ABSTRACT

CONOVER, BRANDON LEE. Quantitative Microfluidic Dynamics Of Spheroidal Particles Within Periodic Optical Landscapes. (Under the direction of Dr. Michael. J. Escuti.)

Over the past 4 decades, research and development of optical manipulation techniques has been primarily focused on observable phenomena. Trapping, sorting, mixing, aligning, and organizing particles—often times spheres on the order of $1 - 100\mu m$—has been shown by several groups using many different optical trapping and optical potential techniques. However, relatively little been reported on either the quantification of the various forces on the particles or on the theoretical aspects of the motion of the particles. Even less has been reported regarding the theoretical aspects of the motion of non-spherical particles within optical traps and landscapes. It is the objective of this dissertation to address these deficits by means of modeling and experimentally verifying the behavior of particles within periodic optical landscapes.

First, we report on our development of a quantifiable analysis of these phenomena by means of a form factor model of spheroidal particle motion in periodic optical landscapes. Using this model, we show that shape does indeed have a quantifiable impact on a particle’s motion in an optical landscape. We conclude that a collection of particles will all traverse an optical landscape differently based directly on their respective sizes, refractive indices, and shapes, sometimes with a high degree of dispersion. Next, we report on our development of a second model of spheroidal particle motion in periodic optical landscapes. Based on the $T$-matrix scattering approach, this model addresses the scattering forces and the electric field polarization effects on the particles’ motion. We conclude that as the particle size gets larger, the scattering forces become greater and very quickly rise above an order of magnitude larger than the gradient forces of the optical landscape. Our conclusions provide quantifiable conditions for when scattering forces and electric field-induced torques within an optical landscape are significant and should not be neglected.

We then report on our creation of pathways to a microfluidic optical manipulation testbed
for interrogating spheroidal particle behavior within optical landscapes and microfluids. We have experimentally implemented a periodic optical landscape and microfluidic system that reasonably approximates the ideal periodic landscape assumed in our models. Furthermore, our apparatus is shown to effectively lock-in or organize microscale particles within an optical landscape and a stationary microfluid. Close approximations of microscale spheroidal particles have also been designed and fabricated via photolithographic means within SU-8 photoresist and then also controlled with the apparatus.

Finally, we report on our creation of a hands-on teaching laboratory on organic electronics and liquid crystal displays that effectively teaches their operational principles, fundamentals, and practical aspects of fabrication, within a reasonable budget and broadly accessible way. Four modules have been developed: a liquid crystal display (LCD) pixel, an organic light-emitting diode (OLED), an organic photovoltaic (OPV) solar cell, and an organic thin-film transistor (OTFT). This effort has been achieved with budgetary restrictions and has been experienced by students from all manners of engineering, physics, chemistry, and materials.

In the final portion of this dissertation, we evaluate the work, summarize the contributions, and make suggestions for how future researchers can take our work and contributions to new application spaces and new research areas.
Quantitative Microfluidic Dynamics Of Spheroidal Particles Within Periodic Optical Landscapes

by
Brandon Lee Conover

A dissertation submitted to the Graduate Faculty of North Carolina State University in partial fulfillment of the requirements for the Degree of Doctor of Philosophy in Electrical Engineering

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DEDICATION

For Brenda.
Brandon Lee Conover was born in Jefferson City, MO, on August 27, 1981 to Arthur Lee and Karen Waite Conover, currently of Columbia, SC. His sole sibling, Brian Scott Conover, resides in Charleston, SC.

In 2003, Brandon graduated the University of Pittsburgh in Pittsburgh, PA, earning a BSE Degree in Computer Engineering (*summa cum laude*) and a Certificate in Photonics. The same year he began graduate studies at North Carolina State University (NCSU), supported by both departmental assistantships, a Department of Education GAANN Fellowship, and the teachings and patience of Dr. Michael Escuti. In 2006, Brandon earned a MS Degree in Electrical Engineering with his thesis “Analytical Model of Particle Motion in Optical Interference Landscapes and Laminar Flow.” Afterward, he continued this research in this general area with both a theoretical and experimental focus.

