The power-law reaction rate coefficient for barrierless reactions

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Abstract. We study the power-law reaction rate coefficient for barrierless reactions, when the reactions take place in systems with power-law distributions, and derive a generalized rate formula for the barrierless reactions in the Gorin model. We show that, unlike those for bimolecular and unimolecular reactions, due to the lack of barriers, the power-law rate coefficient for barrierless reactions does not have a power-law function, and thus is not very strongly dependent on the $\nu$-parameter. Four barrierless reactions are taken as application examples to calculate the new rate coefficients, which with larger fitting $\nu$-parameters can be exactly in agreement with measurements in the experimental studies.

Keywords: chemical kinetics, kinetic theory of gases and liquids, molecular dynamics.

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1. Introduction

Phase space theory (PST) provides a useful and easily implemented reference theory for barrierless reactions. The basic assumption in PST is that the interaction between two reacting fragments is isotropic and does not affect internal fragment motions. Essentially, PST is one version of transition state theory (TST) that focuses on the energetics of the separated fragments in a completely loose transition state (i.e. the rotations of the fragments are completely unhindered). The simplest algorithms are based on locating the transition state at the centrifugal barriers for spherically symmetric \( r^{-n} \) potentials. For example, for \( n = 4 \) it is the model of Langevin–Gioumousis–Stevenson; and for \( n = 6 \), Gorin’s model [1]. In the latter, the thermal rate coefficient is given [2] by

\[
k_{\text{Gorin}}(T) = 2^{11/6} \Gamma(2/3) C^{4/3} \sqrt{\pi / \mu} (k_B T)^{1/6},
\]

where \( \mu \) is the reduced mass of the collision partners, \( C \) is a constant, \( k_B \) is the Boltzmann constant, and \( T \) is temperature.

Like all other formations of TST, the formulae in PST are also based on the assumption of thermal equilibrium [1–3]. However, in reaction rate theory we are interested in the processes of evolution from one metastable state to a neighboring state of metastable equilibrium; therefore, the assumptions would be quite far-fetched. A lot of theoretical work and experimental studies on the physical, chemical, biological and technical processes taking place in complex systems have revealed that in many situations the statistical property of complex systems is not Boltzmann–Gibbs (BG) distributions, but often follows power-law distributions (e.g. see [4] and the references therein). Power-law distributions in complex systems have chiefly been studied in processes such as single-molecule conformational dynamics [5, 6], chemical reactions [7], gene expressions [8], cell reproductions [9], complex cellular networks [10], small organic molecules, [11] etc. In these processes, the reaction rate coefficients are often energy-dependent.
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(and/or time-dependent [12–14]) with power-law forms [15, 16], which thus are beyond the scope of conventional reaction rate formulae with BG exponential forms. In such situations, the rate formulae in conventional reaction rate theories based on BG statistics have to be modified.

The statistical mechanical theory of power-law distribution has been developed. For example, the generalized Gibbsian theory for power-law distribution was presented for systems away from equilibrium [17]. In stochastic dynamical theory on Brownian motion in a complex system, power-law distributions can be discovered by introducing generalized fluctuation–dissipation relations and solving the Fokker–Planck equations [4, 18]. It is especially worth mentioning that in recent years nonextensive statistical mechanics (NSM) based on Tsallis entropy has received much attention and very wide application to a variety of interesting problems in physics, chemistry, astronomy, biology, engineering and technology [19]. NSM has also been the statistical basis of the kappa-distributions observed in space plasmas [20–24]. In NSM, the power-law distribution can be derived using the extremization of Tsallis entropy. When one generalizes BG statistical mechanics to NSM, the usual exponential and logarithm can be replaced respectively by the $q$-exponential and the $q$-logarithm. Here we can write some of the distributions known in NSM. We can introduce the power-law energy $\nu$-distribution

$$P(\varepsilon) \sim \left[1 - (\nu - 1)\frac{\varepsilon}{k_B T}\right]^{1/(\nu-1)},$$

if the energy $\varepsilon$ is small. Or we can write $P(\varepsilon) \sim \varepsilon^{-\alpha}$ if the energy $\varepsilon$ is large [4], where $\nu \neq 1$ is a parameter. This power-law $\nu$-distribution represents the statistical property of the systems being at a nonequilibrium stationary state [24, 25]. Equation (2) is reduced to a BG distribution if the $\nu$-parameter is set to $\nu \to 1$, where the parameter $\nu \neq 1$ measures the distance away from thermal equilibrium.

