# OBSERVATION OF INERTIA EFFECTS IN MOLECULAR ROTATIONAL BROWNIAN MOTION

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**Annotation:** Inertial effects in molecular rotational Brownian motion represent a fundamental area of study in molecular dynamics and statistical mechanics. The thermal agitation of molecules results in rotational Brownian motion, which induces additional fluctuations and changes in their rotational energy. These effects have a significant impact on molecular dynamics, particularly at elevated temperatures, by altering molecular interactions and their behavior in the surrounding environment.
***Keywords:*** *rotational motion, Gaussian distribution, diffusion, molecule, inertia, tensor.*

## НАБЛЮДЕНИЕ ИНЕРЦИОННЫХ ЭФФЕКТОВ В МОЛЕКУЛЯРНОМ ВРАЩАТЕЛЬНОМ БРОУНОВСКОМ ДВИЖЕНИИ.

**Аннотация**: Инерционные эффекты в молекулярном вращательном броуновском движении представляют собой основную область изучения в молекулярной динамике и статистической механике. Термальное движение молекул приводит к возникновению вращательного броуновского движения, которое вызывает дополнительные колебания и изменения в их вращательной энергии. Эти эффекты значительно влияют на молекулярную динамику, особенно при повышенных температурах, изменяя взаимодействия молекул и их движения в окружающей среде.
***Ключевые слова:*** *вращательное движение, гауссовское распределение, диффузия, молекула, инерция, тензор.*

## AYLANMA BROUN HARAKATIDA MOLEKULALARDA INERSION TA’SIRLARNING KUZATILISHI

**Annotatsiya:** Aylanma Braun harakatidagi molekulalardagi inersial ta'sirlar molekulyar dinamika va statistik mexanikada o‘rganishning asosiy sohasini ifoda etadi. Molekulalarning termal qo‘zg‘alishi oqibatida yuzaga keladigan aylanma Braun harakati ularning aylanish energiyasida qo‘shimcha tebranishlar va

o‘zgarishlarga olib keladi. Ushbu ta'sirlar molekulyar dinamikaga, ayniqsa yuqori haroratlarda, molekulalarning o‘zaro ta'sirini va ularning atrof-muhitdagi xatti-harakatlarini o‘zgartirish orqali sezilarli ta'sirini ko‘rsatmasdan qolmaydi.

***Kalit so‘zlar:*** *aylanma harakat, Gauss taqsimoti, diffuziya, molekula, inersiya, tenzor.*

**Introduction.** In the fields of statistical mechanics and molecular dynamics, the unique significance of rotational Brownian motion is evident. This motion arises from the thermal agitation of molecules, and during this process, additional fluctuations and energy changes in their rotational motion are observed. This thesis is dedicated to the study of molecular inertial effects, which can significantly alter intermolecular interactions and their movements in the environment, particularly at elevated temperatures. The aim is to achieve a clear understanding and prediction of molecular behavior through the dynamics of their rotation and correlation functions.

This work is based on the theoretical analysis of inertial effects in molecular rotational Brownian motion, employing methods developed by Still to derive scientifically grounded results and conclusions.

**Inertial effects and their calculation.**

The theory accounting for inertial effects of particles, namely molecules, during rotational Brownian motion was first developed by Still. The orientation distribution probability of the Still function can be represented as a continuous function as follows:

$$\frac{\partial P}{\partial t} = \nabla_{\varepsilon} j \qquad (1)$$

Here, the current density $j$ is given by the following equation

$$j = R\nabla_{\varepsilon} P \qquad (2)$$

$$R_{ij}(t) = \int_0^t < \omega_i(0)\omega_j(t) > dt \qquad (3)$$

Here $\omega_i$ - represents the projection of the angular velocity, or its shadow. Now we will calculate $R_{ij}$

$$R_{ij}(t) = (kT/\xi_i)\left[1 - \exp(-\xi_i t/I)\right]\delta_{ij} \qquad (4)$$

To calculate $R_{ij}$ we need to write the general form of the rotational diffusion equation as follows:

$$\partial P/\partial t = \sum_i R_{ii}(t)\partial^2 P/\partial \xi_i^2 \qquad (5)$$

If $\xi_i t / I >> 1$ is present, the form of the rotational motion equation can be expressed as follows:

$$\partial P / \partial t = \sum_i (kT / \xi_i) \partial^2 P / \partial \varepsilon_i^2 \quad (6)$$

here, $kT / \xi_i = D$ represents the components of the diffusion tensor. The solution of equation (5) can be understood to be valid for any $t$ , $\xi_x = \xi_y$ arbitrary condition.

