Circulation of a particle trapped in an optical tweezer

Bo Sun, Yohai Roichman and David G. Grier
Department of Physics and Center for Soft Matter Research
New York University
April 4, 2008

1 Steady-state circulation of a driven trapped particle

Our goal is to calculate the circulation $\nabla \times S$ of the probability flux $S$ due to a specified force $F$ that both traps and drives a particle. We will focus our attention on a stably trapped particle, so that the circulating state is a non-equilibrium steady state.

Consider a particle of mobility $\mu$ subject to a spatially varying force $F$. The flux of probability for finding this particle is given by

$$S = \mu F \rho - D \nabla \rho,$$

(1)

where $\rho(r)$ is the density of particles at $r$ and where $D = \mu k_B T$ is the single-particle self-diffusion coefficient at temperature $T$. Continuity of the probability density requires

$$\nabla \cdot S = -\frac{\partial \rho}{\partial t}.$$  

(2)

In steady state, furthermore, $\partial_t \rho = 0$, which yields

$$\nabla \cdot S = 0.$$  

(3)

Equation (3) yields the Fokker-Planck equation for this system:

$$D \nabla^2 \rho = \mu\rho \nabla \cdot F + \mu F \cdot \nabla \rho \quad \text{or}$$

$$\nabla^2 \rho = \beta (\rho \nabla \cdot F + F \cdot \nabla \rho),$$

(4)

(5)

where $\beta^{-1} = k_B T$. In principle, we can solve Eq. (4) for $\rho(r)$ and then use Eq. (1) to obtain $S$. In the following sections, we will use first-order perturbation theory to obtain a closed-form expression for the probability flux of an optically trapped particle.

2 Model for an optical tweezer

We model an optical tweezer as a radially symmetric Gaussian optical intensity field. This gives rise both to intensity-gradient forces and to radiation pressure. We model the intensity-gradient force as

$$F_0 = -k \exp\left(-\frac{r^2}{2\sigma^2}\right) r,$$

(6)

where $k$ is the stiffness of the trap, and $\sigma$ is its effective width. This force is derived from the gradient of the light’s intensity, and so is manifestly conservative. It resembles a conventional harmonic well for small displacements with

$$\lim_{r \to 0} F_0 = -kr.$$  

(7)

The effective spring constant is proportional to the intensity of the laser light used to create the trap.
We model the radiation pressure as arising from the same Gaussian intensity distribution

\[ F_1 = k\sigma \exp \left( -\frac{r^2}{2\sigma^2} \right) \hat{z}, \]  

(8)

but being directed along the trapping beam’s direction of propagation, \( \hat{z} \). This is a simplified model because the radiation pressure actually should be directed along the local wave vector of the focused beam. Equation (8) expresses the force of radiation pressure in terms of the trap’s natural force scale, \( k\sigma \). In fact, the strength, \( f_1 \), of this term’s contribution to the total force also is proportional to the light’s intensity, but must be smaller than \( k\sigma \) to achieve stable trapping.

Unlike \( F_0 \), \( F_1 \) is not conservative. This can be seen because

\[ \nabla \times F_1 = k\sigma \left( \nabla \exp \left( -\frac{r^2}{2\sigma^2} \right) \right) \times \hat{z} \]

\[ = -k\sigma \frac{r}{\sigma^2} \exp \left( -\frac{r^2}{2\sigma^2} \right) \hat{r} \times \hat{z} \]

\[ = k \frac{r}{\sigma} \exp \left( -\frac{r^2}{2\sigma^2} \right) \sin \theta \hat{\phi} \]  

(9)

(10)

(11)
in spherical coordinates. Because \( \nabla \times F_1 \) does not vanish in general, \( F_1 \) is not the gradient of a potential energy. Consequently, \( F_1 \) is not conservative.

For the sake of comparison, the comparable exercise for the intensity-gradient force yields

\[ \nabla \times F_0 = -k \exp \left( -\frac{r^2}{2\sigma^2} \right) r \]

\[ = k \frac{r}{\sigma} \exp \left( -\frac{r^2}{2\sigma^2} \right) \hat{r} \times \hat{r} \]

\[ = 0. \]  

(12)

(13)

(14)
The total force acting on a trapped particle is then

\[ F = F_0 + \epsilon F_1, \]  

(15)

where \( \epsilon = f_1/(k\sigma) \) is the relative strength of radiation pressure. The particle becomes trapped at the point of mechanical equilibrium where \( F = 0 \). From Eqs. (6) and (8), this occurs at \( z_0 = \epsilon \sigma \), provided that \( \epsilon < 1 \). The particle must be trapped for the system to enter a steady state. Consequently, we can treat \( \epsilon \) as a small parameter in what follows.