Most recently, TST for nonequilibrium systems with power-law distributions was studied and the generalized reaction rate formulae of these cases were derived for one-dimensional and $n$-dimensional Hamiltonian systems [15]. The power-law TST reaction rate coefficients for the elementary bimolecular reactions [26] and the unimolecular reactions [27], and the collision theory power-law rate coefficients [28] were also studied. These facts tell us that energy distribution plays a key role in reaction rate theories, if the reaction takes place in nonequilibrium complex systems. In addition, the mean first passage time [29] and the escape rate for power-law distributions in both overdamped systems [30] and low-to-intermediate damping [31] were studied, and showed new and important characteristics. As we can imagine, this is a complicated and exciting field in exploring the understanding of open nonequilibrium reaction rate theory.

The purpose of this work is to generalize the barrierless reaction rate formula to a nonequilibrium system with the power-law $\nu$-distribution. In section 2, we study the power-law reaction rate coefficient of the barrierless reactions. In section 3, we conduct numerical analyses to show the dependence of the power-law reaction rate coefficient on the $\nu$-parameter. As application examples of the new formula, in section 4 we calculate the power-law reaction rate coefficients of four barrierless reactions, and compare them with the rate values in the experiment studies, and then determine the $\nu$-parameter. Finally, in section 5 we conclude and discuss the results.
2. The power-law rate coefficient for barrierless reactions

In this section, we will follow the standard line of textbooks to derive the power-law reaction rate formula. For barrierless reactions, the relation between the state-selected rate constant \( k_{ij} \) and the reaction cross section \( \sigma_{ij} \) \(^{(2)}\) is

\[
 k_{ij} (u_r) = u_r \sigma_{ij} (u_r),
\]

where \( u_r \) is the relative velocity between the two reactant particles. The average reaction cross section \( \sigma_r \) is given by the average over all the reactants internal states,

\[
 \sigma_r = \sum_{i,j} w_i^A w_j^B \sigma_{ij} (u_r),
\]

where \( w_i^A \) and \( w_j^B \) represent the weighting factors of \( i \)th and \( j \)th reactant internal states, respectively. The thermal rate constant for the process is defined by the average on \( u_r \sigma_r \) over all \( u_r : 0 \rightarrow \infty \),

\[
 k = \int_0^\infty \sigma_r u_r f(u_r) \, du_r,
\]

where \( f(u_r) \) is the relative velocity distribution function of the particles.

There are many ways to calculate the reaction cross \( \sigma_r \). In PST, the effective potential method is an often-used convenient method. The effective potential is given \(^{(2)}\) by

\[
 V_{\text{eff}}(R) = V(R) + L^2 / 2\mu R^2,
\]

where \( R \) is a distance between the collision partners, \( L \) is the orbital angular momentum, and \( V(R) \) is the isotropic fragment–fragment interaction energy. For neutral reactions without the barrier, the efficient potential in the Gorin model \(^{(1, 2)}\) is

\[
 V_{\text{eff}}(R) = -C / R^6 + L^2 / 2\mu R^2.
\]

The first term in this equation is the ionization potential, and the second term is the centrifugal potential. Because of \( L = \mu u_r b \), using the relative translational energy \( E_r = \mu u_r^2 / 2 \) we obtain

\[
 V_{\text{eff}} = -C / R^6 + E_r (b / R)^2.
\]

Equation (8) has a single maximum at a radius \( R_c = (3C / E_r b^2)^{1/4} \) and the maximum is

\[
 V_{\text{eff},*} = 2E_r^{3/2}b^{3}3^{-3/2}C^{-1/2},
\]

where \( C \) is a constant determined by the nature of the molecules, and \( b \) is an impact parameter, defined as the distance between the closest two molecules in the absence of inter-particle forces. If \( E_r < V_{\text{eff},*} \), the centrifugal barrier cannot be penetrated when the tunneling is neglected, and no reaction occurs (in fact, the absence of a barrier also leads to quantum tunneling effects which are usually not important for calculating the thermal rate constant \(^{(2)}\)). If \( E_r = V_{\text{eff},*} \), one particle is captured in a circular orbit of radius \( R_c \) around the other particle. If \( E_r < V_{\text{eff},*} \), the two particles can move inside each other and the reaction probability is approximately equal to one. The critical impact parameter \( b_* \) is obtained from \( V_{\text{eff},*} \) by

\[
 b_* = 2^{-1/3}E_r^{-1/6}3^{1/2}C^{1/6},
\]