At the same time, Brandon participated in the Preparing the Professoriate program at NCSU in which he co-taught an undergraduate and graduate course on Soft Electronics, resulting in a slate of novel, hands-on laboratory modules. Throughout his time at NCSU, Brandon served The Science House first as an instructor and later as a curriculum advisor, a role in which he helped develop new photonics teaching laboratories and methods for minority and underrepresented high school students.

The most significant moment of Brandon’s time at NCSU occurred in 2005 when he met and quickly fell in love with Brenda who, at the time, was working in the ECE departmental office. Don’t worry, skeptical reader, she was not Brandon’s supervisor. She didn’t assume that role until August 22, 2009, when she and Brandon were married in the mountains of North Carolina.

Upon graduation, Brandon will continue his career with Bennett Aerospace, a prime contractor for the United States Department of Defense (among other things), located in Cary, NC.
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Chapter 1

Introduction

1.1 Light As a Tool

Many would say a toolbox is incomplete without a sturdy claw hammer. It is a beacon of simplicity among its sister tools. But with it, the skilled craftsman can deftly drive iron nails and wooden pegs to build any manner of conceived structure from the grand palace to the humble bird house. While the claw hammer can be employed for creation on an infinite scale, it may also be exploited for various degrees of destruction—from removing a carefully placed tack in an antique armoire or knocking down the final beam of a home too weathered to stand. As a tool, the claw hammer is perhaps much more than its inventor originally intended. It is an extension of he or she that swings it, and only as good as the skills of its master.

In much the same way, the light that fills our world is both simple and multifaceted. No skills are required to marvel at the warm and illuminating glow of the late summer sunset or the early winter sunrise. However, the trained engineer knows that light may be harnessed as a tool for myriad purposes: magnifying the microscopic world beyond our vision to develop cutting-edge metamaterials and life-saving medicines or for revealing malignant tissues via process that allow treatment to occur in time to increase our own survival. In much the same way, light may also be used for delicate destruction of an ill-advised tattoo or the magnificent
demolition of an in-bound ballistic missile.

1.1.1 Optical Trapping and Optofluidics

Optical trapping and manipulation are possible because light carries energy. In fact, light is energy. Comprising wavelengths shorter than radio waves and microwaves but longer than X-rays and gamma rays, what we call light is one small portion of the electromagnetic spectrum, the whole of which defines the various forms of electromagnetic radiation.

In 1970, Arthur Ashkin and his colleagues were the first pioneers to detect that light interacting with micrometer sized particles resulted in optical scattering and gradient forces [1]. This discovery soon led to the advent of the optical trap [2–4] and, ultimately, to a family of techniques—optofluidics—having only recently achieved important landmark innovations. Optofluidics combines optical tools and techniques with microfluidic environments. Microfluidics will be further discussed in Chapter 2 but it is important to note here that physics at the microscale (in low Reynolds number environments) is quite different from physics in the classical sense. Inertia is effectively non-existent and mixing of fluids is dominated by diffusion [5–7]. This provides an optimal environment for optical micromanipulation.

The novelty of optofluidics, arguably, is in what the techniques enable—interaction of light and particles in a well-controlled microfluidic environment. The fluids provide the crucial element of flexibility in these systems. They may be employed as particle carriers with controllable velocities, they may serve as reagents for a chemical or biological assay, and they may be modified or mixed to adjust the refractive index of the medium locally or throughout the system. Having access to such versatility when engineering a light-particle interaction system is paramount when the particles of interest are less than accommodating (changing the refractive index of a red blood cell, for instance, would likely cause much greater difficulty).
1.1.2 Optical Manipulation In Practice

By properly harnessing and conserving this energy we can move, hold, and otherwise manipulate microscale particles. The first and, perhaps, simplest method is the optical trap: a single beam of tightly focused light resulting in three-dimensional capture of microscopic particles [2]. The trapping of smaller particles—atoms [8]—resulted in a Nobel Prize in Physics for Stephen Chu, Claude Cohen-Tannoudji, and William D. Phillips while the trapping and manipulation of biological particles has increased our understanding of their mechanisms [9–12].

Biology has continued to benefit from optical trapping, notably in terms of cell sorting. With a periodic optical intensity pattern, also called an optical landscape, interacting with particles in a microfluidic flow, MacDonald, Spalding, and Dholakia [13] and Grier [14, 15] have shown experimentally that cells can be sorted using their own intrinsic properties such as size and refractive index. This non-contact and minimal-damage technique of particle control has revolutionized colloidal sorting, offering an effective alternative to more invasive options such as fluorescence activated systems [16].