$$\xi_x = \xi_y \frac{\partial P}{\partial t} = R_{xx}(t)\left[\frac{\partial^2 P}{\partial \theta^2} + ctg\theta \frac{\partial P}{\partial \theta} + \cos ec^2\theta \frac{\partial^2 P}{\partial \varphi^2} + (ctg^2\theta + \frac{R_{zz}(t)}{R_{tt}(t)} \frac{\partial^2 P}{\partial \psi^2} - 2\cos\theta \cos ec\theta \frac{\partial^2 P}{\partial \varphi \partial \psi})\right]$$

(7)

The solution of equation (7) is generalized for spherical functions

$$P = \sum_{l,m,n} C_{mn}^l(t) T_{mn}^l(\varphi, \theta, \psi) \quad (8)$$

If equation (8) is substituted into equation (7), it can be written as $C_{mn}^l$

$$C_{mn}^l(t) = a_{mn}^l D_{l,n}(t) \quad (9)$$

In that case, $D_{l,n}(t)$ satisfies the following condition

$$\partial \ln D_{l,n}(t) / \partial t = \Gamma_{l,n} R_{xx}(t) - n^2 R_{zz}(t) \quad (10)$$

In this case $\Gamma_{l,n} = n^2 - l(l+1)$ is calculated as (10).

$$D_{l.n} = \exp\left\{\left[n^2 - l(l+1)\right]\frac{IkT}{\xi_x^2}\left[\frac{\xi_x t}{I} - \exp\left(-\frac{\xi_x t}{I}\right) - 1\right] - n^2 \frac{IkT}{\xi_x^2}\left[\frac{\xi_z t}{I} + \exp\left(-\frac{\xi_z t}{I}\right) - 1\right]\right\} \quad (11)$$

If $\frac{\xi_i t}{I} >> 1$ is present, $D_{l.n}(t)$ will have an exponential character and depend on $t$

However, if $\frac{\xi_i t}{I} << 1$ is absent, it will exhibit a Gaussian distribution.

$$\lim_{\xi_i t / I \to 0} D_{l,n}(t) = \exp\left[-\frac{1}{2} l(l+1) \frac{kT}{I} t^2\right] \quad (12)$$

The solution of the equation can be computed based on formulas (8), (9) and (11) and $a_{m.n}^l$ can be observed that the coefficient indicates the initial distribution.

When calculating inertial effects for nuclear magnetic resonance and dielectric relaxation time, the correlation function (8) should be expressed in the following form:

$$K_{(l)}^{(m)} = < Y_l^m(\beta(t), \alpha(t)) Y_l^m(\beta(0), \alpha(0)) > \quad (13)$$

The angle of the molecule in $\eta$ for Still's calculations will be expressed in the following form:

$$K_{(0)}^{(1)}(t) = cos^2\eta \exp(-2h_x) + \sin^2\eta \exp[-(h_x + p_z)] \quad (14)$$

$$K_{(2)}^{(m)}(t) = (1-\frac{3}{2}\sin^2\eta)^2 \exp(-6h_x) + \frac{3}{4}\sin^2 2\eta \exp[-(5h_x + h_z)] + \frac{3}{4}\sin^4\eta \exp[-(2h_x + 4h_z)] \quad (15)$$

$$h_i = IkT/\xi_i^2 \left[ (\xi_i t/I) + \exp(-\xi_i t/I - 1) \right] \quad (16)$$

This type of theory is applicable for spherical cavity-type molecules. Additionally, it is necessary to take the rotational coordinate system vector $z$ relative to the axis. If $\eta$=0 or small values of $\xi$ the correlation functions (14) and (15) can be expressed in the following form based on Gaussian distribution:

$$K_{(1)}^{(0)} = \exp(-\tau^{*2}) \quad (17)$$

$$K_{(2)}^{(m)} = \exp(-3\tau^{*2}) \quad (18)$$

Here, $\tau^* = t(kT/I)^{\frac{1}{2}}$ Equations (17) and (18) hold significant importance in Still's theory. To apply such equations, it is necessary to consider additional conditions. In this case, equation (1) cannot be used for calculating the probability of the distribution function. Based on the law of free rotation, it can be shown that the correlation function has the following solution.

$$K_{(1)}^{(0)}(t) = 2/3\,(1-\tau^{*2}) \exp\left(-\tau^{*2}/2\right) + 1/3 \quad (19)$$

$$K_{(2)}^{(m)}(t) = \left(2/5\right)(1-4\tau^{*2}) \exp(-2\tau^{*2}) + \left(2/5\right)(1-\tau^{*2}) \exp\left(-\tau^{*2}/2\right) + 1/5 \quad (20)$$

**Conclusion**. Rotational Brownian motion leads to additional fluctuations in molecular systems. These fluctuations can significantly impact the rotational and translational properties of molecules, thereby influencing their dynamics. This is crucial for accurately modeling molecular systems and predicting their behavior.

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