by means of heavy-ion fusion at near barrier energies [1]. Due to very low production probabilities, investigation of heavy-ion fusion reactions remains a challenging task both experimentally and theoretically. Theoretical investigations are mostly based on transport theory in which heavy-ion fusion is viewed as a diffusion process [2–5]. During the approach phase, a part of the kinetic energy of the relative motion dissipates into intrinsic degrees of freedom, colliding ions overcome the Coulomb barrier and a sticking configuration is formed. Subsequently, the system evolves inward over the conditional saddle to form a spherical compound nucleus. Heavy-ion fusion is described in terms of a few relevant variables, which evolve according to a Langevin dynamics as in a typical diffusion process. In most of these investigations quantum statistical effects are ignored and a classical treatment is employed, in which friction and diffusion properties are related through classical fluctuation-dissipation theorem. Since superheavy elements are stabilized by the shell correction energy, they should be synthesized at reasonably low energies, which corresponds to nuclear temperatures of the order of $T = 0.5 - 1.0$ MeV. On the other hand, the curvature of the conditional saddle is also of the order of $\hbar\Omega = 1.0$ MeV. As a result, it is expected that the quantum statistical effects play an important role in the formation of a compound nucleus by diffusion along the conditional potential barrier [6–8]. In a recent work, using the density matrix formalism, we derived a generalized Fokker-Planck equation for the distribution function of relevant collective variables with non-Markovian transport coefficients and we illustrated the quantum statistical effects on the formation of compound nucleus at low temperatures [9,10]. Here, we consider the same problem, but follow a different description based on generalized Langevin approach. By projection on the collective space, it is possible to deduce stochastic equations of motion for collective variables. The friction term involves memory effect and the random force acts as a correlated noise and they are related according to quantum fluctuation-dissipation theorem [11,12]. As a result, the quantum statistical fluctuations are incorporated into the description and the approach is valid at all temperatures. In principle, the Langevin approach presented here is equivalent to the density matrix formalism, however it has certain advantages as compared to the description by the Fokker-Planck equation [13]. One thing is that, in realistic situations, numerical simulations of Langevin equation require much less numerical effort than the solution of the Fokker-Planck equation. Furthermore, diffusion coefficients presented here are modified by the friction mechanism, which was not considered in the density matrix approach [9,10]. In section 2, we derive generalized Langevin equations for the relevant collective variables. In section 3, we present an analysis of the Langevin equation. In section 4, in order to illustrate the effect of quantum statistical fluctuations, we present calculations to describe the heavy-ion fusion reactions at low temperatures. Finally, we give conclusions in section 5.

II. GENERALIZED LANGEVIN EQUATIONS

It is possible to derive transport equation for the entire dynamics of the heavy-ion fusion process, starting from the entrance channel until formation of a compound nucleus. Here,

we want to investigate the influence of quantum statistical fluctuations on the formation probability of compound nucleus at near barrier energies. For this purpose, we consider a part of the dynamics, namely, evolution of the system along the conditional saddle from sticking configuration until formation of compound nucleus. For simplicity, we describe the evolution in terms of a single collective variable, namely the elongation variable, q, which approximately corresponds to the relative distance between the colliding ions. We consider a model, in which evolution of the system is described by a Hamiltonian of the form,

$$H = H_0 + H_{coll} + V_{coup} \tag{1}$$

where H_0, H_{coll} and V_{coup} represent the Hamiltonian of the intrinsic nucleonic degrees of freedom, the Hamiltonian of the collective variable and the coupling interaction of the collective variable with the intrinsic nucleonic degrees of freedom, respectively. For simplicity, we consider a harmonic form for the collective Hamiltonian $H_{coll} = p^2/2M \pm M\Omega^2 q^2/2$, where M is the mass parameter of the collective variable and $M\Omega^2$ denotes the magnitude of the curvature parameter of the potential energy, 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, $V_{coup} = qF$. The classical equation of motion for the collective variable can be deduced from $dp/dt = -(dH/dq)$, where (..) denotes an average over the intrinsic degrees of freedom, to give,

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

Here, the quantity on the right hand side denotes the force of the intrinsic degrees of freedom on the collective motion. We consider the case where the coupling F is a one-body operator. We then need only the single-particle density matrix ρ 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 $\delta\rho(t) = \rho(t) - \bar{\rho}(t)$, where the bar means taking ensemble average. Assuming fluctuations are small, $\delta\rho(t)$ is determined by a linearized transport equation [14] around the average $\bar{\rho}(t)$,

$$i\hbar\frac{\partial}{\partial t}\delta\rho(t) - [\bar{h}(t), \delta\rho(t)] - [\delta q(t)F, \bar{\rho}(t)] = 0 \tag{3}$$

where $\bar{h}(t) = h + \bar{q}(t)F$, 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,

$$i\hbar\frac{\partial}{\partial t}\bar{\rho}(t) - [\bar{h}(t), \bar{\rho}(t)] = 0\,. \tag{4}$$