The ability to selectively trap, sort, mix, align, and order nano- and micro-scale particles using optical trapping techniques has become progressively more enhanced in recent years. Examples are readily found for in vitro control of DNA [9], molecular motors [15], nanowire manipulation and alignment [17], and even integration of all elements needed for a complete system on a single, miniaturized platform commonly called “lab-on-a-chip”, to which an entire scholarly journal of the same name is dedicated.

While optofluidics and optical trapping techniques are relatively new as research fields go, experimental examples of the utility and potential of the many application areas are already ubiquitous—research groups around the world are built around optofluidic principles and entire scholarly journals and textbooks are dedicated to publishing and explaining the latest findings. Furthermore, companies are finding success providing the infrastructure necessary for building complete systems (e.g., Advanced Liquid Logic) and various sizes, shapes, and functions of particles to be interrogated within such systems (e.g., Liquidia, Bangs Lab-
oratories). Collaborative efforts are leading to new methods of biotheraputics, vaccines, and chemical sensors to name but a few. The future—and the present—of optofluidics and optical manipulation is quite bright.

1.2 Dissertation Approach and Research Contributions

Without diminishing the importance of the current state of optofluidics and the research conducted to date, this dissertation reports the following overarching contribution: quantification of the microfluidic response of spheroidal particles in periodic optical interference landscapes. We note that while optofluidics concerns the interaction of light and realistically shaped and structured particles (blood cells, proteins, etc.) on the microscale, no satisfactory analytical model exists that completely describes the phenomena and unique features of such realistic particles within optical landscapes. We submit that quantifying the response spheroidal particles in optical landscapes is a major step forward in achieving a complete and accurate analytical model.

To clarify our discussion of spheroidal particles, Fig. 1.1 illustrates the three types of spheroids, defined by their aspect ratio, \( AR \). The \( AR \) relates the major axis to the minor axes \( (a_1 : a_2) \) of a given particle. Aspect ratios of 1 represent spheres, whereas aspect ratios less than and greater than 1 are oblate and prolate particles, respectively. Within the scope of this dissertation, we are primarily concerned with sphere and true spheroids, i.e., those particles with equivalent minor axes and a dissimilar major axis.

Within our work, several discoveries have been made and contributions to the field of engineering research have been established. Chapter 2 begins this effort by providing background to the various scientific concepts and principles underlying the overall effort. Throughout this chapter, context is provided by means of the literature—pioneering and pivotal. The interaction of light with material is the pervasive and foundational layer of this dissertation as a whole and space is given to examining relevant physics and capabilities of light and light handling including polarizability, interference, optical traps, and optical landscapes. Because
the systems of interest are optofluidic, an overview of microfluidic principles, including laminar flow, the Reynolds number, and Brownian motion, is appropriate and provided. Finally, we provide an overview of the work reported over the last several decades and the current application spaces of optical manipulation.

Chapter 3 addresses the following question: Does the shape of microscale particles have an appreciable and quantifiable impact on their motion within a spatially periodic optical potential? Others have shown that size, refractive index, and other intrinsic particle properties determine a particle’s motion [18]. We submit that shape cannot be neglected. To address our question, we have constructed an analytical model of particle-light interaction within spatially periodic optical potential energy landscapes, also known as optical landscapes. Chapter 3 is presented in a pre-print form of a manuscript intended for publication in Physical Review E. The findings presented therein positively answer our question in that particle shape does matter and, in fact, that the aspect ratio of a particle is exponentially related to the optical force it experiences within an optical landscape and a laminar, microfluidic flow.

