Research on thermal effects in optical trap in vacuum

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Abstract: The escape phenomenon, mainly caused by thermal effects, is known as an obstacle to the further practical application of optical levitation system in vacuum. Irregular photophoresis induced by thermal effects can act as an “amplifier” of Brownian motion. Studies on this topic provide interpretation for particle escaping phenomenon during the pressure decreasing process, as well as valuable insights into the micro- and nanoscale thermal effects in optical trap in vacuum. In this paper, we derive and test a dynamic model for the motion of an optically levitated particle in a non-equilibrium state and demonstrate the escaping mechanism of heated particles. The result of theoretical investigations is consistent with experimental escape at 0.1mbar. This work reveals and provides a theoretical basis for the stable operation of laser levitated oscillator in high vacuum and pave the way for the practicability of ultra-sensitive sensing devices.

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1. Introduction

Levitated particles in vacuum can be applied in a wide range of fields, including precision measurement of acceleration [1,2] and mass [3], ultrasensitive force [4,5] and torque detection [6,7], high-speed rotation [8,11], optical refrigeration [12], quantum ground-state cooling [9-15], and stochastic thermodynamics [16-18]. Unlike in liquid or air, optical tweezers operating in vacuum are well isolated from the thermal environment, making them an excellent candidate for ultrasensitive sensing. However, the effects of laser heating are stronger in vacuum, since the interaction between particles and surroundings become insufficient with decreased pressure. These interactions cause the dissipation of the center-of-mass motion and are the source of random forces acting on the particles.

The thermal effects of a levitated particle have been suspected to be the cause of particle loss at decreased gas pressure in numerous researches [19-24]. Photophoretic force arising from the internal temperature gradient has proved to be the mechanism for the loss at ~30 mbar [24]. In this case, the particle is assumed to have a constant accommodation coefficient, and the photophoretic force is induced by variation in temperature on the particle surface (\(\Delta T_s\)-force). This occurs if illumination provides uneven heat and points along the direction of temperature gradient. As a matter of fact, there always exists a variation in accommodation coefficient over the surface of particle due to the impurities and non-ideal particle shape. This results in a body-fixed force (\(\Delta \alpha\)-force) [25], which yields particle motion in any possible direction. As a result, random walk depending on the irradiation occurs, which adds to the Brownian motion [26].

In this paper, the motion of a heated trapped sphere is investigated. First, we study the dynamics of the sphere under both types of photophoretic forces in connection with Brownian motion. It is shown that irregular photophoresis enhances the stochastic process of Brownian motion. Then, we test the model
by comparing the calculated results with the experimental data and previous work. The dynamic model allows us to assess the difference accommodation coefficient over the levitated sphere, implying the application of levitodynamics to material science study. Since maintaining the trapping stability of levitated sphere is a critical task for an optical levitated system, our study paves the way for the stable operation of oscillator in high vacuum.

2. Principle of photophoretic force

Photophoresis is a well-known phenomenon of the light-induced motion of particles suspended in gas [32]. There are two types of photophoretic force, namely, $\Delta T_s$-force and $\Delta \alpha$-force. These are respectively induced by variation in temperature over the surface of particles and by variation in the thermal accommodation coefficient $\alpha$. Both can cause a temperature variation in the gas surrounding the particle. After inelastic collision, hotter gas molecules leave the particle surface faster than colder ones, which results in a net force on the particle pointing from the hot to the cold side.

The $\Delta T_s$-force is directed along or against the direction of incident light (Fig.1(a)). A semi-empirical expression for $F_{\Delta T}$ has been given by Rohatschek [27] on spherical particles for the entire range of pressure, such as:

$$F_{\Delta T} = \frac{2}{p + p_{max}}$$

$$p_{max} = D \frac{2}{\alpha \pi a}$$

$$F_{max} = D \sqrt{\frac{\alpha \pi a}{2} \frac{J_1}{k_p}}$$

$$D = \frac{\pi \kappa}{2} \sqrt{\frac{c \eta}{T}}$$

$$\bar{c} = \frac{8RT}{\pi M}$$

where $\bar{c}$ denotes the average thermal velocity of gas molecules at temperature $T$, $M$ denotes the molar mass of the gas, and $\eta$ represents the dynamic viscosity of gas, and $R=8.31J/(mol\cdot K)$ is the gas constant. The thermal creep coefficient $\kappa$ is related to the thermal accommodation coefficient $\alpha$; therefore, $D$ is a factor determined entirely by the gas properties, independent of the pressure $p$ and particle size (radius $a$). $J_1$ represents the asymmetry parameter that involves an integration of normalized absorbed light intensity over the particle volume [28]. For a weakly absorbing sphere with a complex refractive index of $m = n + ik$, $J_1$ can be obtained by the formula [29,30]:

$$J_1 = 2nK\left(\frac{3(n-1)}{8n^2} - \frac{2}{5}nkx\right)$$

where $x = 2\pi a / \lambda$ and $nkx \ll 1$. We assume that the light is $+z$-propagating, $J_1 < 0$ leads to a repulsive photophoretic force, namely, positive photophoresis. $I$ represents the flux density of illumination at the particle position, and $k_p$ is the thermal conductivities of the particle. The expression of $F_{\Delta T}$ can achieve a maximum force $F_{max}$ at a pressure $p_{max}$, where the particle size is comparable to the mean free path of gas molecules.

The particle can experience pure $\Delta T_s$-force only if the accommodation coefficient $\alpha$ is uniform. However, the accommodation coefficient $\alpha$ shall have variation over the particle surface, e.g., that arising from the difference in surface shape and roughness or different material composition of the particle. Therefore, even if the particle is heated evenly, there is still $\Delta \alpha$-force acting on the particle (Fig.1(a)). For a simple model in which the surface of spherical sphere is divided into two hemi-spheres with two different accommodation coefficient $\alpha_1$ and $\alpha_2$, the expression for instantaneous $\Delta \alpha$-force is given by the
following equation [28]:

\[
F_{\Delta \alpha} = \frac{1}{2\varepsilon} \cdot \frac{\gamma - 1}{\gamma + 1} \cdot \frac{1}{1 + \left(\frac{p'}{p}\right)^2} \cdot \frac{\Delta \alpha}{\bar{a}} \cdot H \tag{3}
\]

where \(\gamma = \frac{c_p}{c_v}\) represents the ratio of the specific heats of the gas, and \(H\) denotes the net energy flux transferred by gas molecules. For a sphere in air, \(\gamma = 1.4\) [31,32]:

\[
F_{\Delta \alpha} = \frac{1}{12\varepsilon} \cdot \frac{1}{1 + \left(\frac{p'}{p}\right)^2} \cdot \frac{\Delta \alpha}{\bar{a}} \cdot H \tag{4}
\]

Here, \(\Delta \alpha = \alpha_2 - \alpha_1\), \(\bar{a} = (\alpha_1 + \alpha_2)/2\), \(p' = \sqrt{\alpha'/2}p_{\text{max}} = 3\Delta T/\pi a\) is a characteristic pressure inversely proportional to the radius. The energy flux absorbed by the sphere is \(H = Q_a \pi a^2 I\), and \(Q_a\) is the absorption efficiency of the sphere [32]. The direction of \(\Delta \alpha\)-force \((F_{\Delta \alpha})\) points from the side of the higher accommodation coefficient to the lower one. This force is irrelevant to the direction of incident light and is determined by the particle orientation, and is also called body-fixed force here. Since the effect of collisions between a particle and surrounding gas molecules can result in random force and random angular momentum, all particles perform Brownian displacement and Brownian rotation. As a result, the direction of \(\Delta \alpha\)-force is randomly distributed, which will make Brownian motion more vigorous. Illuminated particles may perform irregular photophoresis and exhibit an irregular motion shown in the insert of Fig.1(b), which is similar to Brownian motion but stronger and clearly distinguishable from it.