For simplicity of derivation, we neglect the collision term on the right hand side of eq.(3) and eq.(4) [15–17], however subsequently, we incorporate the damping width of single-particle states. Starting from an initial state $\delta\rho(s)$ at some time s, the formal solution of eq.(3) can be given as,

$$\delta\rho(t) = -\frac{i}{\hbar}\int_s^t dt'\delta q(t')\left[G(t,t')FG^\dagger(t,t'),\bar{\rho}(t)\right] + G(t,s)\delta\rho(s)G^\dagger(t,s) \tag{5}$$

where the first term describes the effects of the perturbation during the time interval $t-s$ with $G(t,s) = \exp\left[-(i/\hbar)\int_s^t dt'\bar{h}(t')\right] \approx \exp\left[-(i/\hbar)(t-s)\bar{h}(t)\right]$ 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 $\delta\rho(s)$ 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.(5). 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.(5), we approximate the average density matrix in terms of the instantaneous single-particle wave functions as $\bar{\rho}(t) \approx \sum |\phi_l(t)\rangle n_l \langle\phi_l(t)|$, where we neglect the off diagonal elements. In this expression, the instantaneous wave functions $\phi_l(t) = \phi_l[q(t)]$ are determined from $(h + qF)|\phi_l(q)\rangle = \varepsilon_l(q)|\phi_l(q)\rangle$ 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,

$$\delta\rho_{ij}(t) = -\frac{i}{\hbar}\int_s^t dt'\delta q(t')G_{ij}(t,t')\langle i|F|j\rangle(n_j - n_i) + G_{ij}(t,s)\delta\rho_{ij}(s) \tag{6}$$

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 $\delta\rho(s)$ is a Gaussian random quantity with zero mean $\overline{\langle i|\delta\rho|j\rangle} = 0$ and a second moment. In accordance with the fluctuation-dissipation relation of the single-particle density matrix, we specify the second moment of $\delta\rho(s)$ as,

$$\overline{\langle i|\delta\rho|j\rangle\langle j'|\delta\rho|i'\rangle} = \delta_{ii'}\delta_{jj'}\frac{1}{2}\left[n_i(1-n_j) + n_j(1-n_i)\right] . \tag{7}$$

In the special case of diagonal elements this formula gives the known result for fluctuations of occupation numbers, $\overline{\langle i|\delta\rho|i\rangle\langle i|\delta\rho|i\rangle} = n_i(1-n_i)$ [18]. Substituting eq.(5) into the right hand side of eq.(2), we find a generalized Langevin equation for the fluctuations of the collective variable,

$$\frac{d}{dt}\delta p(t) \pm M\Omega^2\delta q(t) = \int_s^t dt'\gamma(t-t')\delta q(t') + \xi(t) \tag{8}$$

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

$$\gamma(t-t') = \frac{i}{\hbar}\Sigma|\langle i|F|j\rangle|^2 G_{ji}(t,t')\left[n_i(1-n_j) - n_j(1-n_i)\right] \tag{9}$$

and

$$\xi(t) = -\Sigma\langle i|F|j\rangle G_{ji}(t,s)\langle j|\delta\rho|i\rangle. \tag{10}$$

Using eq.(7), the auto-correlation function of the random force can be expressed as,

$$\overline{\xi(t)\xi(t')} = \Sigma|\langle i|F|j\rangle|^2 G_{ij}(t,t')\frac{1}{2}\left[n_i(1-n_j)+n_j(1-n_i)\right] . \tag{11}$$

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.(8). For evolution over a short time interval from t' to t, by neglecting the right hand side of eq.(8), we find the following relation,

$$\delta q(t') \approx C(t-t')\delta q(t) - S(t-t')\delta p(t) . \tag{12}$$

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

$$C(t-t') = \cos\Omega(t-t') \qquad \text{and} \qquad S(t-t') = \frac{1}{M\Omega}\sin\Omega(t-t') . \tag{13}$$

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

$$C(t-t') = \cosh\Omega(t-t') \qquad \text{and} \qquad S(t-t') = \frac{1}{M\Omega}\sinh\Omega(t-t') . \tag{14}$$

The first term in eq.(12) 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.(12) into the right hand side of eq.(8). Note that, since the fluctuations are linear, the same equation as eq.(8), 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 $q(t) = \bar{q}(t) + \delta q(t)$,

$$\frac{d}{dt}p(t) \pm M\Omega^2 q(t) = -\beta p(t) + \xi(t) . \tag{15}$$

Here, the reduced friction coefficient is given by,

$$\beta = \frac{i}{\hbar}\int_0^{t-s} d\tau \Sigma|\langle i|F|j\rangle|^2 e^{-\frac{i}{\hbar}\tau(\varepsilon_j-\varepsilon_i)} n_i(1-n_j)S(\tau) + c.c. . \tag{16}$$