The motion of spheroids in these environments is determined by two hydrodynamic balance equations: the force balance equation which defines the trajectory and the torque balance equation which defines the orientation. Chapter 3 provides the mathematical formulation and results of our model based on these equations, each of which depends on a particle’s form factor—-a representation of the interaction between material and light based on refractive index, polarizability, shape, and size. We assert that our analysis is a major step forward in quantify-
Chapter 4 addresses the following questions: (1) Is it reasonable to assume that the scattering forces imposed on both spherical and non-spherical particles by an optical landscape can be neglected? (2) Under what conditions does the torque produced by the optical gradient force on prolate and oblate particles overwhelm the torque caused by the electric field? We have asked these questions because the form factor approach of Chapter 3 may not adequately address particles whose size is nearly equivalent to the period optical landscape or those particles heavily impacted by scattering forces. In these cases, it is likely that the scattering of the electric field and its polarization are significant. To address these special case, we have developed a T-Matrix scattering model based on the linear scattering of the electric fields at the surfaces of the particles.

Chapter 4 is presented in a pre-print form of a manuscript intended for publication in Applied Optics. The contributions gleaned from this model include a quantification of the significance of the scattering and polarization effects brought about by an optical landscape on spheroidal particles.

The T-Matrix method is employed to calculate the amplitude scattering matrix in the far-field which, as the literature shows [19], has numerous applications. We employ the method to transform the incoming electric fields (incident plane waves) into outgoing electric fields (scattered spherical waves). The Maxwell stress tensor (MST) is then used to find the optically-induced gradient forces, the scattering forces, and the torque on the particle. Chapter 4 will provide the development and results of our T-Matrix Scattering model. As was the case for the form factor model, we aim for the T-Matrix model to be one more tool available to the optofluidic system designer for analysis of techniques including optical fractionation, nanoscale assembly, and organic matter stress response to name a few.

Chapter 5 aims to support the two modeling efforts of the previous chapters by providing experimental pathways. Three questions are posed: (1) Can we experimentally implement a periodic optical landscape and microfluidic system that reasonably approximates the ideal periodic landscape assumed in Chapters 3 and 4? (2) Can this apparatus be shown to effectively lock-in or organize
microscale particles within an optical landscape and a stationary microfluid? (3) Can close approximations of microscale spheroidal particles be designed and fabricated via photolithographic means and then also controlled with the apparatus? To our knowledge, no such optical trapping / optical landscape apparatus has been reported that relies solely on interference of coherent beams of light and a low-NA objective to create the landscapes. As Chapter 5 will address we can create and, therefore, contribute a viable and effective optical manipulation apparatus and will demonstrate its utility.

Several other fabricated and experimental methods exist for fractionating and manipulating various types of microparticles but these rely on spatial light modulators or high-NA objectives, among other techniques, to produce similar results. This work confirms, albeit on a preliminary level, the possibility of constructing an operational optical fractionation system based on optical interference techniques and provides a pathway for connecting model predictions to experimental results. We have also determined and employed a method for fabricating spheroidal particles—particles not readily available on the open market—and will provide our detailed approach in Chapter 5.

Chapter 6 takes a turn toward the broader focus of the Ph.D. program, preparing scientists for a role in teaching and in research. We pose the following question: Can a hands-on teaching laboratory on organic electronics and liquid crystal displays be developed that effectively teaches their operational principles, fundamentals, and practical aspects of fabrication, within a reasonable budget and broadly accessible way? To address this question, we have developed four laboratory teaching modules offering hands-on experience with organic semiconductor devices and liquid crystal display technologies, i.e. Soft Electronics: a liquid crystal display (LCD) pixel, an organic light-emitting diode (OLED), an organic photovoltaic (OPV) solar cell, and an organic thin-film transistor (OTFT). Building upon traditional semiconductor device and optics education, these hands-on lab activities address concepts central to Soft Electronics.

This slate of lab activities is the first of its kind to provide students with the knowledge and materials to build and evaluate LCD pixels, OLEDs, OPVs, and OTFTs all within a semester-
long undergraduate/graduate course. Based on the positive feedback from students and the success of the laboratory modules, we definitively answer Yes, such a laboratory-based course can be created and offers a worthwhile educational opportunity and constitutes a significant contribution to the educational community. Chapter 6 is a pre-print form of a manuscript intended for The American Journal of Physics. The work reported is additionally intended to display the level of professorial preparation provided by the NCSU Ph.D. experience.

