Optomechanical interaction between single-walled carbon nanotubes of various structures

D Kislov¹, O Kushchenko¹ and A S Shalin¹,²

¹ITMO University, 49 Kronverksky Pr., St. Petersburg 197101, Russia
²Kotel’nikov Institute of Radio Engineering and Electronics of Russian Academy of Sciences (Ulyanovsk branch), Goncharova Str.48, Ulyanovsk, Russia, 432000
denis.a.kislov@gmail.com

Abstract. We consider optomechanical interaction in an asymmetric structure of a carbon nanotubes dimer of different orientations and/or different atomic structures in the field of a plane wave or a focused Gaussian beam. Here we show that optical coupling in such the system can lead to nonreciprocal interactions between the constituents. We demonstrate that a non-conservative force is applied to the center of mass of an optically coupled nanotube dimer, resulting in an unexpected lateral action. The sign and magnitude of this force depend on abrupt phase transitions in the properties of the asymmetric dimer.

1. Introduction

Carbon nanotubes are an interesting object for optics, optoelectronics, nanoelectronics, lab-on-a-chip, etc. When designing various devices, it is often necessary to manipulate individual nanotubes or several nanotubes at once.

Optical tweezers are a good tool for this. The capture of various nano- and microparticles and manipulations with them have been widely developed in various fields of science [1,2]. Recently, in optomechanics, the interaction with plasmonic particles has been studied rather well [3-6]. However, such particles have a disadvantage - significant ohmic losses. Particles made of materials with high refractive index n > 3 [7-12], which are a competitive alternative to resonant metal nanoparticles, are widely used, for example, in the development of metasurfaces [13] and optical or optoelectronic devices [14-17], and are free from this drawback.

Along with this, there are a few works in which the optical capture of nanotubes in optical traps and binding in optical fibers are shown experimentally [18]. There are several theoretical works in which optical binding of nanocylinders and nanowires made of glass, titanium dioxide, and other materials is considered [19,20]. However, there are still no works in which the optomechanical interaction of nanotubes, depending on their atomic structure, would be studied in detail.

2. Theoretical formalism

In this work, we consider single-wall carbon nanotubes of two types: "armchair" (x, x) and "zig-zag" (x, 0). The indices are written in brackets that specifies the coordinates of the chiral vector. In this work, x = 8, 10, 12. The imaginary part of the dielectric constant in the visible wavelength range for a given nanotubes type, simulated from first principles, was taken from the work [21]. Then, using the Kramers-Kronig relation, the real part of the dielectric constant was restored (Fig.1).
The mathematical formalism is based on the dipole approximation. To calculate the polarizability of nanotubes, we used a model for the anisotropic polarizability of a nano-needle \((1)-(2)\) (highly elongated ellipsoid) \([22]\). This can be done with good accuracy since the length of the tube is much greater than its diameter.

\begin{equation}
\mathbf{a}_{\text{CNT}} = \begin{pmatrix}
\alpha_{||} & 0 & 0 \\
0 & \alpha_{\perp} & 0 \\
0 & 0 & \alpha_{\perp}
\end{pmatrix}
\end{equation}

\begin{equation}
\alpha_{||} = 4\pi\varepsilon_0 \varepsilon_{\text{CNT}} r_{\text{CNT}}^2 \varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}} \frac{\varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}}}{3\varepsilon_{\text{CNT}} + 3L_1 (\varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}})}
\end{equation}

\begin{equation}
\alpha_{\perp} = 4\pi\varepsilon_0 \varepsilon_{\text{CNT}} r_{\text{CNT}}^2 \varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}} \frac{\varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}}}{3\varepsilon_{\text{CNT}} + 3L_2 (\varepsilon_{\text{CNT}} - \varepsilon_{\text{irr}})}
\end{equation}

\begin{equation}
L_1 = \frac{\hbar_{\text{CNT}} r_{\text{CNT}}^2}{2} \int_0^\infty \frac{dq}{d(q + \varepsilon_{\text{CNT}} + q)(\varepsilon_{\text{CNT}})}
\end{equation}

\begin{equation}
L_2 = \frac{\hbar_{\text{CNT}} r_{\text{CNT}}^2}{2} \int_0^\infty \frac{dq}{d(q + \varepsilon_{\text{CNT}} + q)(\varepsilon_{\text{CNT}})}
\end{equation}

here \(\hbar_{\text{CNT}}\) - is the half of the nanotube length; \(r_{\text{CNT}}\) - nanotube radius.