Substituting eqs.(13) and (14) for $S(\tau)$, we find for the friction coefficient for a parabolic well,

$$\beta = -\frac{1}{2iM\Omega}\Sigma|\langle i|F|j\rangle|^2\left[\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i-\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i-\hbar\Omega-i\eta} - \frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i+\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i+\hbar\Omega-i\eta}\right] n_i(1-n_j) + c.c. \tag{17}$$

and for a parabolic barrier,

$$\beta = +\frac{1}{2M\Omega}\Sigma|\langle i|F|j\rangle|^2\left[\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i-i\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i-i\hbar\Omega-i\eta}\right.$$
$$\left.-\frac{e^{-\frac{i}{\hbar}(t-s)(\varepsilon_j-\varepsilon_i+i\hbar\Omega-i\eta)}-1}{\varepsilon_j-\varepsilon_i+i\hbar\Omega-i\eta}\right]n_i(1-n_j)+c.c.\,. \tag{18}$$

In obtaining these results, we include the damping width η of the single-particle states into the propagator in eq.(16) [19]. In further evaluation of the friction coefficients, we neglect the time-dependent terms in eqs.(17) and (18). 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.(17) and eq.(18) 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,

$$\beta = \Sigma|\langle i|F|j\rangle|^2\frac{1}{M\Omega}\left[\frac{\eta}{\left(\varepsilon_j-\varepsilon_i-\hbar\Omega\right)^2+\eta^2}-\frac{\eta}{\left(\varepsilon_j-\varepsilon_i+\hbar\Omega\right)^2+\eta^2}\right]n_i(1-n_j) \tag{19}$$

and for a parabolic barrier,

$$\beta = \Sigma|\langle i|F|j\rangle|^2\frac{1}{M\Omega}\left[\frac{\varepsilon_j-\varepsilon_i}{(\varepsilon_j-\varepsilon_i)^2+(\hbar\Omega-\eta)^2}-\frac{\varepsilon_j-\varepsilon_i}{(\varepsilon_j-\varepsilon_i)^2+(\hbar\Omega+\eta)^2}\right]n_i(1-n_j)\,. \tag{20}$$

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 [20],

$$\overline{\xi(t)\xi(t')} = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\frac{\hbar\omega}{2T}\coth\frac{\hbar\omega}{2T}\cdot 2D(\omega) \tag{21}$$

where,

$$D(\omega) = T\Sigma|\langle i|F|j\rangle|^2\frac{1}{\omega}\left[\frac{\eta}{\left(\varepsilon_j-\varepsilon_i-\hbar\omega\right)^2+\eta^2}-\frac{\eta}{\left(\varepsilon_j-\varepsilon_i+\hbar\omega\right)^2+\eta^2}\right]n_i(1-n_j)\,. \tag{22}$$

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 $\langle i|F|j\rangle^2 \propto \exp[-(\varepsilon_j-\varepsilon_i)^2/2\Delta^2]$ or $\propto 1/\left[1+(\varepsilon_j-\varepsilon_i)^2/2\Delta^2\right]$. Furthermore, because of the Lorentzian factors in eq.(22), 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.(21) of the random force can be expressed as,

$$\overline{\xi(t)\xi(t')}=2D_0\cdot\chi(t-t') \tag{23}$$

where

$$\chi(t-t')=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\frac{\hbar\omega}{2T}\coth\frac{\hbar\omega}{2T}\cdot\exp\left[-(\hbar\omega)^2/2\Delta^2\right]. \tag{24}$$

The correlation function is characterized by two different parameters, the cut-off energy and temperature. Figure 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,

$$\chi_0(t-t')=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\exp\left[-\frac{(\hbar\omega)^2}{2\Delta^2}\right]=\frac{1}{\sqrt{2\pi}\tau_0}\exp\left[-(t-t')^2/2\tau_0^2\right]. \tag{25}$$

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, in the quantal regime i.e. at low temperatures $\hbar\Omega\geq 2T$, we are faced with a stochastic evolution with a correlated noise [11,12].

III. ANALYSIS OF 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 [17,21,22] and we need to adopt suitable algorithms for numerical simulations [23]. However, in the situation that we consider here, the solution of the Langevin eq.(15) can be given analytically [13]. 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,

$$P(q,p,t)=\frac{1}{2\pi X}\exp\left[-\frac{1}{2X^2}\left((q-\overline{q})^2\tilde{\sigma}_{qq}+2(q-\overline{q})(p-\overline{p})\tilde{\sigma}_{qp}+(p-\overline{p})^2\tilde{\sigma}_{pp}\right)\right] \tag{26}$$

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,

$$\frac{d}{dt}\overline{q}(t) = \frac{1}{M}\overline{p}(t) \qquad \text{and} \qquad \frac{d}{dt}\overline{p}(t) \pm M\Omega^2\overline{q}(t) = -\beta\overline{p}(t)\,. \tag{27}$$

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

$$\frac{d}{dt}\delta q(t) = \frac{1}{M}\delta p(t) \qquad \text{and} \qquad \frac{d}{dt}\delta p(t) \pm M\Omega^2\delta q(t) = -\beta\delta p(t) + \xi(t)\,. \tag{28}$$

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

$$\frac{d}{dt}\sigma_{qq}(t) = \frac{2}{M}\sigma_{qp}(t) \tag{29}$$

$$\frac{d}{dt}\sigma_{qp}(t) \pm M\Omega^2\sigma_{qq}(t) = \frac{1}{M}\sigma_{pp}(t) - \beta\sigma_{qp}(t) + D_{qp}(t) \tag{30}$$

$$\frac{d}{dt}\sigma_{pp}(t) \pm 2M\Omega^2\sigma_{qp}(t) = -2\beta\sigma_{pp}(t) + 2D_{pp}(t) \tag{31}$$

