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Computer simulation of the collision frequency of two particles in optical tweezers*

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Optical tweezers have been successfully used in the study of colloid science. In most applications people are concerned with the behaviour of a single particle held in the optical tweezers. Recently, the ability of the optical tweezers to simultaneously hold two particles has been used to determine the stability ratio of colloidal dispersion. This new development stimulates the efforts to explore the characteristics of a two-particle system in the optical tweezers. An infinite spherical potential well has been used to estimate the collision frequency for two particles in the optical trap based on a Monte Carlo simulation. In this article, a more reasonable harmonic potential, commonly accepted for the optical tweezers, is adopted in a Monte Carlo simulation of the collision frequency. The effect of hydrodynamic interaction of particles in the trap is also considered. The simulation results based on this improved model show quantitatively that the collision frequency drops down sharply at first and then decreases slowly as the distance between the two particles increases. The simulation also shows how the collision frequency is related to the stiffness of the optical tweezers.

Keywords: optical tweezers, simulation, collision frequency, multiple trapping
PACC: 6120J, 9430H, 8270D, 3280P

1. Introduction

Optical tweezers have been successfully used in colloid science.[1−4] But mostly the optical tweezers control one single particle in experiments. Actually, optical tweezers can hold more than one particle simultaneously, and this ability has been used in recent research on stability ratio measurement of colloid suspensions.[5] The novel feature of this method is to investigate the characteristics of colloid suspension on an individual particle level, so it is very different from the conventional macroscopic methods like turbidity measurements, low angle light scattering and dynamic scattering.[6−8] In this method, a pair of optical tweezers is used to catch one particle, and then another. After the two particles have stayed in the optical tweezers for some time, this pair of optical tweezers is shut off to release the two particles from the trap, and then one can see the outcomes of their collisions in the optical tweezers. After testing many particle pairs, the sticking probability[9,10] can be deduced from the statistical result of the number of collisions leading to permanent doublets and the total number of particle collisions.

About the dynamics of the two particles in the optical tweezers, a special model is suggested.[5] According to this model, the particle pair in the optical tweezers will experience two different kinds of status named "compact status" and "relaxed status". When the second particle is falling into the trap, there will be an additional directed head-on speed, which makes the two particles closer than they are in their equilibrium points. This kind of status is called "compact status". After the effect of impact dampens down, the particles relax to the equilibrium points. The corresponding status is called "relaxed status" in which the collision frequency is much smaller than that in "compact status". Using this presumption, Sun *et al*[5]

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deduced the stability ratio by subtracting the contribution of the collisions in “relaxed status” from the experimentally measured accumulated contribution of all collisions in a period of time. The resulting stability ratio is consistent with that obtained by the conventional methods.[5]

To confirm the validity of the model, it is necessary to understand the dynamics of the particles in the optical tweezers. This is also of great importance for understanding the particle collision and aggregation behaviour for many systems in different fields, such as cloud physics and aerosol science, in which optical tweezers have also been successfully used.[11,12]

To test that the collision frequency in “compact status” is much larger than that in “relaxed status”,[5] a simulation of the collision frequency of two particles in a simple infinite spherical potential well was performed and verified that the collision frequency drops down sharply as the distance between the two particles increases.[13] However, the characteristic of the potential well formed by optical tweezers is analogous to a harmonic potential.[14] Hence it is more reasonable to consider the particles moving in the harmonic potential wells, in which the particles experience the force of optical tweezers besides thermal random force and the viscosity force. Due to the strong hydrodynamic interaction when the two particles are close to each other, it is also necessary to consider the effect of the hydrodynamic interaction in the simulation. In this article, we use this improved model in a Monte Carlo simulation of the collision frequency of the two particles in the optical tweezers. With this model, we can obtain not only the relationship between the collision frequency and the initial separation of the two particles in optical tweezers, but also the relationship between the collision frequency and the tweezers stiffness which can be adjusted by changing the power of laser beam of the optical tweezers. The knowledge of the dependence of collision frequency on tweezers stiffness will help control the collision frequency of the two particles in the optical tweezers, which will be important in the applications similar to that described in Ref.[5]. The simulation will help understand the dynamics of the particles in a trap, which may also be of interest in the similar researches in cloud physics and aerosol science, and the applications in different types of multiple trapping.[15,16]

2. The simulation method

In the simulation, we adopt the hard sphere model in which particles do not interpenetrate or overlap. The two particles in the optical tweezers undergo a Brownian motion confined by the tweezers. Unlike the free Brownian motion, the two particles in the optical tweezers experience another force when departing from the equilibrium points in the optical tweezers. As pointed out above, the potential of the optical tweezers within a certain range around the trapping position is believed to be a harmonic potential with a spring constant K, which is called tweezers stiffness.[14] But in the problems discussed here, the potential is more complex because there are two particles in the optical tweezers. If the harmonic potentials the two particles experience are the same, the two particles will have a tendency to go to the same equilibrium point, which will lead to very high collision frequency. So according to the result that the collision frequency in the “relaxed status” is low,[5] we suggest that the two particles experience different harmonic potentials so that the two spheres in their equilibrium points are departed from each other. Using this model, we test how the collision frequency is related to the separation of the two particles in the optical tweezers and see if there will be a much greater collision frequency in “compact status” than in “relaxed status”. We also test how the collision frequency is related to the tweezers stiffness.