### 3 Fokker-Planck equation for trapped particle

We will set up our calculation for \( \rho \) as a perturbation expansion in the small parameter, \( \epsilon \). In particular, we will take

\[ \rho(r) = \rho_0(r) + \epsilon \rho_1(r) + \mathcal{O}(\epsilon^2). \]  

(16)

We expect \( \rho_0 \) to reflect the unperturbed trap’s radial symmetry. Hence, it is a function of \( r \) rather than \( \mathbf{r} \).

The probability flux also can be expanded in powers of \( \epsilon \), yielding

\[ S = S_0 + \epsilon S_1 + \mathcal{O}(\epsilon^2), \]  

with

\[ S_0 = \mu F_0 \rho_0 - D\nabla \rho_0 \]  

(17)

(18)

(19)

Requiring \( S \) to satisfy Eq. (3) at all orders of \( \epsilon \) then yields a hierarchy of Fokker-Planck equations,

\[ \epsilon^0: \quad \nabla^2 \rho_0 = \beta (\rho_0 \nabla \cdot F_0 + F_0 \cdot \nabla \rho_0) \]  

\[ \epsilon^1: \quad \nabla^2 \rho_1 = \beta (\rho_1 \nabla \cdot F_0 + \rho_0 \nabla \cdot F_1 + F_0 \cdot \nabla \rho_1 + F_1 \cdot \nabla \rho_0) \]  

(20)

(21)

Because \( F \) only includes terms up to \( \mathcal{O}(\epsilon) \), higher-order Fokker-Planck equations have the form

\[ \epsilon^n: \quad \nabla^2 \rho_n = \beta (\rho_n \nabla \cdot F_0 + \rho_{n-1} \nabla \cdot F_1 + F_0 \cdot \nabla \rho_n + F_1 \cdot \nabla \rho_{n-1}) \]  

(22)
3.1 Solution at order $\epsilon^0$

The leading-order term involves only the conservative force. Assuming further that the particle remains trapped, which is consistent with $\epsilon < 1$, then the system comes to equilibrium with $S_0 = 0$. Equation (1) then yields an easily solved equation for $\rho_0$,

$$\nabla \rho_0 = \beta \rho_0 F_0$$  \hspace{1cm} (23)
$$\nabla \ln \rho_0 = \beta F_0$$  \hspace{1cm} (24)

$$= -\beta k \exp \left(-\frac{r^2}{2\sigma^2}\right) r.$$  \hspace{1cm} (25)

$$\ln \rho_0 = \beta k \sigma^2 \exp \left(-\frac{r^2}{2\sigma^2}\right) + c$$  \hspace{1cm} (26)

$$\rho_0(r) = N_0 \exp \left(\beta k \sigma^2 \exp \left(-\frac{r^2}{2\sigma^2}\right)\right).$$  \hspace{1cm} (27)

Because $\rho_0(r)$ is a solution of $S_0 = 0$, it also is a solution of $\nabla \cdot S_0 = 0$, and thus of the zeroth-order Fokker Planck equation, Eq. (20).

This result looks good at first blush, but has the unfortunate property that $\lim_{r \to \infty} \rho_0(r) = N_0 > 0$. This means that the probability density cannot be normalized unless an artificial limit is placed on the size of the system. Physically, this arises because thermally driven particles have a non-vanishing probability to wander arbitrarily far from a potential well of finite depth.

If, however, we assume that the trap is strong enough that $r < \sigma$, we may approximate

$$\rho_0(r) \approx N_0 \exp \left(-\frac{1}{2} \beta kr^2\right).$$  \hspace{1cm} (28)

This is the result for a particle at equilibrium in a harmonic potential energy well, and is normalized with

$$N_0 = \left(\frac{\beta k}{2\pi}\right)^{\frac{3}{2}}.$$  \hspace{1cm} (29)

