Analytical solution of a multidimensional Langevin equation at high friction limits and probability passing over a two-dimensional saddle*

XING Yong-Zhong(邢永忠)[1)]

(Physics Department of Tianshui Normal University, Tianshui 741000, China)
(Institute of Modern Physics, Chinese Academy of Sciences, Lanzhou 730000, China)
(Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator of Lanzhou, Lanzhou 730000, China)

Abstract The analytical solution of a multidimensional Langevin equation at the overdamping limit is obtained and the probability of particles passing over a two-dimensional saddle point is discussed. These results may break a path for studying further the fusion in superheavy elements synthesis.

Key words Langevin equation, high friction, saddle point, analytical solution

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1 Introduction

The existence of superheavy elements is a long-standing prediction based on the theory of the nuclear shell structure model since extra-stability would be reached due to the shell closure of the nucleons[1]. In the last few decades, enormous efforts have been made both theoretically and experimentally and great achievements have been obtained in the synthesis of superheavy elements[2]. More than twenty elements have been synthesized artificially in the laboratory[3]. So far, however, we are far from completely understanding the mechanism of superheavy elements synthesis. The fusion hindrance, which is described with extra-push energy, is known to exist[4, 5] in the massive systems. Although a lots of attempts have been made to solve this forbidding problem and some achievements have been successfully gained[6, 7], there are a lot of problems which need to be solved in this field.

A new theoretical model for the fusion mechanism of massive unclear systems has been proposed by Y. Abe and his cooperators in Ref. [8,9], in which the fusion process is divided into two steps: an approaching phase up to the contact of two incident ions and shape evolutions from the amalgamated configuration to the spherical shape. In the approaching phase of passing over the Coulomb barrier, the system can be described as collision processes under frictional forces. The evolutions of the amalgamated mono-nuclear system toward the spherical shape are also under the frictional forces acting in collective motions of excited nuclei. Since the two steps are connected successively, the results of the first step not only give a probability for incident ions to stick to each other, but also give the initial conditions for the second step. Because the heat-up processes during two-body collisions, the collective shape motions of the system are under a strong dissipation stemming from frequent interactions with the nucleons at a finite temperature. Thus the whole process is described by dissipation-fluctuation dynamics. That is to say briefly, the process of synthesis of superheavy elements via the way of massive nuclear collision is a dissipation-fluctuation dynamics, in which there is an additional saddle which must be dealt with carefully.

Under a series of assumptions, for instance, the internal degrees of freedom are more quickly thermalized than the collective ones, and the dynamical process can be described by the Langevin equation[10].

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1) E-mail: tsxyz@public.lz.gs.cn

However, this equation is not easy to solve for real nuclear interaction. Therefore, the fusion barrier was greatly simplified in order to explore the space-time evolution of the distribution function or the probability. The most popular form of the fusion barrier is taken as an inverted parabola and the study for it has been done in Ref. [11] where the formal solution of the Langevin equation and the probabilities passing over the one-dimensional potential barrier have been gained. Based on the work of Ref. [11], in the present paper, we try to solve analytically the Langevin equation with linear external force at the overdamping limit and try to apply the result to the two-dimensional barrier. Therefore, we first apply the method used in Ref. [11] to solve analytically the two-dimensional Langevin equation under the overdamping condition in the next section. In the third section, we use these results to calculate the probability of nucleons passing over a two-dimensional saddle point.

2 Analytical solution of the multidimensional Langevin equation at the overdamping limit

The spatiotemporal evolution of the many-body system under the action of random force $\mathcal{F}(t)$ and a linear external force is governed by the dynamical equation with a vector of degrees of freedom $Z \equiv \{z_1, z_2, \cdots, z_n\}$, driven by the mass tensor $\boldsymbol{M}$, the friction tensor $\mathcal{G}$ and the spring tensor $\mathcal{S}$ they can be read as

$$\boldsymbol{M}\frac{\mathrm{d}^2 Z}{\mathrm{d}t^2} + \mathcal{G}\frac{\mathrm{d}Z}{\mathrm{d}t} - \mathcal{S}Z = \mathcal{F}(t). \tag{1}$$