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 (A5) and (A6), diffusion coefficients can be expressed in terms of the correlation function of the random force as,

$$D_{pp}(t) = \int_0^t dt' Q(t-t') \cdot \overline{\xi(t')\xi(t)} = 2D_0 \int_0^t ds\, Q(s) \cdot \chi(s) \tag{32}$$

and

$$D_{qp}(t) = \int_0^t dt' S(t-t') \cdot \overline{\xi(t')\xi(t)} = 2D_0 \int_0^t ds\, S(s) \cdot \chi(s)\,. \tag{33}$$

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 (A7) and (A8) 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 $S(s)$. For 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 [9,10]. Figures 2 and 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 on diffusion coefficients, we calculate diffusion coefficients by replacing $\overline{\Omega}$ with Ω in the propagators $Q(s)$ and $S(s)$. Figures 4 and 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 (29), (30) and (31). However, it is much easier to obtain these variances directly from the Langevin equation (15) with the help of one-sided Fourier transform [18], as shown in Appendix A.

IV. QUANTUM STATISTICAL 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 [5,24,25],

$$P_f(t) = \int_0^\infty dq \frac{1}{\sqrt{2\pi\sigma_{qq}(t)}} \exp\left[-\frac{(q-\overline{q}(t))^2}{2\sigma_{qq}(t)}\right] = \frac{1}{2}\mathrm{erfc}\left(-\frac{\overline{q}(t)}{\sqrt{2\sigma_{qq}(t)}}\right). \tag{34}$$

Here, $\overline{q}(t)$ and $\sigma_{qq}(t)$ are the mean value and the variance of the elongation parameter, which are given by (A10) and (A11) 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 $(\overline{q}_0, \overline{p}_0)$ 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 [10], 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 a analytical expression given by (A14), while in the quantum limit

it is given by (A18), and involves a one dimensional numerical integration over the frequency ω. Figure 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 [10]. 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 $\overline{\Omega}$.

V. CONCLUSIONS

Since several years, much effort has been made for synthesis of superheavy elements by heavy-ion fusion at near barrier energies. Even though, the reaction mechanism of heavy-ion fusion is not well understood, in most theoretical descriptions fusion is viewed as a diffusion process, which can be described by a Fokker-Planck approach or a stochastic Langevin approach [2–5,24,25]. In these descriptions the quantum statistical effects are ignored and a classical treatment is employed. In a recent work, we introduced a description based on a generalized Fokker-Planck approach, which incorporates quantum effects through non-Markovian transport coefficients [9,10]. In the present work, we follow a different description based on a generalized Langevin approach. The friction term and the random force both involve memory effects and they are related to each other in accordance with the fluctuation-dissipation theorem. As a result, the quantum statistical fluctuations are incorporated into the description. In principle, both approaches provide an equivalent description, however the Langevin approach has certain advantages in practical applications. In general, for a complex potential energy surface, it is much easier to carry out simulations of Langevin equation than solving the Fokker-Planck equation. Furthermore, diffusion coefficients presented here are strongly modified by the friction mechanism, which was not considered in the Fokker-Planck approach [10]. In this work, we consider a simple model in which the fusion barrier is represented by an inverted parabola. In this case, the joint distribution function of the collective variable and the conjugate momentum becomes a Gaussian, and the fusion probability can be given in an analytical form. Calculations illustrate that the quantum statistical effects enhance the fusion probability at low temperatures. However, the enhancement is somewhat less pronounced than that reported in the previous investigation [10]. For a realistic potential energy surface, analytical solution is not possible and distribution function of collective variables should be constructed by generating sufficient number of events of the generalized Langevin equation. Since, the random force is not a white noise, we cannot use standard methods for numerical simulations [21,22]. Therefore, it is necessary to develop suitable algorithms for simulations of the Langevin equation with a correlated random force [23].

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APPENDIX

In this Appendix, we analyze solutions of the Langevin eq.(15) together with $dq/dt = p/M$ by employing one-sided Fourier transform [18]. After performing the Fourier transform, we obtain

$$-q_0 - i\omega q(\omega) = \frac{p(\omega)}{M} \qquad \text{and} \qquad -p_0 - i\omega p(\omega) \pm M\Omega^2 q(\omega) = -\beta p(\omega) + \xi(\omega) \tag{A1}$$

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. Combining two equations in (A1), the Fourier transforms of the collective variables are given by,

$$q(\omega) = iq_0 \frac{\omega + i\beta}{\omega^2 \mp \Omega^2 + i\omega\beta} - \frac{1}{M} \frac{p_0 + \xi(\omega)}{\omega^2 \mp \Omega^2 + i\omega\beta} \tag{A2}$$

$$p(\omega) = \frac{\pm M\Omega^2 q_0}{\omega^2 \mp \Omega^2 + i\omega\beta} + i\omega \frac{p_0 + \xi(\omega)}{\omega^2 \mp \Omega^2 + i\omega\beta} \ . \tag{A3}$$