Finally, Chapter 7 aims to tie the contributions of this dissertation together and to present the reader with a clear message regarding the novelty of our work. In addition, some of the challenges faced in arriving at our conclusions will be provided. Chapter 7 will provide some detail as to where additional research efforts would be best focused.
1.3 Related Publications

The work contained in this dissertation has been peer-reviewed and presented at 7 professional conferences and is in preparation for 3 journal submissions:


Chapter 2

Background

2.1 Light and Materials: A Primer

We will begin our background discussion by briefly exploring the physics of light and matter interactions as they pertain to this dissertation. What follows in this section will be an overview of Maxwell’s equations, a description of dielectric polarizability, and an introduction to electromagnetic interference.

2.1.1 An Analytical Description Of Light: Maxwell’s Equations

As Chapters 3 and 4 will develop two separate analytical models for particle behavior in optical fields, a discussion of time-dependent electromagnetic fields and their behavior is warranted. We must begin with Maxwell’s equations. Credit is due to James Clerk Maxwell for realizing that the independent nature of electric and magnetic phenomena disappear when in a time-dependent regime (e.g., Ampère’s law, $\nabla \cdot J = 0$, is incorrect except for steady-state currents) [20].
As a set, Maxwell’s equations in SI units and differential form are:

\[
\begin{align*}
\nabla \cdot D &= \rho \quad &\text{(2.1a)} \\
\nabla \times E &= -\frac{\partial B}{\partial t} \quad &\text{(2.1b)} \\
\nabla \cdot B &= 0 \quad &\text{(2.1c)} \\
\nabla \times H &= J + \frac{\partial D}{\partial t}, \quad &\text{(2.1d)}
\end{align*}
\]

where all five vector quantities are implicitly assumed to have a time-dependence, unless otherwise noted. Electrical quantities are represented as \( E \) (electric field, \( V/m \)), \( D \) (electric displacement, \( W/m^2 \)), \( J \) (electric current density, \( A/m^2 \)), and \( \rho \) (electric charge density, \( A/m^2 \)). Magnetic quantities consist of \( H \) (magnetic field, \( A/m \)) and \( B \) (magnetic induction, \( C/m^3 \)).

The quantities here, as well as in the remainder of this work, in bold notation are vectors.

It will benefit us to relate \( E \) and \( B \), the electric and magnetic field quantities, to \( D \) and \( H \), the corresponding derived fields, via the polarization \( P \) and the magnetization \( M \) of the material medium. Assuming vacuum conditions, we write these relations as

\[
\begin{align*}
D &= \varepsilon_0 E + P \\
H &= \frac{1}{\mu_0} B - M,
\end{align*}
\]

where \( \varepsilon_0 \) is the electric permittivity and \( \mu_0 \) is the magnetic permeability. Ohm’s law may be used to find \( J \),

\[
J = \sigma[r]E,
\]

where \( \sigma \) is the conductivity of the material. Concerning our dielectric particles of interest, we can neglect any magnetization (allowing \( \mu \) to be always equal to \( \mu_0 \)) and assume a source-free space, i.e., \( \sigma \) and \( \rho \) are zero. However, concerning dielectric particles, vacuum conditions cannot be assumed, and particle permittivities must be considered. As a result, Maxwell’s
equations can now be written as [20]:

\[
\begin{align*}
\nabla \cdot E &= \frac{\rho}{\varepsilon} = 0 \quad (2.5a) \\
\nabla \times E &= -\mu \frac{\partial H}{\partial t} \quad (2.5b) \\
\nabla \cdot H &= 0 \quad (2.5c) \\
\nabla \times H &= \varepsilon \frac{\partial E}{\partial t}. \quad (2.5d)
\end{align*}
\]

We may now write the electromagnetic wave equation. Using Eqs. (2.5b) and (2.5d) to eliminate \( H \), we find

\[
\nabla^2 \times E = -\frac{1}{\nu^2} \frac{\partial^2 E[r, t]}{\partial^2 t},
\]

where \( \nu = (\mu \varepsilon)^{-1/2} \), the speed of light in this system. We note that the speed of light in a vacuum is

\[
c = (\mu_0 \varepsilon_0)^{-1/2} = 2.998 \times 10^8 \text{ m/s}, \quad (2.7)
\]

and that the index of refraction of the dielectric particle is

\[
n_p = \left( \frac{\varepsilon}{\varepsilon_0} \right)^{1/2}. \quad (2.8)
\]