In experiments, the second particle trapped by the same optical tweezers is just above the first one in the trap. So we consider that the equilibrium points of the first and the second particles are (0, 0, 0) and (0, 0, c) respectively, where $c > 2R$, R is the radii of the particles.

The differential equations of the particle in the trap are

$$m\frac{\mathrm{d}^2 x_i}{\mathrm{d}t^2} = -\alpha\frac{\mathrm{d}x_i}{\mathrm{d}t} - K_i(x_i - x_{0i}) + F_i(t), \quad i = 1,2,3, \tag{1}$$

where x denotes the position of the particle, K is the tweezers stiffness, $F(t)$ is the random force, and the subscript i means ith direction. m is the mass of the particle, and $\alpha = 6\pi\eta R$. Here η is the viscosity of the liquid. x_{0i} is the equilibrium point of the particle in ith direction.

Then the equations can be transformed to the following:

$$\begin{cases} \dfrac{\mathrm{d}x_i}{\mathrm{d}t} = v_i, \\ \dfrac{\mathrm{d}v_i}{\mathrm{d}t} = -\gamma v_i - f_i(x_i - x_{0i}) + \Gamma_i(t), \end{cases} \quad i = 1,2,3, \tag{2}$$

where $\gamma = \alpha/m$, $f_i = K_i/m$, $\Gamma_i(t) = F_i(t)/m$.

Due to the independence of the random forces in the three different directions, we have[17]

$$\langle \Gamma_i(t)\Gamma_j(t')\rangle = 2\gamma(kT/m)\delta(t-t')\delta_{ij}. \tag{3}$$

However, for the case discussed here, the viscosity force term $-\gamma v$ needs correction due to the hydrodynamic interaction of the two particles in the trap. As mentioned in Ref.[17], the random force is the total force of the molecules of the liquid acting on the particle except for the viscosity force. So, the trapping force and the random forces are not affected by the hydrodynamic interaction. They need not be corrected.

As is theoretically analysed by Batchelor[18] and tested experimentally by Crocker,[1] for two spheres of the same radius, the expressions for the diffusion relative to the centre of mass are

$$D_{\rm RM}^{\parallel} = \frac{D_0}{2}\left[1 - \frac{3}{2r/R} + \frac{1}{(r/R)^3} - \frac{15}{4(r/R)^4} + O((r/R)^{-6})\right], \tag{4}$$

$$D_{\rm RM}^{\perp} = \frac{D_0}{2}\left[1 - \frac{3}{4r/R} - \frac{1}{2(r/R)^3} + O((r/R)^{-6})\right], \tag{5}$$

where r is the centre–centre separation of the two particles, D_0 is the diffusivity for a single particle with no hydrodynamic interactions, $D_{\rm RM}^{\parallel}$ is the corrected diffusivity along the centre–centre line taking into consideration the hydrodynamic interaction of the two particles, and $D_{\rm RM}^{\perp}$ is the corrected diffusivity perpendicular to the centre–centre line.

The corresponding expressions for the diffusion of the centre of mass itself are

$$D_{\rm CM}^{\parallel} = \frac{D_0}{2}\left[1 + \frac{3}{2r/R} - \frac{1}{(r/R)^3} - \frac{15}{4(r/R)^4} + O((r/R)^{-6})\right], \tag{6}$$

$$D_{\rm CM}^{\perp} = \frac{D_0}{2}\left[1 + \frac{3}{4r/R} + \frac{1}{2(r/R)^3} + O((r/R)^{-6})\right], \tag{7}$$

where $D_{\rm CM}^{\parallel}$ is the diffusivity along the centre–centre line and $D_{\rm CM}^{\perp}$ is perpendicular to it.

For the correction of the viscosity force, the connection of the diffusivity and the viscosity coefficient $D = \dfrac{k_{\rm B}T}{6\pi\eta R}$ is also needed.

Using these equations, we can make a correction of $-\gamma v$. Then we can use the simulation method in Ref.[17] to do the simulation of x and v.

In the simulation, c is set to be $2R+0.1\mu$m, where R=0.5μm to match the experimental situation in Ref.[5]. About the tweezers stiffness, we use the same value for the two transverse directions (x and y), and a much smaller one for the longitudinal one (z).[14,19] Here we set K_z to be one tenth of $K_{x,y}$.