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

$$q(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \exp(-i\omega t) q(\omega) \qquad \text{and} \qquad p(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \exp(-i\omega t) p(\omega) \, . \tag{A4}$$

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,

$$q(t) = q_0 R(t) + p_0 S(t) + \int_0^t dt' S(t - t') \xi(t') \tag{A5}$$

and

$$p(t) = q_0 \left(M\Omega\right)^2 S(t) + p_0 Q(t) + \int_0^t dt' Q(t - t') \xi(t') \tag{A6}$$

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

$$Q(t) = \exp\left(-\frac{\beta}{2} t\right) \left(\cosh \overline{\Omega} t - \frac{\beta}{2\overline{\Omega}} \sinh \overline{\Omega} t\right) \tag{A7}$$

$$S(t) = \frac{1}{M\overline{\Omega}} \exp\left(-\frac{\beta}{2} t\right) \sinh \overline{\Omega} t \tag{A8}$$

and

$$R(t) = \exp\left(-\frac{\beta}{2}t\right)\left(\cosh\overline{\Omega}t + \frac{\beta}{2\overline{\Omega}}\sinh\overline{\Omega}t\right) \tag{A9}$$

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 (A5) and (A6),

$$\overline{q}(t) = \overline{q}_0 R(t) + \overline{p}_0 S(t) \qquad \text{and} \qquad \overline{p}(t) = \overline{q}_0 \left(M\Omega\right)^2 S(t) + \overline{p}_0 Q(t)\,. \tag{A10}$$

The variances are given by,

$$\sigma_{qq}(t) = \sigma_{q0}R^2(t) + \sigma_{p0}S^2(t) + \int_0^t ds \int_0^t ds' S(s)S(s')2D_0\chi(s-s') \tag{A11}$$

$$\sigma_{qp}(t) = \sigma_{q0}\left(M\Omega\right)^2 R(t)S(t) + \sigma_{p0}S(t)Q(t) + \int_0^t ds \int_0^t ds' S(s)Q(s')2D_0\chi(s-s') \tag{A12}$$

and

$$\sigma_{pp}(t) = \sigma_{q0}\left(M\Omega\right)^4 S^2(t) + \sigma_{p0}Q^2(t) + \int_0^t ds \int_0^t ds' Q(s)Q(s')2D_0\chi(s-s')\,. \tag{A13}$$

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 $\sigma_{qq}(t)$ [5],

$$\begin{aligned}\sigma^{\chi}_{qq}(t) &= \int_0^t ds \int_0^t ds' S(s)S(s')2D_0\chi(s-s') \to \int_0^t ds \int_0^t ds' S(s)S(s')2D_0\delta(s-s') \\ &= \frac{T}{M\Omega^2}e^{-\beta t}\left[\frac{\beta^2}{2\overline{\Omega}^2}(\sinh\overline{\Omega}t)^2 + \frac{\beta}{2\overline{\Omega}}(\sinh 2\overline{\Omega}t) - e^{+\beta t} + 1\right]. \end{aligned} \tag{A14}$$

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

$$\begin{aligned}\sigma^{\chi}_{qp}(t) &= \int_0^t ds \int_0^t ds' S(s)Q(s')2D_0\chi(s-s') \to \int_0^t ds \int_0^t ds' S(s)Q(s')2D_0\delta(s-s') \\ &= \frac{\beta T}{\overline{\Omega}^2}e^{-\beta t}(\sinh\overline{\Omega}t)^2 \end{aligned} \tag{A15}$$

and

$$\begin{aligned}\sigma^{\chi}_{pp}(t) &= \int_0^t ds \int_0^t ds' Q(s)Q(s')2D_0\chi(s-s') \to \int_0^t ds \int_0^t ds' Q(s)Q(s')2D_0\delta(s-s') \\ &= MT\frac{\beta}{\overline{\Omega}}e^{-\beta t}\sinh\overline{\Omega}t\left[\cosh\overline{\Omega}t - \frac{\beta}{2\overline{\Omega}}\sinh\overline{\Omega}t\right] + MT\left(1 - e^{-\beta t}\right). \end{aligned} \tag{A16}$$

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

$$\chi(s-s') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(s-s')} \tilde{\chi}(\omega) \tag{A17}$$

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

$$\sigma_{qq}^{\chi}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left|\tilde{S}_t(\omega)\right|^2 \tilde{\chi}(\omega) 2D_0 \tag{A18}$$

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

$$\sigma_{qp}^{\chi}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \tilde{S}_t(\omega) \tilde{Q}_t^*(\omega) \tilde{\chi}(\omega) 2D_0 \quad \text{and} \quad \sigma_{pp}^{\chi}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \left|\tilde{Q}_t(\omega)\right|^2 \tilde{\chi}(\omega) 2D_0 \tag{A19}$$