The harmonic approximation is valid if the particle’s thermally driven excursions are small compared with the Gaussian trap’s width. This is the case if $\sigma^2$ is larger than

$$\langle r^2 \rangle = 4\pi \int_0^\infty r^2 \rho_0 r^2 \, dr$$  \hspace{1cm} (30)
$$= 4\pi N_0 \int_0^\infty r^4 \exp \left(-\frac{1}{2} \beta kr^2\right) \, dr$$  \hspace{1cm} (31)
$$= 4\pi N_0 3\sqrt{\frac{\pi}{2}} \frac{1}{(\beta k)^{\frac{3}{2}}}$$  \hspace{1cm} (32)
$$= \frac{3}{\beta k}.$$  \hspace{1cm} (33)

The harmonic approximation therefore is valid for

$$\beta k \sigma^2 > 3.$$  \hspace{1cm} (34)

In the discussion that follows, we will model the conservative part of the tweezer force in the harmonic approximation, Eq. (7), but retain the Gaussian dependence of the non-conservative part. This is reasonable because $F_1$ varies with distance as $O \left(r^2/\sigma^2\right)$, whereas the next term in $F_0$ would appear at $O \left(r^3/\sigma^3\right)$.
3.2 Solution at order $\epsilon^1$

To write out the Fokker-Planck equation for $\rho_1$ explicitly, we first need

$$\nabla \cdot \mathbf{F}_1 = k\sigma \hat{z} \cdot \nabla \exp \left( -\frac{r^2}{2\sigma^2} \right) - k\sigma \exp \left( -\frac{r^2}{2\sigma^2} \right) \nabla \cdot \hat{z}$$

$$= -k \frac{z}{\sigma} \exp \left( -\frac{r^2}{2\sigma^2} \right).$$

(35)

From this, we obtain the Fokker-Planck equation:

$$\nabla^2 \rho_1 = -3\beta k \rho_1 - \beta k \frac{z}{\sigma} \rho_0 - \beta k \mathbf{r} \cdot \nabla \rho_1 + \beta k \sigma G \rho_0$$

$$= -\beta k \left[ 3\rho_1 + \mathbf{r} \cdot \nabla \rho_1 + (1 + \beta k \sigma^2) \frac{z}{\sigma} \rho_0 \right],$$

(36)

where, for notational convenience, we have introduced $G(r) = \exp \left( -\frac{r^2}{2\sigma^2} \right)$.

The finite and real-valued solution to Eq. (38) can be obtained with Mathematica

$$\rho_1(r) = H(r) \frac{z}{\sigma} \rho_0(r),$$

(39)

where

$$H(r) = \frac{\beta k \sigma^2}{1 + \beta k \sigma^2} \frac{\sigma^3}{r^3} \left[ \sqrt{\frac{\pi}{2}} (1 + \beta kr^2) \text{erf} \left( \frac{r}{\sqrt{2} \sigma} \right) \right].$$

(40)

This solution is bounded,

$$\lim_{r \to 0} \rho_1(r) = 0$$

(41)

and does not affect the normalization of the probability density,

$$\int \rho_1(r) \, d^3r = 0.$$ 

(42)

The first-order correction therefore resembles a p-wave distortion of the normalized zeroth-order solution.

Taylor expanding $H(r)$ around $r = 0$, we obtain

$$\rho_1(r) \approx \beta k \sigma^2 \frac{1 + 3\beta k \sigma^2}{3(1 + \beta k \sigma^2)} \frac{z}{\sigma} \rho_0(r).$$

(43)

This approximation captures the leading-order dependence on laser power in the circulation rate and power dissipation.

4 The circulation

The local circulation of the probability flux is

$$\nabla \times \mathbf{S} = \mu \rho \nabla \times \mathbf{F} + \mathbf{F} \times \nabla \rho - D \nabla \times \nabla \rho$$

$$= \mu \rho \nabla \times \mathbf{F} + \mu \mathbf{F} \times \nabla \rho.$$ 

(44)

(45)

Anticipating that the flux traces out a toroidal roll centered on the $z$ axis, the mean circulation rate is

$$\Omega_0 = \frac{1}{2\pi} \int \nabla \times \mathbf{S} \cdot \hat{\phi} \, d^3r,$$

(46)

where

$$\hat{\phi}(r) = -\frac{y}{\xi} \hat{x} + \frac{x}{\xi} \hat{y}.$$ 

(47)
and where \( \xi = \sqrt{x^2 + y^2} \). Equation (46) then can be simplified with vector identities:

\[
(\nabla \times \mathbf{S}) \cdot \hat{\phi} = \nabla \cdot (\mathbf{S} \times \hat{\phi}) + \mathbf{S} \cdot (\nabla \times \hat{\phi})
\]

\[
= \nabla \cdot (\mathbf{S} \times \hat{\phi}) + \frac{S_z(r)}{\xi}.
\]