By using a transformation,

$$\begin{aligned} Y &\equiv \boldsymbol{O}^{-1}\boldsymbol{M}^{1/2}Z, \quad \boldsymbol{\beta} \equiv \boldsymbol{O}^{-1}\boldsymbol{M}^{-1/2}\mathcal{G}\boldsymbol{M}^{-1/2}\boldsymbol{O}, \\ \mathcal{R}(t) &\equiv \boldsymbol{O}^{-1}\boldsymbol{M}^{-1/2}\mathcal{F}(t). \end{aligned} \tag{2}$$

Equation (1) can be transformed into the following form,

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}t^2} + \boldsymbol{\beta}\frac{\mathrm{d}Y}{\mathrm{d}t} - \boldsymbol{\Omega}^2 Y = \mathcal{R}(t), \tag{3}$$

where $\boldsymbol{O}$ is a orthogonal matrix with which the matrix $\boldsymbol{M}^{-1/2}\mathcal{S}\boldsymbol{M}^{-1/2}$ can be diagonalized, i. e. $\boldsymbol{O}^{-1}\boldsymbol{M}^{-1/2}\mathcal{S}\boldsymbol{M}^{-1/2}\boldsymbol{O} \equiv \boldsymbol{\Omega}^2$. Assuming the random force is the Gaussian one, the first and second moments of them have the properties

$$\langle \mathcal{R}(t) \rangle = 0, \quad \langle \mathcal{R}(t)\mathcal{R}^{\mathrm{T}}(t') \rangle = 2T\boldsymbol{\beta}\delta(t-t'). \tag{4}$$

In general, it is not easy to get the analytical solution of the above-mentioned equation. However, Professor Abe and his collabrators[11] have, fortunately, paved a way to solve it analytically and the formal solution has been obtained under the assumption that

$$Y_{\mathrm{i}} = \frac{\mathrm{d}Y_{n+i}}{\mathrm{d}t}, \quad \text{for} \quad i = 1, 2, \cdots, n. \tag{5}$$

In fact, the method proposed by Abe can be directly used to solve the multidimensional Langevin equation at the overdamping limit without this assumption.

In the strong friction limit, eliminating the faster degrees of freedom, the Eq. (3) can been reduced as

$$\boldsymbol{\beta}\frac{\mathrm{d}Y}{\mathrm{d}t} - \boldsymbol{\Omega}^2 Y = \mathcal{R}(t). \tag{6}$$

This expression is just a dynamical equation of the Gaussian stochastic processes in the configuration space under the assumption that the relaxation of momentum variables is much faster than the coordinate freedoms in the light of Smoluchowski's opinion[12, 13].

It is easier to get the solution of Eq. (6) both analytically and numerically than of Eq. (3) in the same dimensional cases because not only is the number of variables less but the order of Eq. (6) is lower than Eq. (3). For the n-dimensional situation, multiplying Eq. (6) by $\boldsymbol{\beta}^{-1/2}$ and replacing Y with $Q = \boldsymbol{\beta}^{1/2}Y$, we have the following one-order equation

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \boldsymbol{\beta}^{-1/2}\boldsymbol{\Omega}^2\boldsymbol{\beta}^{-1/2}\boldsymbol{Q} + \boldsymbol{\beta}^{-1/2}\mathcal{R}(t). \tag{7}$$

Here $\boldsymbol{Q} = \{q_1, q_2, \cdots, q_n\}^{\mathrm{T}}$ and $\boldsymbol{\beta}^{-1/2}\mathcal{R}(t)$, $\boldsymbol{\beta}$ is the $n \times n$ matrix while $\boldsymbol{\Omega}^2$ is the $n \times n$ diagonalized one. Diagonizing symmetric matrix $\boldsymbol{\beta}^{-1/2}\boldsymbol{\Omega}^2\boldsymbol{\beta}^{-1/2}$ with orthogonal matrix $\boldsymbol{U}$ as $\boldsymbol{U}^{-1}\boldsymbol{\beta}^{-1/2}\boldsymbol{\Omega}^2\boldsymbol{\beta}^{-1/2}\boldsymbol{U} = D = \sum_i |i > \lambda_i < i|$. And defining

$$X = \boldsymbol{U}^{-1}\boldsymbol{Q}, \quad R(t) = \boldsymbol{U}^{-1}\boldsymbol{\beta}^{-1/2}\mathcal{R}(t), \tag{8}$$

then the solutions of Eq. (7), in the component form are

$$X_i = \mathrm{e}^{\lambda_i t}X_{i0} + \int_0^t \mathrm{e}^{\lambda_i(t-\tau)}R_i(\tau)\mathrm{d}\tau, \quad (i = 1, 2, \cdots, n). \tag{9}$$