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and the reaction cross section is,
\[ \sigma = \pi b^2 = 2^{-2/3}\pi E_{r}^{-1/3}3C^{1/3}. \]  
(11)

Then the thermal rate coefficient is given by
\[ k = \int_{0}^{\infty} du_r \sigma u_r f(u_r). \]  
(12)

It is clear that this rate formula depends strongly on the relative velocity distribution function. Selecting the velocity distribution function depends on the statistical property of the systems under consideration. In conventional theories, it used to be thought that systems always maintained their thermodynamic equilibrium. Under this assumption, the statistical distribution used to be naturally a BG distribution, and therefore the relative velocity distribution has the exponential form [32]

\[ f(u_r) = \left( \frac{\mu}{2\pi k_B T} \right)^{3/2} \exp \left( -\frac{\mu u_r^2}{2k_B T} \right). \]  
(13)

However, generally speaking, the chemical reaction is not always in a thermodynamic equilibrium with a BG distribution, but usually in a nonequilibrium state with non-BG distributions. In the reaction rate theory, what we are interested in is the process of evolution from one metastable state to another neighboring state; so the thermodynamic equilibrium assumption is quite far-fetched. In particular, in some complex systems, the system far away from equilibrium does not relax to a thermodynamic equilibrium with a BG distribution, but often asymptotically approaches a stationary nonequilibrium with a power-law distribution. In this case, the relative velocity distribution function, equation (13), is not the case, and consequently the reaction rate coefficient equation (1) should be modified.

In NSM, the power-law distribution (2) can be derived using the extremization of Tsallis entropy. When BG statistics are generalized to nonextensive statistics, the usual exponential and logarithm can be replaced respectively by the corresponding \( q \)-exponential and \( q \)-logarithm [19]. Here the \( \nu \)-exponential [33, 34] can be defined as

\[ \exp_{\nu} x = \left[ 1 + (\nu - 1) x \right]^{1/(\nu - 1)}, \]  
(14)

if \( 1 + (\nu - 1)x > 0 \) and as \( \exp_{\nu} x = 0 \) otherwise. And the inverse function, the \( \nu \)-logarithm, can be defined as

\[ \ln_{\nu} x = \frac{x^{\nu - 1} - 1}{\nu - 1}, \]  
(15)

In this framework, using the energy distribution (2), the relative velocity distribution (13) can be generalized to the power-law \( \nu \)-distribution,

\[ f_{\nu}(u_r) = Z_{\nu} \left[ 1 - (\nu - 1) \frac{\mu u_r^2}{2k_B T} \right]^{1/(\nu - 1)}, \]  
(16)

where \( Z_{\nu} \) is the normalization constant [35],

\[ Z_{\nu} = \left( \frac{m}{2\pi k_B T} \right)^{3/2} \left\{ \begin{array}{ll}
\left( \nu - 1 \right) \frac{\Gamma \left( \frac{1}{\nu - 1} + \frac{5}{2} \right)}{\Gamma \left( \frac{1}{\nu - 1} \right)} & \text{if } \nu > 1, \\
\left( 1 - \nu \right) \frac{3}{2} \Gamma \left( \frac{1}{1 - \nu} \right) & \text{if } 1/3 < \nu < 1.
\end{array} \right. \]  
(17)
In the limit $\nu \to 1$, (16) is reduced to (13), the form in conventional BG thermodynamic statistics. Here, it would be helpful to introduce the physical meaning of the power-law parameter $\nu \neq 1$. In 2004, an equation of the parameter $\nu \neq 1$ was found in both self-gravitating and plasma systems with long-range interactions; hence, a clear physical explanation for $\nu \neq 1$ was presented [24, 25]. The equation can be written as

$$k_B T \left( \frac{\nabla T}{m_e r} \right) (1 - (\nu - 1))$$

for the self-gravitating system [25] and

$$k_B T \left( \frac{\nabla C}{m_e r} \right) (1 - (\nu - 1))$$

for the plasma system [24], where $T(r)$ is space-dependent temperature, $m$ is particle mass, $e$ is electron charge, $\phi_g(r)$ is a gravitational potential function, and $\phi_C(r)$ is a Coulombian potential function. The equation shows that the $\nu$-parameter is $\nu \neq 1$ if and only if $\nabla T(r) \neq 0$ and hereby the power-law distribution represents the nature of an interacting many-body system in a nonequilibrium stationary-state. For a chemical reaction system, the equation of the $\nu$-parameter should be similar to that for the self-gravitating system (although one needs to study the precise expression), and $\phi_g(r)$ should be construed as an intermolecular interaction potential function.

