Particle binding over a nanofiber

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Abstract. We propose a configuration for optical binding of nanoparticles over a thin fiber under a plane wave illumination. We have shown that the interference of the field scattered into a guided mode of a nanofiber results in the formation of optomechanically stable configurations. Our estimations of the binding force and the trapping parameter for dielectric particles show that it is potentially possible to observe particle binding over a nanofiber experimentally.

1. Introduction

Optical manipulation has been extensively studied during the last few decades [1]. Following the realization of optical trapping, a new phenomenon, termed optical binding, was observed when two dielectric particles were trapped and bound transversely in a large beam waist [2]. This was due to the modification of the field caused by the presence of the particles and governed by their relative positions.

Using an evanescent wave of nanofibers for an optical trapping is already a well known process [3, 4, 5, 6]. All the above-mentioned dealt with the use of external laser beams to excite the waveguide mode. In contrast to such an approach, we advance a consideration of a normal incidence of a laser beam (see figure 1). This configuration has not yet been studied.

![Figure 1. Configuration for stable optical binding: (a) studied before; (b) studied in this paper.](image)

This is also an alternative configuration of optical binding (contrary to surface binding [2, 7, 8]). We suggest placing two dielectric nanoparticles close to a thin optical fiber and applying laser illumination perpendicular to the nanofiber axis (see figure 2). The electric field induces dipole moments in the particles. The particles start to radiate into free–space and...
the fiber. The field is scattered into the waveguide mode from the interference pattern, and nanoparticles bind into stable long-range states with forces of several pN.

Figure 2. Two nanoparticles under plane wave illumination.

2. Theoretical description
2.1. Binding force
There are many different ways to describe such electromagnetic systems. One approach is to use the scattering matrix approach [3], and another option is to use the finite element method (FEM), which requires a lot of computation power. In this paper, we used a comprehensive method based on the Green’s function.

The formulation of the problem is the following: plane wave illumination is scattered on nanoparticles, after which the scattered field propagates through a nanofiber for a longer distance without significant losses compared with surface plasmon binding [7].

We used the following approximations:

1. Only the HE$_{11}$ mode is considered as being propagated in a fiber. In other words, we assume that the single-mode condition is fulfilled [9]:

\[ V = k \rho_c \sqrt{\varepsilon_f - \varepsilon_m} < V_c \approx 2.405, \]  

where $\rho_c$ is the fiber radius, $k = \omega/c$ is the free-space wavenumber of the incident wave, $\varepsilon_f$ and $\varepsilon_m$ are the permittivities of the fiber and the background media.

2. The dipole approximation. We assume that the external field induces only the electric dipole moment in particles.

3. Only the $z$ dipole component is induced. In other words, we assume that $\mathbf{p} \parallel \mathbf{E}^{\text{inc}}$ and $|\mathbf{p}| \approx p_z$, where $\mathbf{E}^{\text{inc}}$ is the electric field of the incident wave.

4. The effective polarizability tensor is a slow function of $z$, so $\partial_z \hat{\alpha}_{\text{eff}} \approx 0$.

5. 1D motion along the $z$-axis. We assume that the distance from the particle centres to the fiber $z$-axis is constant and the polar angle $\varphi$ is equal and fixed for both particles.

The main goal is to calculate the force between two nanoparticles placed over the fiber. As soon as we use the dipole approximation, the force acting on the particle in $r_2$ may be written as [10]:

\[ \mathbf{F}_{12} = \frac{1}{2} \sum_{i=x,y,z} \text{Re} \left\{ p_{2,i}^* \nabla E_i(r) \right\}_{r=r_2}, \]  

where $\mathbf{p}$ is the dipole moment, $\nabla = \partial_r$ is the nabla operator and $\mathbf{E}$ is the total electric field. The problem then is formulated as a self-consistent problem of finding $\mathbf{E}$ and $\mathbf{p}$.

To find the electric field in the system, we apply the Green’s function formalism. The total field in the system at the point $r_2$ is the sum of the incident and scattered fields

\[ \mathbf{E}(r_2) = \mathbf{E}^{\text{inc}}(r_2) + \mathbf{E}^{\text{sc}}(r_2), \]
where the scattered field in $\mathbf{r}_2$ is the sum of the scattered fields from the dipole located in $\mathbf{r}_1$ and the effective dipole induced by the nanofiber in $\mathbf{r}_2$. In SI units, it may be written as [10]

$$
\mathbf{E}^{sc}(\mathbf{r}_2) = \frac{k^2}{\varepsilon_0} \left( G_0(\mathbf{r}_2, \mathbf{r}_1) + \hat{G}_s(\mathbf{r}_2, \mathbf{r}_1) \right) \mathbf{p}_1 + \frac{k^2}{\varepsilon_0} \hat{G}_s(\mathbf{r}_2, \mathbf{r}_2) \mathbf{p}_2.
$$

(4)

where $\varepsilon_0$ is the vacuum permittivity, $G_0$ is the dyadic vacuum Green’s function and $\hat{G}_s$ is the dyadic fiber Green’s function.