From the formula, it is also obvious that photophoretic forces strongly depend on the pressure and reach their maximum if the particle size is comparable to the mean free path of gas molecules. For a pressure of a few mbar, the mean free path is approximately at the scale of tens of microns. This means that the photophoretic force is an important force for \(\mu\)-sized particles at pressures of few mbar or below. Thus, for a levitated microsphere in an optical trap in low-pressure environments, the motion of sphere can be highly influenced by photophoresis.

3. Motion of heated particle

Typically, due to a non-ideal shape and impurities, the particle in the optical trap will absorb part of the trapping light and convert it into heat. If the gas pressure is low, the interaction between the gas molecules and the particle is insufficient. Then, the energy absorbed by the particle cannot be dissipated and the particle will be in a state of thermal non-equilibrium. In addition, differences in surface roughness and composition will result in variations in the accommodation coefficient over the particle surface. Thus, particle motion is also affected by the photophoretic force. In our experiment, we observed a phenomenon that the microspheres can easily escape from the optical trap with no feedback when the pressure in the chamber drops to below a few mbar.

3.1. Dynamical model in single-beam optical trap

There are two kinds configurations for capturing micron particles: upward single beam and counter-propagation beams. The dual-beam optical trap can offer 3D manipulation of particles ranging from hundreds of nanometers to tens of microns in vacuum. It is more suitable for precision sensing in various environments in the future and we employ this configuration in experimental setup. In our study, we found that the escaping mechanism makes no essential difference between a single-beam optical trap or a dual-beam optical trap. However, the case of a dual-beam optical trap requires huge computation and we think it is not necessary considering the analysis of escaping mechanism. Thus, we choose the case of a single-beam trap to demonstrate the escaping mechanism of levitated particles in vacuum.
Figure 1. (a) Photophoretic $\Delta T$-force and $\Delta \alpha$-force. A particle having different accommodation coefficients on the two hemispheres ($\alpha_1 > \alpha_2$) experiences a resultant force pointing upwards. (b) Schematic of levitated sphere in an upward optical trap. The inset is a diagram of the trajectory of sphere in the radial plane.

In order to study the mechanism for loss of sphere during pumping down without cooling, we model the motion of a spherical particle in a single-beam optical trap. The schematic of the model is shown in Fig.1(b). A vertically oriented 1064 nm Gaussian beam is used to levitate the sphere. The beam waist radius is 3 $\mu$m and optical power is set to 100 mW. The sphere is composed of silica with a radius of $r=5$ $\mu$m. To simplify the model, we assume that the accommodation coefficient of one half of the sphere surface is $\alpha_1$ and that of the other is $\alpha_2$ (see Fig.1(a)). The equation of center-of-mass motion can be described classically and is given by Newton’s second law [17,19]:

$$\ddot{r}(t) + \Gamma_{\text{CM}} \dot{r}(t) = \frac{1}{m} \left[ F_{\text{fluc}}(t) + F_{\text{det}}(\mathbf{r}, t) \right]$$

(5)

where $\mathbf{r}$, $m$ represents the position and mass of particle, and $\Gamma_{\text{CM}}$ represents the damping rate. $F_{\text{fluc}}(t)$ and $F_{\text{det}}(\mathbf{r}, t)$ represent stochastic forces and deterministic forces, respectively.

In our model, we assume that the temperature of sphere is higher than that of the surroundings. Gas molecules impinge on the sphere surface at temperature $T_{\text{imp}}$ and leave at temperature $T_{\text{em}}$ ($T_{\text{em}} > T_{\text{imp}}$). $\Gamma_{\text{imp}}$ and $\Gamma_{\text{em}}$ are the damping rates for the sphere in connection with the impinging gas and emerging gas, respectively[19]. Accordingly, the random fluctuation force $F_{\text{fluc}}(t)$ has two contributions, $F_{\text{imp}} = \sqrt{2k_B T_{\text{imp}}} \zeta(t)$ and $F_{\text{em}} = \sqrt{2k_B T_{\text{em}}} \zeta(t)$. Here, $\zeta(t)$ encodes a white-noise process, such that $\langle \zeta(t) \rangle = 0, \langle \zeta(t) \zeta(t+\tau) \rangle = \delta(\tau)$ [33]. In Fig.1(b), the gravity force $F_G = mg$, photophoretic force $F_{\Delta T}$, and optical trapping force $F_x = k_x$(radial) and $F_z = k_z$ (axial)($k_x, k_z$ the stiffness of optical trap) belong to the deterministic forces $F_{\text{det}}(\mathbf{r}, t)$. Then, the equation of motion for particle in the x and z directions reads as:

$$m\ddot{z}(t) = F_z - F_G + F_{\Delta T} + F_{\text{imp}}(t) + F_{\text{em}-z}(t) + m(\Gamma_{\text{imp}} + \Gamma_{\text{em}-z}) \dot{\zeta}(t) - m(\Gamma_{\text{imp}} + \Gamma_{\text{em}-z}) \dot{\zeta}(t)$$

(6)

$$m\ddot{x}(t) = F_x + F_{\text{imp}}(t) + F_{\text{em}-x}(t) + F_{\text{axial}}(t) - m(\Gamma_{\text{imp}} + \Gamma_{\text{em}-x}) \dot{\zeta}(t) - m(\Gamma_{\text{imp}} + \Gamma_{\text{em}-x}) \dot{\zeta}(t)$$

(7)

Here, since the $\Delta \alpha$-force has a random direction and is independent of illumination, we assume that the photophoretic force $F_{\Delta \alpha}$ fluctuates on the same time scale as the random forces $F_{\text{imp}}(t)$ and $F_{\text{em}}(t)$. Then, $F_{\Delta \alpha}(t) = F_{\text{fluc}}(t)$. In the axial direction, the thermal effects induce both types of photophoretic force $F_{\Delta T}$ and $F_{\Delta \alpha}$, as shown in Equation (7).
Similar conclusions can be obtained for a dual-beam optical trap, which is essentially consistent with the dynamic model of single-beam optical trap (see Section 3 in Supplement). Therefore, this dynamic model of the motion of heated particle is universal for both the single-beam optical trap and the dual-beam optical trap. Fig.2 show the experimental and calculated standard deviation (STD) of x displacement for a trapped sphere in a dual-beam optical trap. Here, we assume that the complex refractive index \( n = 1.45 + 1 \times 10^{-4} i \). Then, we can obtain \( Q_x = 0.056 \) by three-dimensional numerical simulation using FDTD methods. By fitting the experimental data to our model, we find that \( \Delta \alpha = 3 \times 10^{-8} \). Since particles are easily escape at 0.1 mbar in experiment, we are more concerned about the change of displacement amplitude when the pressure drops from 10 mbar to 0.1 mbar, shown in Fig.2. The experimental results are in good agreement with the calculated ones in the tendency. The standard deviation of displacement increases as the pressure decreases, and the ratio of that at 0.1 mbar and 10 mbar are about 2.7 and 2.9 for experimental and calculated data respectively.

![Figure 2](image_url)  
Figure 2. Experimental and calculated standard deviation of x displacement. The ratio of STD is obtained by dividing the standard deviation at a certain pressure by the standard deviation at 10 mbar in each case. The sphere (r=5 μm) is trapped in a dual-beam optical trap. The wavelength of two Gaussian beams is 1064 nm, the waist radius is 5 μm, and the power is 150 mW.

In 2008, Hans Rohatschek [26] gave a simple description of stochastic processes associated with photophoresis. The mean square deviation of the particle random walk reads,

\[
\langle x^2 \rangle = \frac{2kt}{\gamma} \left( T + \frac{mF_{\Delta \alpha}^2}{3k\gamma^2} \right)
\]