The force action of the nanotubes was calculated using the expression for the effective electromagnetic field based on the formalism of the Green's function for free space \([23,24]\).

\begin{equation}
\mathbf{E}(\mathbf{r}_1) = \left[1 - \omega^2 \mu_0 G_{21}(\mathbf{r}_1) \mathbf{a}_{\text{CNT},2} G_{12}(\mathbf{r}_2) \mathbf{a}_{\text{CNT},1}\right]^{-1} \left[\mathbf{E}_{\text{inc}}(\mathbf{r}_1) + \omega^2 \mu_0 G_{21} G_{12} \mathbf{a}_{\text{CNT},2} \mathbf{E}_{\text{inc}}(\mathbf{r}_2)\right]
\end{equation}

\begin{equation}
\mathbf{E}(\mathbf{r}_2) = \left[1 - \omega^2 \mu_0 G_{21}(\mathbf{r}_1) \mathbf{a}_{\text{CNT},2} G_{12}(\mathbf{r}_2) \mathbf{a}_{\text{CNT},1}\right]^{-1} \left[\mathbf{E}_{\text{inc}}(\mathbf{r}_2) + \omega^2 \mu_0 G_{21} G_{12} \mathbf{a}_{\text{CNT},2} \mathbf{E}_{\text{inc}}(\mathbf{r}_1)\right]
\end{equation}

Time averaged optical force on each nanotube in the dipolar approximation can be written as follows:

\begin{equation}
\mathbf{F}_{\text{CNT},1}(\mathbf{r}_1) = \frac{1}{2} \text{Re} \left[\sum_i \mathbf{p}_{\text{CNT},1}^* \nabla \mathbf{E}_i(\mathbf{r}_1)\right] \quad \mathbf{F}_{\text{CNT},2}(\mathbf{r}_2) = \frac{1}{2} \text{Re} \left[\sum_i \mathbf{p}_{\text{CNT},2}^* \nabla \mathbf{E}_i(\mathbf{r}_2)\right] \quad i = x, y, z
\end{equation}

here \(\mathbf{p}_{\text{CNT},1} = \mathbf{a}_{\text{CNT},1} \mathbf{E}(\mathbf{r}_1), \quad \mathbf{p}_{\text{CNT},2} = \mathbf{a}_{\text{CNT},2} \mathbf{E}(\mathbf{r}_2)\) - dipole moment of nanotubes.

It is known that when illuminated by an external field, identical nano- and microscopic particles can form stable structures due to their mutually acting optical forces on each other. This effect is known as optical binding (fig.2a). Potential forces act on two identical connected particles, which are
equal in magnitude and oppositely directed - thereby the principle of "actio et reactio" is fulfilled. However, this is not always the case. Forces on optically interacting but dissimilar particles are not necessarily reciprocal. Dissimilar particles experience forces that do not compensate each other, which results in an overall movement of the system. In our case, a similar scenario can be obtained by considering the interaction between two tubes of the same type, but different in orientation (Fig. 2b), as well as between tubes of different types (Fig. 2c).

Figure 2. Transverse optical force acting on nanotubes in a plane wave field, depending on the distance between the centers of the tubes: a) tubes of the same type and the same orientation; b) tubes of the same type and different orientations; c) tubes of different types of the same orientation. The insets show the geometry of the calculation. Designations ZZ - zig-zag, ARM - armchair. Wavelength is 800 nm.

The apparent contradiction with the principle of “actio et reactio” can be resolved via taking into account that particles interacting with an external field constitute an open system, since part of the momentum is carried away by an asymmetrically scattered electromagnetic field. Optical forces between particles are mediated by their interaction with an external field and include not only conservative, but also non-conservative parts.

3. Conclusions
We have demonstrated that two dissimilar and optically interacting nanotubes experience common nonreciprocal interaction forces. This apparent violation of the principle of "action and reaction" occurs due to the presence of non-conservative optical forces that arise due to the interaction with the external field.