The explicit forms of the Green’s functions are the following. The vacuum part is:

$$
G_{0,ij}(\mathbf{r}, \mathbf{r'}) = \frac{e^{ik_1 R}}{4\pi R} \left[ \left( 1 + \frac{ik_1 R - 1}{k_1^2 R^2} \right) \delta_{ij} + \frac{3 - 3ik_1 R - k_1^2 R^2 R_i R_j}{k_1^2 R^2 R^2} \right], \quad \mathbf{R} = \mathbf{r} - \mathbf{r'}.
$$

(5)

The fiber Green’s function [9, 11] is:

$$
G_{s,zz}^{11}(\mathbf{r}, \mathbf{r'}) = -\frac{1}{2} \rho^{11}_s(\beta) \frac{k_2^2}{k_1^2} H_1^{(1)}(k_1 \rho_1) H_1^{(1)}(k_2 \rho_2) \cdot e^{i|z_1 - z_2|},
$$

(6)

where $k_{\rho_1} = \sqrt{\varepsilon_0 k^2 - \beta^2}$, $k_{\rho_2} = \sqrt{\varepsilon_1 k^2 - \beta^2}$, $\beta = \beta(\omega)$ is the fiber propagation constant, which comes from the solution of the transcendental equation; $H_n^{(1)}(z)$ is the Hankel function of the first kind. Other coefficients are given in Appendix A.

In order to find the dipole moments, we need to notice two things:

(1) An ordinary polarizability connects a dipole moment and an external field as

$$
\mathbf{p} = \alpha_0 \mathbf{E},
$$

(7)

where $\alpha_0 = \alpha_0(a, \omega, \varepsilon_\rho, \varepsilon_m)$ is the polarizability, which has an exact expression given by the Mie theory [12]. The explicit expression is given in Appendix B.

(2) The detailed consideration of the scattered field in form (4) allows us to notice that $\mathbf{E}^{sc}$ depends on the dipole moments:

$$
\mathbf{E}^{sc}(\mathbf{r}) = \mathbf{E}^{sc}(\mathbf{r}, \mathbf{p}_1, \mathbf{p}_2).
$$

(8)

This means that we need to solve the following system of equations:

$$
\begin{cases}
\mathbf{p}_1 = \alpha_0 \left( \mathbf{E}^{inc}(\mathbf{r}_1) + \mathbf{E}^{sc}(\mathbf{r}_1, \mathbf{p}_1, \mathbf{p}_2) \right), \\
\mathbf{p}_2 = \alpha_0 \left( \mathbf{E}^{inc}(\mathbf{r}_2) + \mathbf{E}^{sc}(\mathbf{r}_2, \mathbf{p}_1, \mathbf{p}_2) \right),
\end{cases}
$$

(9)

which gives the solution of the self-consistent problem. In terms of the effective polarizability, we have:

$$
\hat{\alpha}_i^{\text{eff}} = \alpha_0 \left[ \mathbf{I} - \alpha_0 \frac{k^2}{\varepsilon_0} \hat{G}^{ss} - \alpha_0 \frac{(k^2)}{\varepsilon_0} \hat{G}_{ij} \hat{\alpha}_j^{\text{ss}} \hat{G}_{jj} \right]^{-1} \left( \mathbf{I} + \frac{k^2}{\varepsilon_0} \hat{G}_{ij} \hat{\alpha}_j^{\text{ss}} \right),
$$

(10)

where we used the notation $\hat{G} = \hat{G}^s + \hat{G}^0$, $\hat{G}_{ij}^{\text{def}} = \hat{G}(\mathbf{r}_i, \mathbf{r}_j)$ and $\hat{\alpha}_i^{\text{ss}} = \alpha_0 \left[ 1 - \alpha_0 \frac{1}{\varepsilon_0} \hat{G}_i^{ss} \right]^{-1}$. We have introduced an effective polarizability such that the induced dipole moment may be found as the product of polarizability and the vector magnitude of the incident wave:

$$
\mathbf{p}_i = \hat{\alpha}_i^{\text{eff}} \mathbf{E}_0, \quad i = 1, 2.
$$

(11)
Considering \(|p| \approx p_z\) and \(\partial_z \hat{\alpha}_{\text{eff}} \approx 0\), we can finally write the expression for the binding force

\[
F_{12,z} = \frac{1}{2} \text{Tr} \left( \hat{\alpha}_{\text{eff}}^* \hat{\alpha}_{\text{eff}} \right) \left| E_0 \right|^2 \frac{k_T}{\varepsilon_0} \text{Re} \left\{ \partial_z \left[ G_{zz}^s(r, r_2) + G_{zz}^0(r, r_2) \right]_{r=r_1} \right\},
\]

which was used for the numeric simulation afterwards.