Where \( \gamma = m\Gamma_{imp} \) is the damping coefficient in vacuum and \( \eta \) represents the dynamic viscosity coefficient. Equation (9) indicates that the actual temperature is added by a kinetic energy corresponding to the asymptotic velocity \( F_{\Delta \alpha}/\gamma \). In our model, an asymptotic velocity \( F_{\Delta \alpha}/\gamma = 0.26 \text{mm/s} \) (\( r = 5 \mu \text{m}, \Delta \alpha = 5 \times 10^{-8} \)) at 0.1 mbar yields an effective temperature contribution of approximately \( 2.7 \times 10^3 \text{K} \). The \( \Delta \alpha \)-force just acts as a “simplifier” for the Brownian motion. The effective temperature \( T_{eff} = mF_{\Delta \alpha}^2/3k\gamma^2 \) is an equivalent describing the photophoretic contribution to stochastic particle displacement as modified Brownian motion. As a result, we consider the photophoretic contribution as a bath with temperature \( T_{eff} \), which is similar to the bath with temperature \( T_{imp} \). Then the equation of motion for particle in radial direction reads,

\[
m\ddot{x}(t) = F_x + F_{imp}(t) + F_{\text{em-x}}(t) + F_{\text{eff-x}}(t) - m(\Gamma_{imp} + \Gamma_{\text{em-x}} + \Gamma_{\text{eff-x}}) \dot{x}(t)
\]

Thus, we can obtain the radial motion position trace in the range of 0.1-10 mbar. The trajectories in Fig.3(a) are calculated from separately from equation (9) and equation (7), corresponding to two methods. Fig.3(b)
show 50-times average of x displacement standard deviation calculated by two the methods. It is seen that the tendency of two curve is consistent and the magnitude of the standard deviation of the displacement is also the same, which verifies the reliability of our model.

Fig 3. Comparison of our results to previous work[26]. Radial motion position(x) trace for a trapped sphere(r=5μm) with Δα = 5×10⁻⁷. (a) Top: the trajectory of x position at 1mbar calculated from equation (9). Bottom: the trajectory of x position at 1mbar calculated from equation (7). (b) 50-times average of x displacement standard deviation calculated by two the methods.

3.2. Effective capture region

Two factors determine whether a particle in the light field can be captured: the range of motion and the region of capture. To further explain the escape process of the particle, we introduce the definition of effective capture region (ECR) proposed by Fu [34]. The effective capture region is defined as a criterion for the capture of particles, whose initial condition can be considered as the equivalent to a later-in-time situation of actual trajectories.

For our modeled single-beam optical trap, since the gravity force is in the z-axis direction, the motion of sphere is symmetrical along the radial direction. This means that the shape of ECR is cylindrically symmetric about the z-axis. In this study, we pay more attention to the extreme value of ECR in the radial direction. Fig.4 shows simulated ECR at pressures of 10mbar and 0.1mbar. Theoretically, the size of the ECR along each axis decreases with pressure because of the decrease in viscous force [34]. Our calculation results (see Fig.S2 in Supplement) allow for a consistent conclusion as demonstrated in Fig.4. For 10 mbar, the viscous force is enough to counteract the kinetic energy from gravitational acceleration, while the optical trapping force in the axial direction plays a minimal role, thus the sphere can be loaded far above the trap radially in a wide range. However, for 0.1 mbar, the viscous force becomes much smaller and the optical trapping force makes a major contribution in the loading process, thus decreasing the volume of ECR. The extreme coordinates x_edge at different pressures ranging from 0.1 mbar to 100 mbar are shown in Fig.5(b). It can be seen that, with the pressure decreasing, the extreme value that marks the farthest boundary at which a microsphere can reach while remaining trapped has shrunk.
Fig. 4. 3D simulation of the ECR of a single-beam trap. 3D display of ECR at (a) 10 mbar and (c) 0.1 mbar. The ECR in vertical section at (b) 10 mbar and (d) 0.1 mbar. Compared with result under the condition of 10 mbar, the volume of ECR at 0.1 mbar appeared significantly shrunk.