The simulation of the collision frequency is performed as follows: The initial smallest distance between the surfaces of the two particles is d_0. During the simulation, both the positions of the two particles are measured at each time step (or increment). Whenever the distance between the two particles (from their centres) is less than or equal to $2R$, they are considered to collide and then the two particles move back to the starting point to do the diffusion motion over again. In the simulation, the time step is taken to be 1×10^{-8}s, and for each simulation the particle moves 1×10^{8} steps. To justify the time step, we have done some simulation with time step 1×10^{-9}s. The simulation gives the same result as that in the case of 1×10^{-8}s time step, which means the time step of 1×10^{-8}s is appropriate in the simulation. For each initial distance d_0, more than 10 independent calculations are carried out and the collision frequency for each distance is averaged over the calculations.

3. Results and discussion

Figure 1, where $K_{x,y} = 1\times10^{-6}$N/m, $K_z = 0.1\times10^{-6}$N/m, and $c = 2R + 0.1\mu$m, shows how the collision frequency of our simulation is related to the separation between the two particles. The result shows that when the separation of them increases, the collision frequency drops rapidly. Therefore, our simulation provides a direct evidence to support the assumption in Ref.[5] that there is a much greater collision frequency in "compact status" than in "relaxed status".

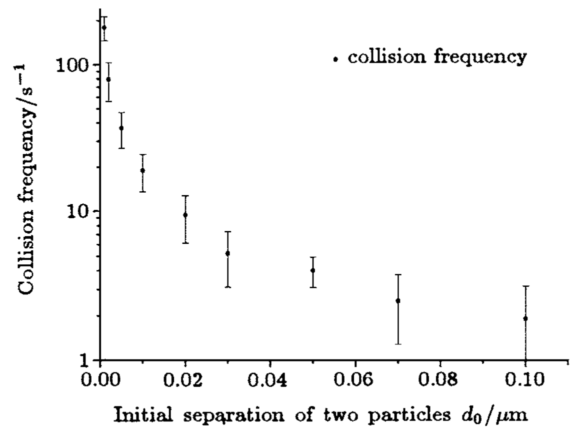

Fig.1. The collision frequency versus initial separation of two particles d_0. Here $K_{x,y} = 1\times10^{-6}$N/m, $K_z = 0.1\times10^{-6}$N/m, and $c = 2R + 0.1\mu$m, with $R = 0.5\mu$m.

As for the tweezers stiffness K, the simulation can also test how the collision frequency is related to K. As mentioned in Ref.[5], there is only one collision in the compact status, and the collision frequency in the "relaxed status" will affect the experiment result.[5] So we take c=2R+0.1μm and d_0=0.1μm in the simulation; this means that the two particles are in "relaxed status". The results show that when the tweezers stiffness in the transverse directions, $K_{x,y}$, changes from 0.1pN/μm to 4pN/μm, the collision frequencies are almost the same (about 1.9). However, if the tweezers stiffness changes from very low to very large, the collision frequency will first increases and then decreases. The result of the simulation can be explained as follows: when the stiffness increases, the particles will be more strongly confined so that their collision frequency decreases; on the other hand, the particles will oscillate more quickly, and the collision frequency increases. The result of our simulation shows that when the stiffness is low, the latter case will be dominant and the collision frequency increases with the increase of the stiffness. When the stiffness is high, the situation changes and the former effect becomes dominant. Actually, the tweezers stiffness being too large or too low has little physical sense because it seldom reaches such values. Whereas for the tweezers stiffness within the range normally used, the result is helpful to the measurement of stability ratio, in which we can conclude that the tweezers stiffness has little influence on the collision frequency in "relaxed status". From this result it can be concluded that the method used in Ref.[5] can be applied widely for different types of optical tweezers, regardless of their stiffness.

Compared with Ref.[13], the difference is that the hydrodynamic interaction of the two particles and the tweezers stiffness are considered in the simulation of this article. These two kinds of factors make the collision frequency lower than that in Ref.[13]. For initial separation of the two particles to be 1nm, the collision frequency calculated in this article is about 200, lower than 500 in Ref.[13]. The collision frequency of the two particles in "relaxed status" is about 1.9, much lower than 25 in Ref.[13]. Compared with the result in experiments (around 1),[5] the result 1.9 in this article is more appropriate. In addition, the relationship between the collision frequency and the tweezers stiffness is studied in this article, which is important in the applications similar to Ref.[5].

4. Conclusions

In this article, the authors suggested a simulation method to simulate the collision behaviour of two particles in optical tweezers. The simulation result supports the assumption of Ref.[5] that the collision frequency in "relaxed status" is much smaller than that in "compact status". The result also shows that the tweezers stiffness has little influence on the collision frequency of the two particles in the "relaxed status" in optical tweezers normally used. It will help improve the theory of the collision processes of two particles in optical tweezers, giving more knowledge of optical tweezers. Also, this kind of simulation can be used in similar researches of trapping multiple particles to understand the motion of the particles in the trap.

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