Acknowledgements
This work has been supported by the Russian Science Foundation (Grant No. 20-72-10141).

References
[1] Canós Valero A., Kislov D., Gurvitz E.A., Shamkhi H.K., Pavlov A.A., Redka D., Yankin S., Zemánek P. and Shalin A.S. 2020 Adv. Sci. 7 1903049
[2] Favre-Bulle I.A., Stilgoe A.B., Scott E.K. and Rubinsztein-Dunlop H. 2019 Nanophotonics 8, 1023
[3] Kislov D., Novitsky D., Kadochkin A., Redka D., Shalin A.S. and Ginzburg P. 2020, Phys.Rev.B 101 035420
[4] Kucherenko M. G. and Kislov D. A. 2018 J. Photochem. Photobiol. A Chem. 354 25
[5] Izmodenova S. V., Kislov D. A., and Kucherenko M. G. 2014 *Colloid J.* **76** 683
[6] Shalin A.S., Sukhov S.V. 2013 *Plasmonics* **8** 625
[7] Zhigunov D., Evlyukhin A.B., Shalin A.S., Zywietz U., and Chichkov B.N. 2018 *ACS Photonics* **5** 977
[8] Baryshnikova K., Filonov D., Simovski C., Evlyukhin A., Kadochkin A., Nenasheva E., Ginzburg P. and Shalin A.S. 2018 *Phys. Rev. B* **98** 165419
[9] Barhom H., Machnev A.A., Noskov R.E., Goncharenko A., Gurvitz E.A., Timin A.S., Shkoldin V. A., Koniaikhin S.V., Koval O.Yu., Zyuzin M.V., Shalin A.S., Shishkin I.I. and Ginzburg P. 2019 *Nano Lett.* **19** 7062
[10] Terekhov P.D., Baryshnikova K.V., Greenberg Y. et al. 2019 *Sci Rep* **9** 3438
[11] Kozlov V., Filonov D., Shalin A.S., Steinberg B.Z. and Ginzburg P. 2016 *Applied Physics Letters* **109** 203503
[12] Terekhov P.D., Shamkhi H.K., Gurvitz E.A., Baryshnikova K. V., Evlyukhin A.B., Shalin A.S. and Karabchevsky A. 2019 *Opt. Express* **27** 8
[13] Ivinskaya A., Kostina N., Proskurin A., Petrov M.I., Bogdanov A.A., Sukhov S., Krasavin A. V., Karabchevsky A., Shalin A.S. and Ginzburg P. 2018 *ACS Photonics* **5** 4371
[14] Kostina N., Petrov M., Ivinskaya A., Sukhov S., Bogdanov A., Toftul I., Nieto-Vesperinas M., Ginzburg P. and Shalin A. 2019 *Phys. Rev. B* **99** 125416
[15] Shalin, A.S., Moiseev, S.G. 2009 *Opt. Spectrosc.* **106** 916
[16] Shalin, A.S. 2010 *Jetp Lett.* **91** 636
[17] Ivinskaya A., Petrov M.I., Bogdanov A.A., Shishkin I., Ginzburg P. and Shalin A.S. 2017 *Light Sci. Appl.* **6** e16258
[18] Li Y., Xin H., Xu X., Liu X., Li B. 2018 *Adv. Mater. Lett.* **9** 8
[19] Simpson S.H., Zemánek P., Maragó O. M., Jones P.H. and Hanna S. 2017 *Nano Lett.* **17** 6
[20] Ha S., Tang Y., van Oene M., Janissen R., Dries R. M., Solano B., Adam A. J. L. and Dekker N.H. 2019 *ACS Photonics* **6** 5
[21] Cho T. H., Su W. S., Leung T. C., Ren W. and Chan C. T. 2009 *Phys. Rev. B* **79** 235123
[22] Bohren C. F., Huffman D. R. 1998 *Absorption and Scattering of Light by Small Particles* (Wiley, New York)
[23] Kostina N.A., Kislov D.A., Ivinskaya A.N., Proskurin A., Redka D.N., Novitsky A., Ginzburg P. and Shalin A.S. 2020 *ACS Photonics* **7** 425
[24] Sukhov S., Shalin A., Haefner D. and Dogariu A. 2015 *Opt. Express* **23** 247