As has been done in Ref. [11], take $\mathcal{R}(t) = \boldsymbol{\Gamma}\boldsymbol{\nu}(t)$. Here $\boldsymbol{\Gamma}$ is a $n \times n$ matrix and $\boldsymbol{\nu}_i(t)$ is a $n \times 1$ one with the following properties,

$$\langle \boldsymbol{\nu}_i(t) \rangle = 0, \quad \langle \boldsymbol{\nu}_i(t)\boldsymbol{\nu}_j(t') \rangle = \delta_{ij}\delta(t-t'). \tag{10}$$

$\{\boldsymbol{\nu}_i(t)\}$ is the ith element of matrix $\boldsymbol{\nu}(t)$. Taking into account the symmetry of matrix $\boldsymbol{\beta}^{-1/2}$, we calculate the correlation of $R(t)R(t')$ directly with Eqs. (8) and (10), the matrix $\boldsymbol{\Gamma}$ and $\alpha \equiv \boldsymbol{U}^{-1}\boldsymbol{\beta}^{-1/2}\boldsymbol{\Gamma}$ fulfill the following relations

$$\boldsymbol{\Gamma}\boldsymbol{\Gamma}^{\mathrm{T}} = 2T\boldsymbol{\beta}, \quad \alpha\alpha^{\mathrm{T}} = 2T. \tag{11}$$

Here T is the temperature while the superscript T indicates transposition of the matrix.

For the case of the inverted parabolic potential, $V=-\frac{1}{2}\boldsymbol{\Omega}^2\boldsymbol{Q}^2$, we can readily get the solution by using the formulae given above. Let

$$x_j(t)\equiv X_i\mathrm{e}^{-\lambda_j t}-X_{j0}=\int_0^t \mathrm{e}^{-\lambda_j(\tau)}R_j(\tau)\mathrm{d}\tau\ , \qquad (12)$$

the distribution of $\{x_j(t)\}$ taking a set of sharp values $\{x_j\}$ can be calculated with definition

$$w(\{x_j\},t;\{X_{j0}\}) = \langle\delta(x_1-x_1(t))\cdots\delta(x_n-x_n(t)\rangle = \int\frac{\mathrm{d}k_1}{2\pi}\cdots\int\frac{\mathrm{d}k_n}{2\pi}\exp\{i[k_1\cdots k_n]\times \begin{bmatrix} x_1\\ \cdots\\ x_n\end{bmatrix}\}\langle p(k_1\cdots k_n)\rangle. \qquad (13)$$

With the functional integration technique and the properties of the Gaussian random force as well as the natures of the Markovian process, we finally have

$$w(x_1,\cdots,x_n,t;X_{10},\cdots,X_{n0})=\frac{1}{\sqrt{(2\pi)^n}\sqrt{\mathrm{Det}\mathcal{A}(t)}}\times \exp\{-\frac{1}{2}[x_1,\cdots,x_n]A^{-1}(t)\begin{bmatrix} x_1\\ \cdots\\ x_n\end{bmatrix}\}, \qquad (14)$$

with

$$\mathcal{A}(t)=\frac{1}{2}\alpha D^{-1}\alpha^{\mathrm{T}}(1-\mathrm{e}^{-2tD}). \qquad (15)$$

The signs are the same as in Eq. (12).