If we assume a source-free space and an isotropic material such that \( \varepsilon \) is the same for all field vectors, then the dispersion relation is \( k \cdot r = \omega/\nu \) and the Helmholtz equation may be written as:

\[
\nabla^2 E[r] + k^2 E[r] = 0,
\]

where \( k^2 \) is the wavenumber, equal to \((\omega/\nu)^2\), and \( \omega \) is the angular frequency. We may find similar expressions for \( H \).
2.1.2 Polarizability Of Dielectric Particles

Now that we have outlined the physics of electromagnetic fields, we will now summarize how matter responds to a surrounding electromagnetic field. The particles and microfluids we discuss in this dissertation are assumed to be lossless dielectrics with linear and isotropic permittivities. Dielectrics differ from conductors in that a steady current cannot flow in them and in that the external field will penetrate to their interior [21]. As such, dielectric particles respond differently than conductors when in the presence of an electromagnetic field. This response is termed the “dielectric polarization”, or “polarization” of the particle, denoted as $P$, first defined in Eq. (2.2). Any dielectric in which $P$ is not zero is said to be polarized. We pay special attention to the polarization relation, Eq. (2.2), in this section while neglecting the magnetization relation, Eq. (2.3), because we are using nonmagnetic materials. This will also be an assumption of our models in Chapters 3 and 4.

The polarization produced within a dielectric is due to bound molecular charge. As these charges experience the applied field, they execute perturbed motions, thus distorting the molecular charge density. Therefore, multipole moments in each molecule are altered from their unperturbed state, the dominant moment being the dipole [20]. These responses are illustrated in Fig. 2.1, where a dielectric and its component molecules is shown in the absence of an electric field, (a), and again in a uniform electric field, (b). Note how the molecules align themselves with the electric field, thus polarizing the entire particle. Therefore, it is the sum of the dipole responses that comprises the electric polarization. The polarization may now be referred to as the dipole moment per unit volume [20].

Let us look again at Eq. (2.2) and suppose the medium is isotropic. The induced polarization, $P$, is now parallel to $E$ with a coefficient independent of direction,

$$P = \varepsilon_0 \chi_e E,$$  \hspace{1cm} (2.10)

where $\chi_e$ is the electric susceptibility of the medium. Solving Laplace’s equation considering
the boundary conditions of an electric field crossing a dielectric particle in which the susceptibility takes a discontinuous jump, we find that the polarization of the particle is

\[ P = (\epsilon_p - \epsilon_m) E_{int} \]  \hspace{1cm} (2.11)

where \( \epsilon_p \) is the dielectric constant of the particle, \( \epsilon_m \) is the dielectric constant of the surrounding medium, and \( E_{int} \) is the field inside the particle,

\[ E_{int} = \frac{3\epsilon_m}{\epsilon_p + 2\epsilon_m} E_m. \]  \hspace{1cm} (2.12)

Using the real part of the Claussius-Mossotti factor, \( K^* \equiv (\epsilon_p^* - \epsilon_m^*) / (\epsilon_p^* + 2\epsilon_m^*) \), we can rewrite the polarization as

\[ P = 3\epsilon_m \Re\{ K^* \} E_m. \]  \hspace{1cm} (2.13)

The polarizability of a dipole may be referred to as the coefficient of the polarization in this form. Using a spherical dielectric \[22\] then allows us to write the polarizability of the matter-light interaction as

\[ \alpha = n_m^2 a^3 \left( \frac{m^2 - 1}{m^2 + 2} \right), \]  \hspace{1cm} (2.14)

in which the radius of the sphere is \( a \), the index of refraction of the surrounding medium.
is $n_m$, and $m = n_p/n_m$. We can now have some analytical insight into how non-spherical particles may respond in electromagnetic fields such as those that will be described later. If a uniform field is applied to a non-spherical particle as in Fig. 2.2, the induced dipoles will attempt align themselves with the field as for the spherical case. However, if the particle is not in an initial equilibrium alignment with the field, not all dipoles will find their optimum alignment simultaneously. This has the effect of causing a rotation of the particle into an equilibrium condition such that the dipoles experience maximum field line interaction.