2.2. Trapping parameter
In order to understand how stable each equilibrium point is, we need to define a dimensionless parameter. The main source of instability is the thermal motion, so we define the trapping parameter as the ratio of the potential energy of the trap \(U_{tr}\) to the energy of thermal motion

\[
\gamma_{tr} \overset{\text{def}}{=} \frac{\text{potential energy of the trap}}{\text{energy of thermal motion}} = \frac{U_{tr}}{kT}.
\]

The question naturally arises whether we can reason in terms of potential energy. Indeed, the binding force has two components: a gradient part and a radiation (scattering) part. The contribution of each part is defined by the real and imaginary parts of polarizability \(\text{Re} \{ \hat{\alpha}_{\text{eff}} \}\) and \(\text{Im} \{ \hat{\alpha}_{\text{eff}} \}\). Numerical computations show that the scattering part of the binding force is negligible (figure 3), so the definition of the trapping parameter according to equation (13) makes sense.

Considering a linear dependence near the equilibrium point, we can introduce an effective stiffness \(k_{eff} = -\partial F_z / \partial z\), so \(U \approx \frac{1}{2} k_{eff} (\Delta x)^2\). The period of the binding force over \(z\) is about the wavelength value. This means that we can put \(\Delta x \approx \lambda / 2\). Now we have an approximate analytical expression for the trapping parameter:

\[
\gamma_{tr} = \frac{\lambda^2}{8kT} \left| \frac{\partial F_z}{\partial z} \right|_{z=z_{eq}},
\]

where \(F_z\) is given by (12).

This dimensionless parameter is very convenient because we can distinguish two cases:

1. \(\gamma_{tr} \ll 1\) — unstable configuration.
2. \(\gamma_{tr} \gg 1\) — stable configuration.

Within this context, stability (or unstability) is understood in terms of thermal perturbation.

3. Results
In order to make some numerical estimations, we have taken the typical parameters of nanoparticles and nanofibres which potentially may be manufactured [13].

All the taken parameters are presented in table 1. The longitudinal component of the force \(F_z\) for such parameters has been calculated using (2) (see figure 3). The maximum amplitude is about several pN. As expected, the interaction does not tend to zero with a large distance between particles \(\Delta z\) as a consequence of a long-range interaction through the guided mode.

Let us estimate the trapping parameter \(\gamma_{tr}\). At the second equilibrium point:

\[
\gamma_{tr}^{\text{near}} = \frac{U_{tr}}{kT} \approx 40,
\]

where \(U_{tr} \approx F_{\text{max}} \cdot \Delta z \approx 1\) pN \cdot 200 nm and \(T = 300\) K. The obtained result is very promising from the experimental point of view. At distant equilibrium points, the trapping parameter appears to be:

\[
\gamma_{tr}^{\text{far}} \approx 5.
\]
Table 1. Parameters of the model

| Parameter | laser power | focus radius | appropriate intensity |
|-----------|-------------|--------------|----------------------|
| Notation  | $P$         | $R_{\text{focus}}$ | $I$                  |
| Value     | 100 mW      | 1 $\mu$m     | $3.2 \times 10^{10}$ W/m$^2$ |

| Parameter | particle radius | fiber radius | medium permittivity | fiber permittivity | particle permittivity | wave length |
|-----------|-----------------|--------------|---------------------|-------------------|----------------------|-------------|
| Notation  | $a$             | $\rho_c$     | $\varepsilon_m$     | $\varepsilon_f$   | $\varepsilon_p$      | $\lambda$   |
| Value     | 200 nm          | 100 nm       | 1.0                 | 2.09              | 2.5                  | 550 nm      |
|           | (Air)           | (SiO$_2$)    | (Polystyrene)       |                   |                      |             |

Figure 3. (a) The longitudinal force for a longitudinal polarization. (b) The trapping parameter dependence on the fiber radius calculated at the second equilibrium position. The particle radius is $a = 200$ nm and the incident wavelength is $\lambda = 550$ nm. The laser power is set to 100 mW with a beam waist $w_0 = 2 \mu$m.

The main benefit of such system is a long–range interaction due to low losses in a nanofiber, which is now clearly visible.

The trapping parameter depends on many arguments. In order to analyze its dependence on the ratio of the fiber radius and the nanoparticle radius we have fixed the distance between nanoparticles at the second equilibrium point and varied the nanofiber radius (figure 3). The local maximum has been found at the point $\rho_c/a \approx 0.9$. This result helps to match a proper nanofiber radius to observe better binding. It should be noted that one cannot trust the results for a very thin nanofiber, as the approximations of the model will no longer be correct.