Returning to the original variables, the distribution of $\{q_i, i=1,2,\cdots,n\}$ reads

$$w(q_1,\cdots,q_n,t;q_{10},\cdots,q_{n0})=\frac{1}{\sqrt{(2\pi)^n}\sqrt{\mathrm{Det}\mathcal{A}(t)}}\times \exp\{-\frac{1}{2}[q_1-\langle q_1(t)\rangle,\cdots,q_n-\langle q_n(t)\rangle]\times \mathcal{A}^{-1}(t)\begin{bmatrix} q_1-\langle q_1(t)\rangle\\ \cdots\\ q_n-\langle q_n(t)\rangle\end{bmatrix}\}, \qquad (16)$$

with

$$\mathcal{A}(t)=\mathrm{e}^{tD}U\mathrm{A}(t)U^{\mathrm{T}}\mathrm{e}^{tD}. \qquad (17)$$

Inserting (4) and (11) in to (17), we have

$$\mathcal{A}(t)=TD^{-1}(\mathrm{e}^{2tD}-1). \qquad (18)$$

3 The probability of passing over a saddle point with multi-parameters at the overdamping limit

As is well known, in the real problems, a saddle point has a certain range and complex shape. The relative height of the saddle point and the corresponding form of the potential barrier are closely related to the direction in which the particles move. In the processes of heavy ion collisions, for instance, the movement of the incident particles has not only the properties of the directional movement along the incident direction but also thermal motion in other directions. Therefore, the number of parameters needed to describe a saddle point depends both on the form of the potential barrier and the direction of the particles motion. In this section, we use the formulae obtained before to study the probability of a nucleon passing over a saddle point with various parameters at the high friction limit in massive nuclear reactions.

The simpliest case is the one-dimensional motion of the particle, the so-called one-dimensional problem, $n=1$. For this case, the distribution function can be found very easily

$$w(q,t;q_0,0) = \frac{1}{\sqrt{2\pi}}\frac{\omega}{\sqrt{T(\mathrm{e}^{\frac{2\omega^2}{\beta}t}-1)}}\times \exp\left\{-\frac{1}{2}\frac{[q-\langle q(t)\rangle]^2\omega^2}{T(\mathrm{e}^{\frac{2\omega^2}{\beta}t}-1)}\right\}, \qquad (19)$$

with

$$\boldsymbol{U}=1,\ \lambda=\frac{\omega^2}{\boldsymbol{\beta}},\ R(t)=\boldsymbol{\beta}^{-1/2}\mathcal{R}(t), \langle q(t)\rangle=\mathrm{e}^{\lambda t}q_0. \qquad (20)$$

Of course, these are the well known results from solving the Smoluchowski equation.

The slightly more complicated case compared with the one-dimensional one is the two-dimensional problem. This is a more real situation for complex massive nuclear collision which is a subject of considerable current interest. Most recently, C. Y. Wang et al.[14] discussed the diffusion of a particle passing over the saddle point of a two-dimensional quadratic potential via a set of coupled Langevin equations. They found that the passing probability is strongly influenced by the off-diagonal components of inertia and friction tensors and there exists an optimal injection choice for the deformable target and projectile nuclei to maximize the fusion probability. Here, in order to get the analytical solution of the multidimensional Langevin equation at high friction limits and show the fundamental properties, we simply take the friction and spring tensors as

$$\boldsymbol{Q}=\begin{bmatrix} q_1\\ q_2\end{bmatrix},\quad \boldsymbol{\Omega}^2=\begin{bmatrix}\omega_1^2,\ 0\\ 0,-\omega_2^2\end{bmatrix},\quad \boldsymbol{\beta}=\begin{bmatrix}\beta_1,\ \beta_{12}\\ \beta_{12},\ \beta_2\end{bmatrix}. \qquad (21)$$

In this model the first degree of freedom indicates the "valley" direction to the saddle and the second one reflects the "confining" direction.

The matrix $\boldsymbol{\beta}^{1/2}$ and $\boldsymbol{\beta}^{-1/2}$ can be found from solving simultaneous equations. The process is cumbersome but straightforward. The results are

$$\begin{aligned}(\boldsymbol{\beta}^{1/2})_{11} &= \frac{(\boldsymbol{\beta}^{1/2})_{12}}{\beta_{12}}(\beta_1-\sqrt{\beta_1\beta_2-\beta_{12}^2}),\\ (\boldsymbol{\beta}^{1/2})_{22} &= \frac{(\boldsymbol{\beta}^{1/2})_{12}}{\beta_{12}}(\beta_2-\sqrt{\beta_1\beta_2-\beta_{12}^2}),\\ (\boldsymbol{\beta}^{1/2})_{12} &= \sqrt{\frac{\beta_{12}^2(\beta_1+\beta_2+2\sqrt{\beta_1\beta_2-\beta_{12}^2})}{(\beta_1+\beta_2)^2+4\beta_{12}}}\,,\end{aligned} \tag{22}$$