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

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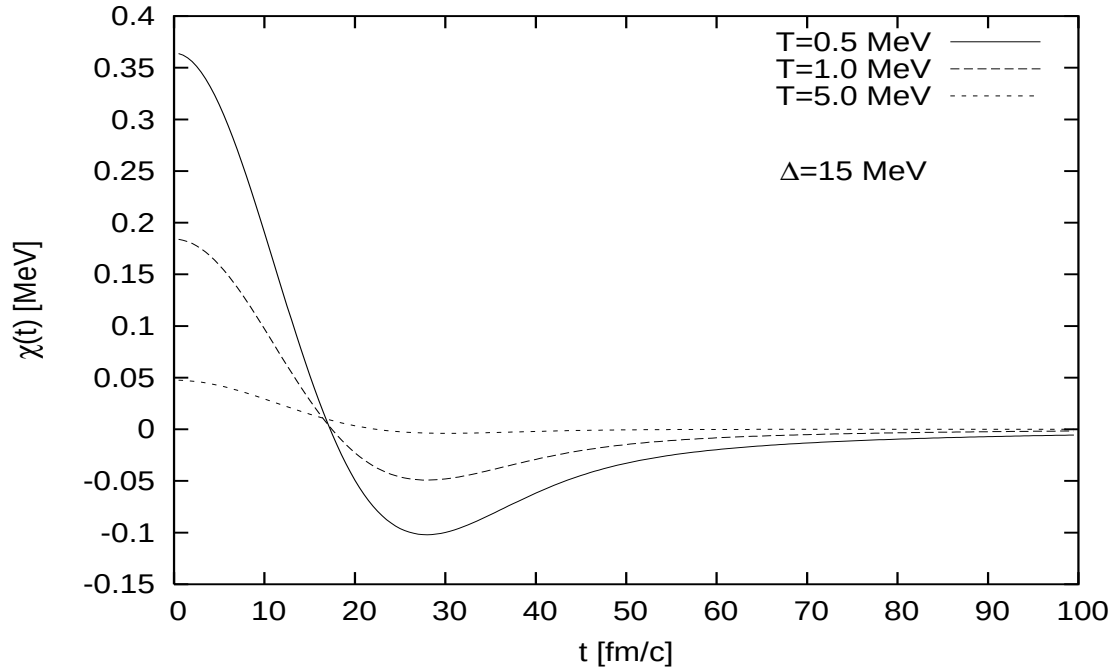


FIG. 1. The correlation function is plotted versus time for $\Delta = 15$ MeV.

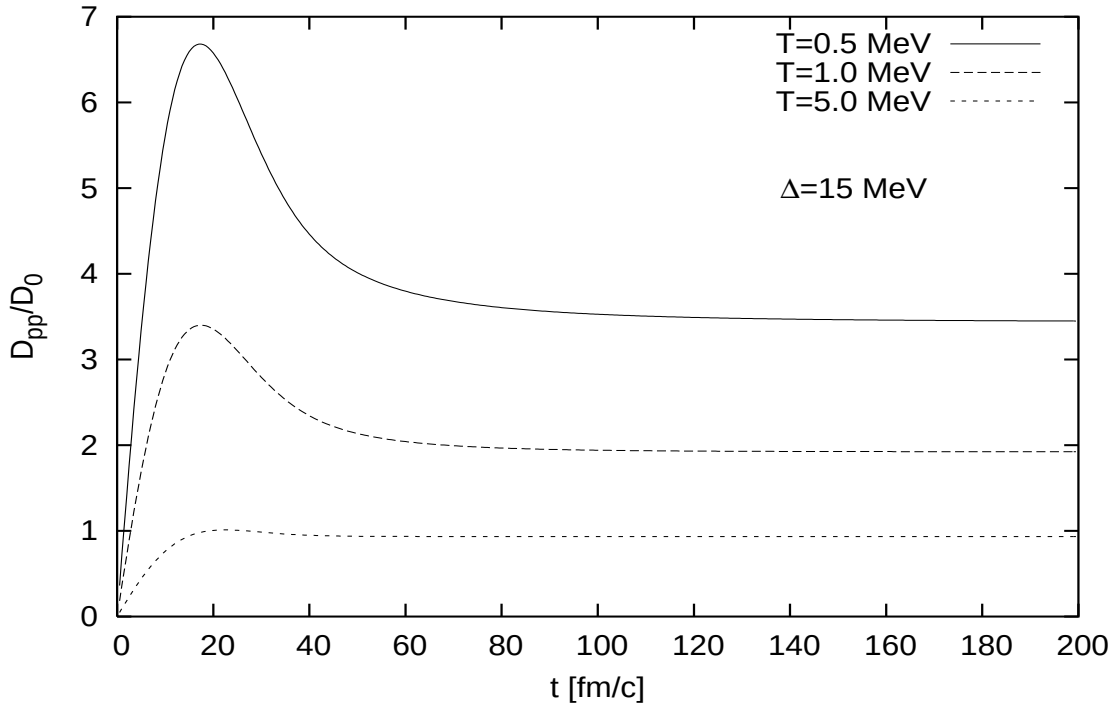


FIG. 2. The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV.