3.3. Analysis of escape of heated sphere

By substituting the complex refractive index of sphere into Equation (2), we can obtain \( J_i = 6.7 \times 10^{-4} \), which means that the photophoretic \( \Delta T \)-force is negative for the weakly absorbing sphere in our calculation. Fig. 5(c) shows the ratio of \( F_{\Delta T} \) and \( F_{\Delta \alpha} \) to the weight of the levitated sphere as a function of pressure. \( F_{\Delta T} \) achieves a maximum value at \( \sim 30 \) mbar when the pressure drops from atmospheric to \( 10^{-2} \) mbar; however, this is only one-tenth of the gravity force. Meanwhile, when we set \( \Delta \alpha = 1 \times 10^{-3} \), \( F_{\Delta \alpha} \) is always much smaller than the gravity force throughout the entire pressure range. As a result, the photophoretic force will change the equilibrium position in the axial direction, but there is always an equilibrium position in this axis.
Figure 5. Analysis of sphere escaping from a single-beam optical trap due to thermal effects. (a) Radial motion position (x) trace for a trapped sphere (r=5 μm) with Δα = 1×10^{-3} as a function of pressure: 1 atm, 10 mbar, 1 mbar, 0.1 mbar. The wavelength of beam is 1064 nm, the waist radius is 3 μm, and the power is 100 mW. (b) Left: simulated extreme coordinates x_{edge} of ECR(start) and calculated extreme coordinates of x position(circle) at different pressures ranging from 0.1 mbar to 100 mbar. Right: calculated x displacement standard deviation at different pressures. (c) The ratio of F_{αT} and F_{αα} to the weight of the trapped sphere.

Fig.5(a) shows the radial motion position trace calculated by Equation (7) for the trapped sphere with Δα = 1×10^{-3}. We consider that the sphere is in a state of thermal equilibrium when the pressure is ≥ 10 mbar, where T_{em} = 0 for Equation (7). When the pressure is lower than 10 mbar, the particles will be heated due to the decrease of gas damping. Since the light intensity in our calculation is on the order of 10^7 W/m^2, we take T_{em} = 500K here according to Ref[19]. Q_{σ} = 0.012 is calculated by three-dimensional numerical simulation using the FDTD method. It is obvious that the motion in the radial direction is increasingly vigorous with the pressure dropping; the contrast is particularly strong for 1 mbar and 0.1 mbar. The maximum displacement is about 6 μm for 1 mbar and 26 μm for 0.1 mbar. However, there is almost no difference for the motion trajectory at 1 atm, calculated with or without considering photophoretic force (see Fig.S1 in Supplement). This indicates that the photophoretic force plays a major role in the intensification of the movement at pressure of a few mbar. In addition, we can see that the ECR shrinks rapidly with the pressure dropping from 10 mbar to 1 mbar in Fig.5(b). At P = 0.1 mbar, the extreme value x_{edge} is about 19 μm, which is smaller than the maximum displacement for this pressure. Consequently, the sphere will escape from the optical trap at a certain pressure between 0.1 mbar and 0.1 mbar. In addition, little difference in Δα makes evident change for the motion according to our simulation. Since the impurities [35] and roughness of surface have an important effect on the accommodation coefficient α, higher purity and better sphericity of sphere are expected for better levitation stability.

In conclusion, the escaping mechanism of particles in an optical trap under vacuum includes two aspects. First, the thermal effects of particles induce a photophoretic force that will enhance the Brownian motions, and this phenomenon becomes increasingly evident during pumping down. Second, the volume of effective capture region shrinks when the pressure decreases. As a result, the range for radial motion
to ensure that particles are trapped in the optical trap also shrinks.

4. Conclusion

We have derived and tested a dynamic model for the motion of a particle in a thermal non-equilibrium state. The motion of particles was simulated on the basis of dynamic equation in the composite force field. Two types of photophoretic forces: $\Delta T$-force and $\Delta \alpha$-force induced by thermal effects have been investigated. It is shown that irregular photophoresis can be described as Brownian motion with increased “effective temperature”. We also simulated the ECR of the particle in our model and observed that the ECR tend to shrink apparently at a specific pressure interval. The processes of particle’s escape due to thermal effects for this interval was demonstrated and were consistent with the escape phenomenon in the experiment. Our work reveals the escaping mechanism of a heated particle in an optical trap in vacuum and open prospects for increasing the trapping stability of levitated particles in optical trap in vacuum.

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

Supplemental document. See Supplement 1 for supporting content.

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