4. Conclusion
We have proposed a configuration for optical binding of nanoparticles over a thin fiber under plane wave illumination. We have shown that the interaction of nanoparticles through a single guiding mode of a nanofiber results in optical binding. Our estimations of the binding force and the trapping parameter for dielectric particles show that it is potentially possible to observe particle binding over a nanofiber experimentally.

Consideration of nanofiber modes of a higher order may increase the binding effect and allow consideration of different frequency ranges, which is a subject of future studies.
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### Appendix A. The fiber Green’s function

Considering the Green’s function of an infinite optical fiber [9, 11], we need to split off only the waveguide part due to its significant contribution to the binding force:

\[
G_{s,zz}(r, r') = -\frac{1}{2} P_{11}^{11}(\beta) \frac{k_p^2}{k_p^1} H_1^{(1)}(k_p \rho) H_1^{(1)}(k_p \rho') e^{i\beta |z_1 - z_2|}, \tag{A.1}
\]

where

\[
P_{11}^{11}(\beta) = \frac{J_1(k_p \rho_c)}{F(\beta) H_1^{(1)}(k_p \rho_c)} \left[ \left( \frac{1}{k_p^2} - \frac{1}{k_p^1} \right) \beta^2 - \left( \frac{J_1(k_p \rho_c)'}{k_p^2 J_1(k_p \rho_c)} - \frac{H_1^{(1)}(k_p \rho_c)'}{k_p^1 H_1^{(1)}(k_p \rho_c)} \right) \right], \tag{A.2}
\]

\[
F(\beta) = -2AA' \beta^2 - 2A^2 \beta + [(B' - C') (k_p^2 B - k_p^2 C) + (B - C) (k_p^2 B' - k_p^2 C')] \rho_c^2.	ag{A.3}
\]

\[
A = \frac{1}{k_p^2} - \frac{1}{k_p^1}, \quad B = \frac{J_1(k_p \rho_c)' k_p^2 J_1(k_p \rho_c)}{k_p^1 H_1^{(1)}(k_p \rho_c)}, \quad C = \frac{H_1^{(1)}(k_p \rho_c)'}{k_p^1 H_1^{(1)}(k_p \rho_c)}, \tag{A.4}
\]

\[
A' = 2\beta \left( \frac{1}{k_p^4} - \frac{1}{k_p^1} \right), \quad B' = -\frac{J_1(k_p \rho_c)'}{k_p^2 J_1(k_p \rho_c)} \beta \frac{J_1(k_p \rho_c)'}{k_p^1 H_1^{(1)}(k_p \rho_c)} \frac{J_1(k_p \rho_c)'}{k_p^2 J_1(k_p \rho_c)} \rho_c^2, \quad \tag{A.5}
\]

\[
C' = -\frac{H_1^{(1)}(k_p \rho_c)'}{k_p^2 H_1^{(1)}(k_p \rho_c)} \beta \frac{H_1^{(1)}(k_p \rho_c)'}{k_p^1 H_1^{(1)}(k_p \rho_c)} \frac{H_1^{(1)}(k_p \rho_c)'}{k_p^2 H_1^{(1)}(k_p \rho_c)} \rho_c^2. \tag{A.6}
\]

where \(k_p \rho_c = \sqrt{\varepsilon_{1w} k_p^2 - \beta^2}, k_p = \sqrt{\varepsilon_f k_p^2 - \beta^2}, \beta = \beta(\omega)\) is the fiber propagation constant, which comes from the solution of the transcendental equation; \(J_n(z)\) is the Bessel function of the first kind, and \(H_n^{(1)}(z)\) is the Hankel function of the first kind, \((J_n(z))' \equiv \frac{\partial J_n(z)}{\partial z}\).

### Appendix B. Polarizability of the sphere (Mie theory results)

The exact expression for the electric polarizability of the sphere can be found using the Mie scattering theory [12]:

\[
a_0 = i \frac{3a^3}{2\pi^3} a_1(x, m), \tag{B.1}
\]

where \(x = \sqrt{\varepsilon_m} ka, m = \sqrt{\varepsilon_p}/\sqrt{\varepsilon_m}\) and

\[
a_1(x, m) = \frac{m\psi_1(mx) (\psi_1(x))' - \psi_1(x) (\psi_1(mx))'}{m\psi_1(mx) (\xi_1(x))' - \xi_1(x) (\psi_1(mx))'}, \tag{B.2}
\]

where

\[
\psi_1(z) = zj_1(z), \quad \xi(z) = zh_1^{(1)}(z), \quad h_1^{(1)}(z) = j_1(z) + iy_1(z), \tag{B.3}
\]

where \(j_1\) and \(y_1\) are the spherical Bessel functions of the first and second kind correspondingly.
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