Now,

\[
\int_V \nabla \cdot (\mathbf{S} \times \hat{\phi}) \, d^3r = \oint_{\partial V} (\mathbf{S} \times \hat{\phi}) \cdot da
\]

by the divergence theorem. Assuming that the flux vanishes far from the origin, then the surface integral over \( \partial V \) also vanishes. Consequently,

\[
\Omega_0 = \frac{1}{2\pi} \int \frac{S_z}{\xi} \, d^3r
\]

Expanding in powers of \( \epsilon \), the first non-vanishing contribution to the circulation rate is

\[
\Omega_0 \approx \frac{\epsilon \mu_1}{2\pi} \int \frac{S_1}{\xi} \, d^3r
\]

\[
= \frac{\epsilon \mu_1}{2\pi} \int \left( F_{r_0} \rho_1 + F_{r_1} \rho_0 - \beta^{-1} \frac{\partial \rho_1}{\partial z} \right) \frac{1}{\xi} \, d^3r
\]

\[
= \frac{\epsilon \mu_1}{2\pi} \int d\theta \int_{-\infty}^{\infty} dz \int_0^{\infty} d\xi \left( -kz \rho_1 + k\sigma G(r) \rho_0 - \beta^{-1} \frac{\partial \rho_1}{\partial z} \right).
\]

The third term vanishes because

\[
\int_{-\infty}^{\infty} \frac{\partial \rho_1}{\partial z} \, dz = \rho_1(r)|_{z=-\infty} = 0.
\]

Therefore,

\[
\Omega_0 \approx \epsilon k\sigma \mu \int_{-\infty}^{\infty} dz \int_0^{\infty} d\xi \left( G(r) - \frac{z^2}{\sigma^2} H(r) \right) \rho_0(r)
\]

\[
\approx \frac{1}{\sqrt{18\pi}} \frac{\mu f_1}{\sigma} \frac{\sqrt{\beta k\sigma^2}}{1 + \beta k\sigma^2}.
\]

Because both \( k \) and \( f_1 \) are proportional to laser power, \( P_0 \), we find that \( \Omega_0 \sim P_0^{\frac{3}{4}} \). The circulation’s nature as a thermal ratchet, furthermore, is confirmed by its \( \Omega_0 \sim T^{\frac{3}{2}} \) scaling with temperature.

### 5 Power dissipated during circulation

The ensemble-averaged viscous drag force density at \( r \) is \( \mu^{-1} \mathbf{S}(r) \). The power density dissipated at \( r \) is therefore

\[
\mathcal{P}(r) = \frac{1}{\mu} \mathbf{S} \cdot \mathbf{v}
\]

where

\[
\mathbf{v}(r) = \frac{1}{\rho(r)} \mathbf{S}(r)
\]

is the mean drift speed of the circulating particle. To lowest order, therefore,

\[
\mathcal{P}(r) \approx \epsilon^2 \frac{S_1^2}{\mu \rho_0}
\]

\[
= \epsilon^2 \frac{1}{\rho_0} \left| \rho_0 \mathbf{F}_1 + \rho_1 \mathbf{F}_0 - D \nabla \rho_1 \right|^2
\]

\[
= \epsilon^2 \mu \left( \frac{\beta k}{2\pi} \right)^2 \frac{(\beta k)^2}{(\sigma^2)^2} \frac{\epsilon^2}{(\sigma^2)^2} \exp \left( - \left( 1 + \frac{1}{2} \beta k\sigma^2 \right) \frac{r^2}{(\sigma^2)^2} \right)
\]

\[
= \mu f_1^2 \left( \frac{\beta k}{2\pi} \right)^2 \exp \left( - \left( 1 + \frac{1}{2} \beta k\sigma^2 \right) \frac{r^2}{(\sigma^2)^2} \right) \frac{z^2 r^2}{(\sigma^2)^2}.
\]
Integrating this over the system’s volume yields the total power dissipated,

\[ P = \int \mathcal{P}(\mathbf{r}) \, d^3r \]  

(64)

\[ = 5\mu f_1^2 \frac{(\beta k\sigma^2)^{\frac{3}{2}}}{(2 + \beta k\sigma^2)^{\frac{7}{2}}} \]  

(65)

Because \( f_1 \) and \( k \) have the same dependence on laser power, Eq. (65) shows that the power dissipated by the circulating sphere is independent of laser power in the limit of strong trapping.