Further, substituting equation (16) with equation (12), one can find that the reaction rate coefficient in the Gorin model becomes $\nu$-dependent

$$k_\nu = 2 \frac{2}{3} 12\pi^2 C^\frac{1}{3} Z_\nu \int_0^\infty \frac{u_r E_r}{\mu} \left( 1 - (\nu - 1) \frac{E_r}{k_B T} \right)^{1/(\nu-1)}.$$

After completing the integration in equation (18), we can derive the reaction rate coefficient for the barrierless reaction in the system with power-law velocity $\nu$-distribution (i.e. the power-law rate coefficient),

$$k_\nu = \frac{2^{11/6} \Gamma \left( \frac{2}{3} \right) \sqrt{\frac{\pi}{\mu}} C^\frac{1}{3} (k_B T)^{1/6} K_\nu}{1 - (\nu - 1)},$$

with the $\nu$-dependent factor,

$$K_\nu = \begin{cases} (\nu - 1)^{-\frac{\nu}{2}} \Gamma \left( \frac{1}{\nu-1} + \frac{5}{2} / \Gamma \left( \frac{1}{\nu-1} + \frac{8}{3} \right), & \text{if } \nu > 1, \\ (1-\nu)^{-\frac{\nu}{2}} \Gamma \left( \frac{1}{1-\nu} + \frac{5}{3} / \Gamma \left( \frac{1}{1-\nu} - \frac{3}{2} \right), & \text{if } \frac{2}{5} < \nu < 1. \end{cases}$$

As compared with the old formula, the new rate coefficient equation (19) has a $\nu$-dependent factor $K_\nu$, but does not have the factor of power-law $\nu$-distribution due to barrierlessness. As expected, in the limit $\nu \to 1$ it is reduced to the standard reaction rate formula for the reactions in systems with a BG distribution [1, 2]

$$k_1 = 2^{11/6} \Gamma \left( \frac{2}{3} \right) \sqrt{\frac{\pi}{\mu}} C^\frac{1}{3} (k_B T)^{1/6}.$$

### 3. Numerical analyses of the power-law barrierless reaction rate coefficient

In order to illustrate the characteristics of the power-law rate coefficient $k_\nu$ in equation (19), and show the dependence of $k_\nu$ on the $\nu$-parameter and the temperature, we conduct numerical analyses.
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Figure 1 shows the dependence of the rate coefficient $k_\nu$ on the parameter $\nu$. The $k_\nu/k_1$-axis was plotted on a logarithmic scale. The range of the $\nu$-axis was chosen from 0.5 to 3.0, a typical range of the values in nonextensive statistics. It was shown that the rate coefficient $k_\nu$ decreases as the parameter $\nu$ increases, which implied that a deviation from a BG distribution, and thus from thermal equilibrium, would result in a significant variation in the reaction rate. However, we find that such a $\nu$-dependent variation in the reaction rate is different for the cases $\nu > 1$ and $\nu < 1$. If $\nu > 1$, the reaction rate will decrease as the $\nu$-parameter deviates from one (i.e. the system deviates from thermal equilibrium). But if $\nu < 1$, the reaction rate will increase as the $\nu$-parameter deviates from one (i.e. the system deviates from thermal equilibrium). This characteristic comes from the different physical states represented by the system in the two cases $\nu > 1$ and $\nu < 1$, respectively. For a deep understanding of this characteristic, we may need to find the exact expression of the $\nu$-parameter of a chemical reaction system.

Figure 2 illustrates the dependence of the rate coefficient $k_\nu$ on the temperature $T$ for three different $\nu$ parameters. The range of $T$-axis was chosen as $100 \sim 1000$ K, the typical temperature range in chemical reactions. The line of $\nu = 1$ corresponds to the conventional reaction rate coefficient $k_1$. It was shown that the power-law rate coefficient increases as the temperature increases; and there are differences, but not very significant, for different $\nu$-parameters about $\nu = 1$.

Nevertheless, different from the power-law rate coefficients for the bimolecular reactions [26], the unimolecular reactions [27] and the collision theory [28], because there are no barriers the power-law rate coefficient equation (19) for the barrierless reactions does not have the factor of power-law $\nu$-distribution and thus it is not very strongly dependent on the $\nu$-parameter, as compared with those for the bimolecular and unimolecular reactions, and the collision theory.