or

$$\begin{aligned}(\boldsymbol{\beta}^{1/2})_{11} &= \frac{(\boldsymbol{\beta}^{1/2})_{12}}{\beta_{12}}(\beta_1+\sqrt{\beta_1\beta_2-\beta_{12}^2}),\\ (\boldsymbol{\beta}^{1/2})_{22} &= \frac{(\boldsymbol{\beta}^{1/2})_{12}}{\beta_{12}}(\beta_2+\sqrt{\beta_1\beta_2-\beta_{12}^2}),\\ (\boldsymbol{\beta}^{1/2})_{12} &= \sqrt{\frac{\beta_{12}^2(\beta_1+\beta_2-2\sqrt{\beta_1\beta_2-\beta_{12}^2})}{(\beta_1+\beta_2)^2+4\beta_{12}}}\,,\end{aligned} \tag{23}$$

$$\boldsymbol{\beta}^{-1/2}=\frac{(\beta_1+\beta_2)^2+4\beta_{12}}{(\beta_1+\beta_2\pm2\sqrt{\beta_1\beta_2-\beta_{12}^2})[2\beta_1\beta_2\mp(\beta_1+\beta_2)\sqrt{\beta_1\beta_2-\beta_{12}^2}]}\begin{pmatrix}(\boldsymbol{\beta}^{1/2})_{22}, & -(\boldsymbol{\beta}^{1/2})_{12}\\ -(\boldsymbol{\beta}^{1/2})_{12}, & (\boldsymbol{\beta}^{1/2})_{11}\end{pmatrix}. \tag{24}$$

The upper line signs in the denominator of Eq. (24) correspond to the values of Eq. (22), and the lower line signs correspond to the values of Eq. (23).

The eigenvalues of matrix $\boldsymbol{\beta}^{-1/2}\boldsymbol{\Omega}^2\boldsymbol{\beta}^{-1/2}$ can be easily gotten. We denote them as λ_1 and λ_2 here and they read

$$\lambda_1=\frac{1}{2}(\eta-\kappa),\qquad \lambda_2=\frac{1}{2}(\eta+\kappa), \tag{25}$$

$$\begin{aligned}\eta &= (\beta_{11}^{-1/2})^2\omega_1^2-(\beta_{22}^{-1/2})^2\omega_2^2\,,\\ \kappa &= \sqrt{4[(\beta_{12}^{-1/2})^2-\beta_{11}^{-1/2}\beta_{22}^{-1/2}]^2\omega_1^2\omega_2^2+\eta^2}\,.\end{aligned} \tag{26}$$

Inserting them into Eq. (17) and with the relations

$$\begin{bmatrix}\langle q_1(t)\rangle\\ \langle q_2(t)\rangle\end{bmatrix}=\mathrm{e}^{tD}\begin{bmatrix}q_{10}\\ q_{20}\end{bmatrix}. \tag{27}$$

We can find that the distribution is

$$w(q_1,q_2,t;q_{10},q_{20})=\frac{1}{2\pi\sqrt{\mathrm{Det}\mathcal{A}(t)}}\times \exp\left\{-\frac{1}{2}[q_1-\langle q_1(t)\rangle,q_2-\langle q_2(t)\rangle]\times \mathcal{A}^{-1}(t)\begin{bmatrix}q_1-\langle q_1(t)\rangle\\ q_2-\langle q_2(t)\rangle\end{bmatrix}\right\}, \tag{28}$$

with

$$\begin{aligned}\mathrm{Det}(\mathcal{A}(t)) &= \frac{T^2}{\lambda_1\lambda_2}(\mathrm{e}^{2\lambda_1t}-1)(\mathrm{e}^{2\lambda_2t}-1),\\ \mathcal{A}^{-1}(t) &= \begin{bmatrix}\frac{\lambda_1}{T(\mathrm{e}^{2\lambda_1t}-1)}, & 0\\ 0, & \frac{\lambda_2}{T(\mathrm{e}^{2\lambda_2t}-1)}\end{bmatrix}.\end{aligned} \tag{29}$$