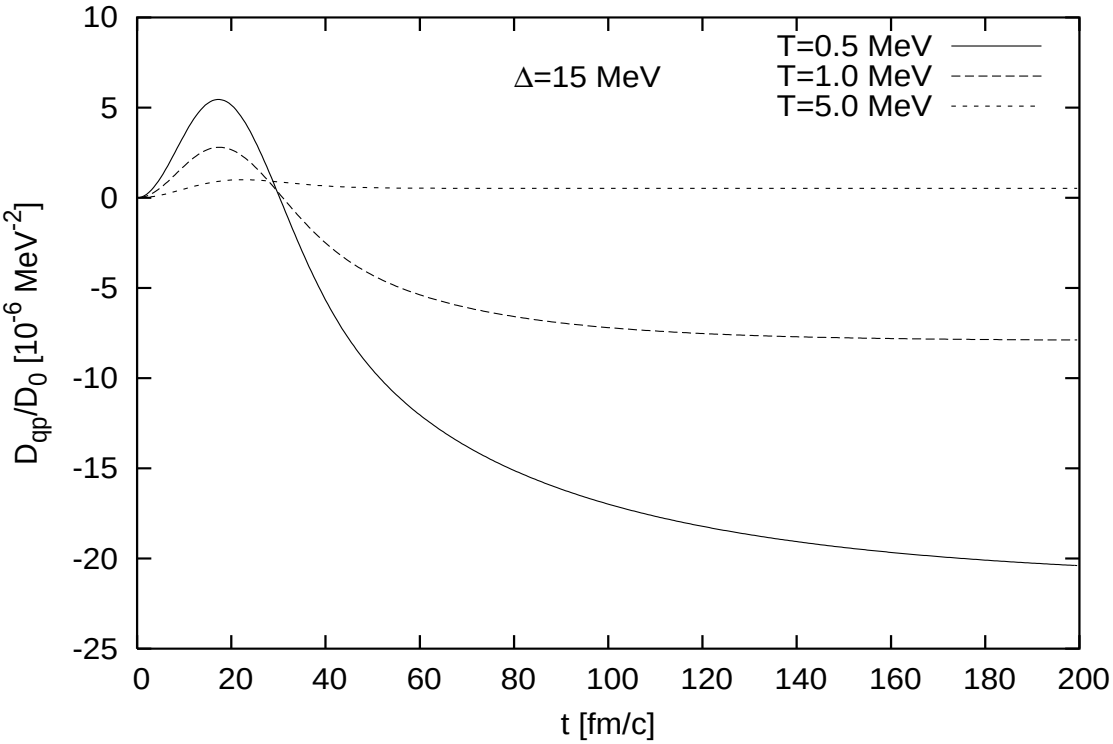


FIG. 3. The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV.

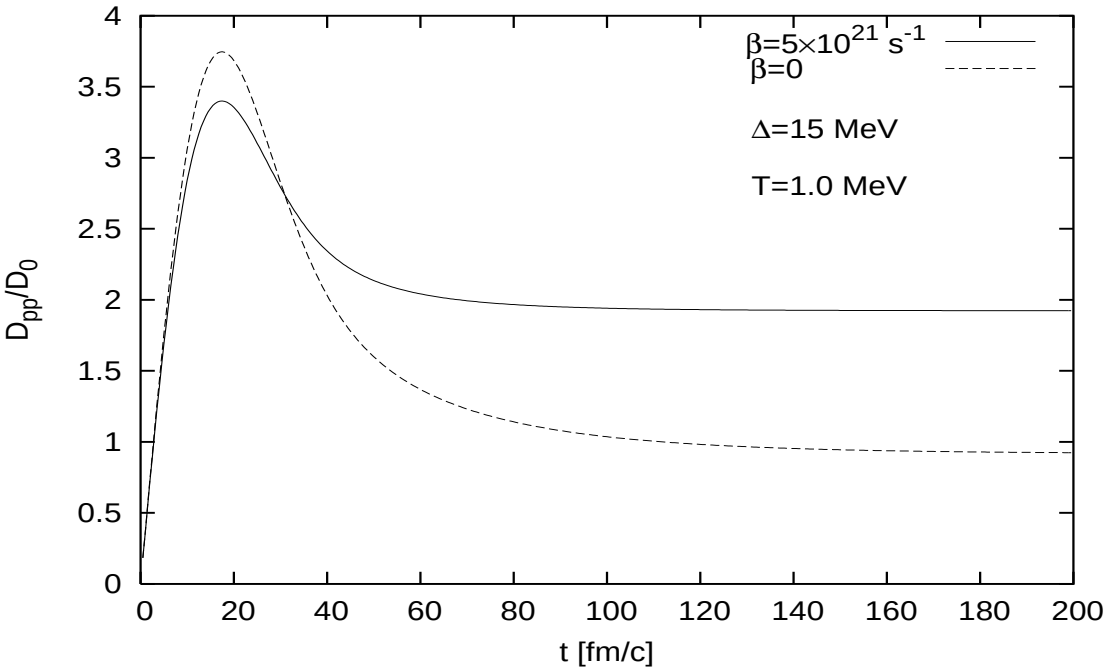


FIG. 4. The momentum diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV and T=1.0 MeV. The cases with and without friction are compared.