4. Application of the new rate coefficient to barrierless reactions

In order to illustrate the application of the new reaction rate formula equation (19) to the barrierless reactions which occur in a nonequilibrium system with the power-law $\nu$-distribution,
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We take four barrierless reactions (see Table 1) to calculate the power-law reaction rate coefficients and compare them with the measurements in the experimental studies.

In Table 1, we list the experimental values and the theoretical values of the rate coefficients for these four reactions: \( k_1 \) is the conventional rate coefficient, calculated by using equation (21), \( k_\nu \) is the power-law rate coefficient calculated by using equation (19), and \( k_{exp} \) is the measured rate coefficient in the experimental studies (taken from the NIST chemical kinetics database at http://kinetics.nist.gov/kinetics).

The quantity \( \delta \) denotes the relative error of \( k_1 \) to \( k_{exp} \), i.e., \( \delta = |k_1 - k_{exp}| / k_{exp} \), and \( \nu \) is the fitting power-law parameter. All the data were obtained at the temperature 400 K.

We find that there are very significant relative errors of \( k_1 \) to \( k_{exp} \), and the values of \( k_\nu \) with different and larger \( \nu \)-parameters can be exactly in agreement with all the experimental studies. A new rate coefficient \( k_\nu \) with larger fitting \( \nu \)-parameters shows that due to barrierlessness the power-law rate coefficient for the barrierless reactions is not very sensitive to the \( \nu \)-parameter. In other words, the reaction rate is not strongly dependent on the form of the energy distribution function, and thus we might need to search for other explanations, besides the nonextensive effect, for the significant relative errors of \( k_1 \) to \( k_{exp} \).

### Table 1. The rate coefficients for four barrierless reactions.

| Reactions          | \( k_1 \) (cm\(^3\)s\(^{-1}\)) | \( k_{exp} \) (cm\(^3\)s\(^{-1}\)) | \( \delta \) | \( k_\nu \) (cm\(^3\)s\(^{-1}\)) | \( \nu \) |
|--------------------|-------------------------------|---------------------------------|-------------|-------------------------------|------|
| CH\(_3^+\) + CH\(_3^+\) | \(1.05 \times 10^{-10}\)     | \(4.03 \times 10^{-11}\)       | 160%        | \(4.03 \times 10^{-11}\)     | 147  |
| C\(_2\)H\(_2\)Cl\(_3^+\) + C\(_2\)H\(_2\)Cl\(_3^+\) | \(8.32 \times 10^{-11}\)     | \(3.43 \times 10^{-11}\)       | 142%        | \(3.43 \times 10^{-11}\)     | 97   |
| CCl\(_3^+\) + Cl \(_-\) | \(8.28 \times 10^{-11}\)     | \(7.29 \times 10^{-11}\)       | 14%         | \(7.29 \times 10^{-11}\)     | 1.55 |
| C\(_2\)H\(_4^+\) + Cl \(_-\) | \(3.31 \times 10^{-10}\)     | \(2.55 \times 10^{-10}\)       | 30%         | \(2.55 \times 10^{-10}\)     | 2.82 |

5. Conclusion

The reaction rate theory for reactions in systems with power-law distributions is beyond the scope of conventional theories of BG distribution. Therefore, the reaction rate
formulae need to be modified for systems with power-law distributions. In this work, we have studied the power-law reaction rate coefficient for barrierless reactions in the Gorin model and have derived the generalized reaction rate formula equation (19). We show that, unlike power-law rate coefficients for bimolecular and unimolecular reactions, as there are no barriers the power-law rate coefficient (19) for barrierless reactions does not have the factor of power-law $\nu$-distribution. Consequently, it is not very strongly dependent on the $\nu$-parameter, as compared with those for bimolecular and unimolecular reactions.

We have made numerical analyses to illustrate the dependence of the power-law reaction rate coefficient $k_\nu$ on the power-law $\nu$-parameter.

We have also taken four barrierless reactions, as application examples of equation (19), to calculate the power-law rate coefficients. We showed that new rate coefficients with larger fitting $\nu$-parameters can be exactly in agreement with measurements in experimental studies. Again, due to barrierlessness the power-law rate coefficient $k_\nu$ for barrierless reactions is not very sensitive to the $\nu$-parameter; thus, the reaction rate is not strongly dependent on the form of the energy distribution function. And the reason for significant relative errors of the conventional rate coefficient $k_1$ to the measured rate coefficient $k_{exp}$ might require a search for other explanations besides the nonextensive effect.

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