The probability of a particle passing over the saddle point can be obtained by performing the following integration over $q_1\geqslant0, q_2\geqslant0$, i. e.

$$p(t;q_{10},q_{20})=\int_{-\infty}^{\infty}\mathrm{d}q_1\int_0^{\infty}\mathrm{d}q_2w(q_1,q_2,t;q_{10},q_{20}). \tag{30}$$

And thus, we finally get the probability passing over the saddle point at time t as

$$p(t;q_{10},q_{20}) = \sqrt{\frac{\pi T(\mathrm{e}^{2\lambda_1t}-1)}{2\lambda_1}}\times \mathrm{erf}c\left[-\sqrt{\frac{\lambda_2\mathrm{e}^{2\lambda_2t}}{2T(\mathrm{e}^{2\lambda_2t}-1)}}q_{20}\right]. \tag{31}$$

For the situation in which two incident nuclei have a large mass asymmetry, the potential energy can be drawn within the liquid drop model (LDM) for heavy nuclear systems. The potential energy surface is a typical two-dimensional problem in the space spanned by the relative distance and the mass-asymmetry coordinates[14]. If we take the relative distance of two incident nuclei as q_1 and the mass-asymmetry coordinates as $q_2=\frac{A_1-A_2}{A_1+A_2}$, here A_1 and A_2 are the mass of incident nuclei. Then the probability of passing over the saddle point is

$$p(t;q_{10},q_{20}) = \int_0^{\infty}\mathrm{d}q_1\int_{-1}^{+1}\mathrm{d}q_2w(q_1,q_2,t;q_{10},q_{20})= \frac{1}{4}\mathrm{e}^{\eta t}\frac{1}{\sqrt{\mathrm{Det}\mathcal{A}(t)}}[1+\mathrm{Erf}(z_1)][1+\mathrm{Erf}(z_2)], \tag{32}$$

$$\begin{pmatrix}z_1\\ z_2\end{pmatrix}= \begin{pmatrix}\sqrt{\frac{\lambda_1}{2T(1-\mathrm{e}^{-2\lambda_1t})}}\cos\theta, & -\sqrt{\frac{\lambda_1}{2T(1-\mathrm{e}^{-2\lambda_1t})}}\sin\theta\\ \sqrt{\frac{\lambda_2}{2T(1-\mathrm{e}^{-2\lambda_2t})}}\sin\theta, & \sqrt{\frac{\lambda_2}{2T(1-\mathrm{e}^{-2\lambda_2t})}}\cos\theta\end{pmatrix}\times \begin{pmatrix}-\beta_{11}^{1/2}q_{10}+\beta_{12}^{1/2}(\mathrm{e}^{-\lambda_2t}-q_{20})\\ -\beta_{12}^{1/2}q_{10}+\beta_{22}^{1/2}(\mathrm{e}^{-\lambda_2t}-q_{20})\end{pmatrix}. \tag{33}$$

η is given in Eq. (26) and θ reads

$$\theta = \frac{1}{2}\tan^{-1}\Big\{\big[2\beta_{12}^{-1/2}(\beta_{11}^{-1/2}\omega_1^2 - \beta_{22}^{-1/2}\omega_2^2)\big]\Big/ \big[[(\beta_{11}^{-1/2})^2 - (\beta_{12}^{-1/2})^2]\omega_1^2 + [(\beta_{22}^{-1/2})^2 - (\beta_{12}^{-1/2})^2]\omega_2^2\big]\Big\}. \quad (34)$$

In summary, the analytical solution of a multidimensional Langevin equation at the overdamping limit is obtained and the probability of particles passing over a saddle point with multi-parameters is discussed. Although we have only given the formal solutions of the equation under the above-mentioned condition without discussing a the detailed application in concrete physical problems, we believe that the method and the results given here may break a path for studying further the fusion in superheavy elements synthesis. As a matter of fact, as has been pointed out in Refs. [6,7], the diffusion motion is a fundamental phenomenon almost everywhere in nature. The issue considered here is a typical problem of diffusion and thus is of important physical relevance. Therefore, both the results and the method used in the present paper are instructive for studying more complicated diffusion motion.

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