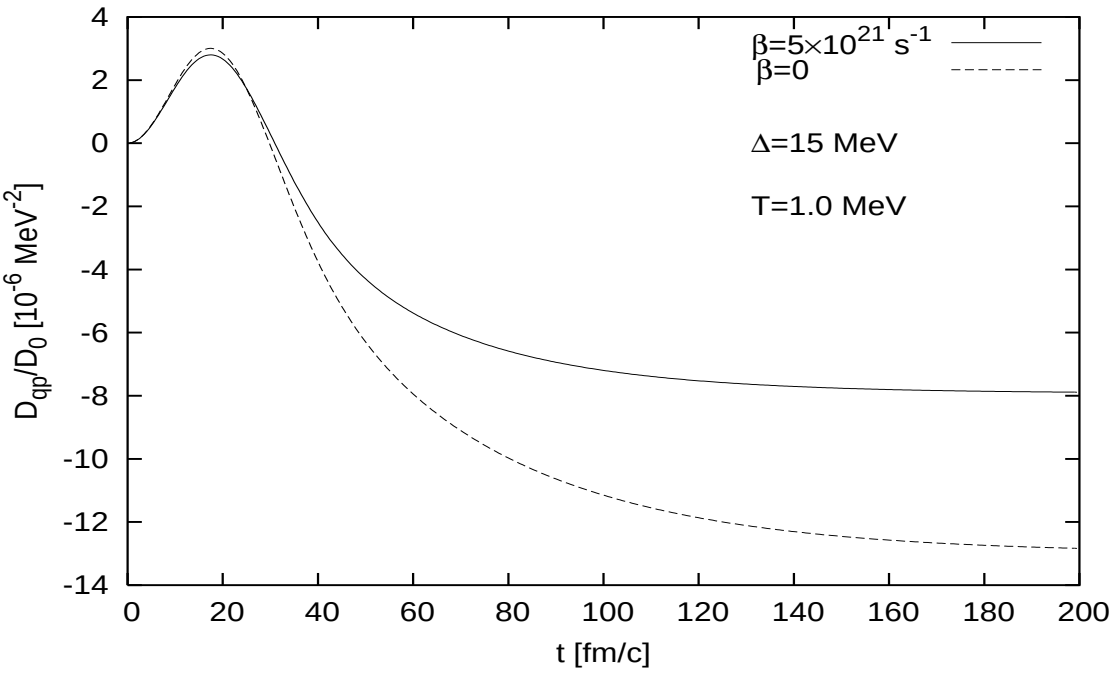


FIG. 5. The mixed diffusion coefficient, in units of classical diffusion coefficient, is plotted versus time for $\Delta = 15$ MeV and T=1.0 MeV. The cases with and without friction are compared.

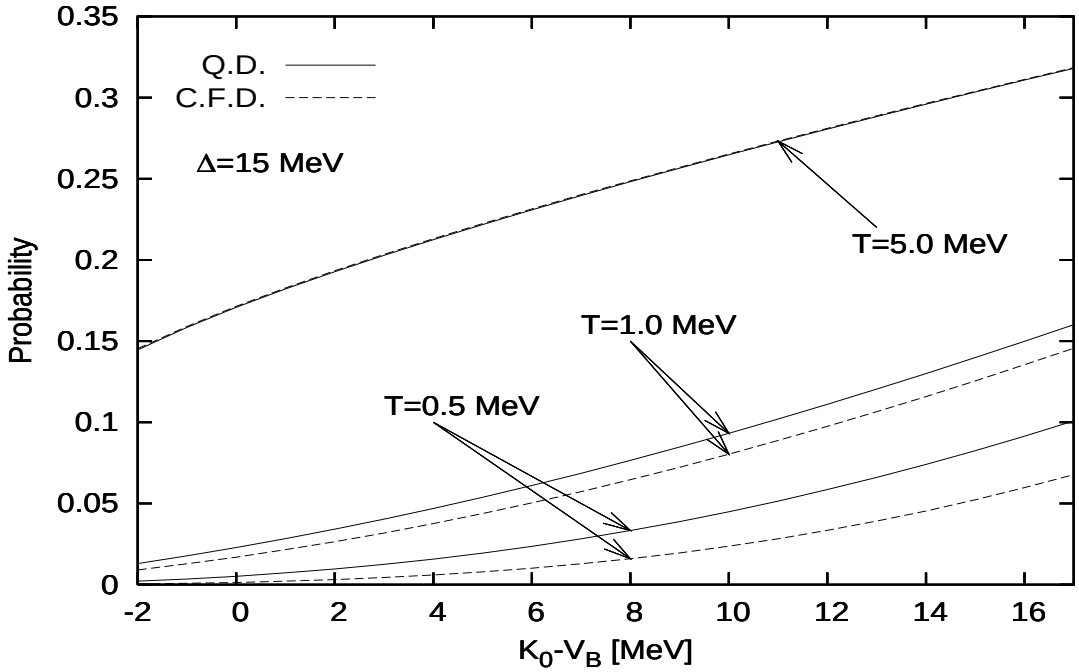


FIG. 6. The formation probability is plotted versus initial kinetic energy minus barrier height. The result of classical diffusion approach is compared with that of quantum diffusion approach for $\Delta = 15$ MeV.