2.1.3 An Introduction To Electromagnetic Interference

Electromagnetic interference is a superposition of two or more electromagnetic waves in which the total electric field intensity at each point is the vector sum of the individual waves. We will now examine certain fundamental principles of energy and momentum leading to an analytic description of interference.

The potential energy density of an electromagnetic wave can be written as

$$u[t] = u_E[t] + u_B[t], \quad (2.15)$$
where \( u_E[t] \) and \( u_B[t] \) are the energy densities of the time-varying electric and magnetic field components defined as

\[
\begin{align*}
    u_E[t] &= \frac{\varepsilon_0}{2} E^2[t] = \frac{1}{2} (E \cdot D) \\
    u_B[t] &= \frac{1}{2\mu_0} B^2[t] = \frac{1}{2} (B \cdot H),
\end{align*}
\]

(2.16) (2.17)

where \( E[t] \) and \( B[t] \) are the magnitudes of the electric and magnetic fields, respectively.

The instantaneous transport of this energy per unit time (power) across a unit area will have units of \( W/m^2 \) and will flow in the direction of the propagating wave. This vector, then, is

\[ S = c^2\varepsilon_0 E \times B = E \times H, \]

(2.18)

termed the Poynting vector.

The electric field itself varies in time at a rate too high for practical detection (\( \sim 10^{14} \) Hz). The irradiance—the average energy per unit area per unit time, or alternatively, the amount of light illuminating a surface [24]—however, is easily measured with sensors such as photodetectors. To measure the irradiance, the time-average of the Poynting vector magnitude, \( \langle |S| \rangle_T \), must be taken, resulting in

\[ I = \langle |S| \rangle_T = \frac{c\varepsilon_0}{2} E^2, \]

(2.19)

where \( E \) is the amplitude of the electric field vector wave.

Interference results whenever two or more coherent electromagnetic waves are superimposed, and generally produces a spatially-periodic irradiance profile (akin to a standing wave) [24]. The total electric field of \( N \) waves is

\[ E_{\text{TOT}} = E_1 + E_2 + \cdots + E_N, \]

(2.20)
where

\[ E_m[r] = A_m \exp(ik_m \cdot r) \]  \hspace{1cm} (2.21)

are the complex amplitudes of the \( m^{th} \) plane waves that vary in space, whereas the amplitude-polarization vectors \( A_m \) can be complex-valued constants. The wave vector has a magnitude \( k = |k| = 2\pi/\lambda \). The total electric field, on the other hand, is a real-valued vector that varies in time and space, more specifically written as

\[
E_{\text{TOT}}[r, t] = \Re \{ E[r] \exp(-i\omega t) \} \\
= \frac{1}{2} \sum_{m=1}^{N} \{ E_m[r] \exp(-i\omega t) + E^*_m[r] \exp(i\omega t) \},
\]  \hspace{1cm} (2.22)

where the notation \( E^* \) refers to the complex conjugate of the vector. The time-average of the electric field, a sinusoidal function of time, is

\[
\langle E^2_{\text{TOT}}[r, t] \rangle_T = \frac{1}{2} E[r] \cdot E^*[r],
\]  \hspace{1cm} (2.23)

and the total irradiance may now be ascertained \[25\]

\[
I[r] = \epsilon_p \frac{c}{n_p} \langle E_{\text{TOT}}[r, t] \rangle_T \\
= \frac{n_p}{2\sqrt{\mu_0 \varepsilon_0}} E[r] \cdot E^*[r] \\
= \frac{n_p}{2\sqrt{\mu_0 \varepsilon_0}} \sum_{l=1}^{N} \sum_{m=1}^{N} A_l \cdot A^*_m \exp \left( i \left( k_l - k_m \right) \cdot r \right).
\]  \hspace{1cm} (2.24)

Interference of two beams \((N = 2)\) may be written as follows, with \( k_1 - k_2 \) as the grating vector,

\[
I[r]_{N=2} \propto A_1^2 + A_2^2 + 2A_1 \cdot A^*_2 \cos \left( k_1 - k_2 \right) \cdot r.
\]  \hspace{1cm} (2.25)

Neglecting phase factors and selecting \( k_1 \) and \( k_2 \) such that they are symmetric about the Z-
where $\phi$ is the half-angle between the two beams. It is important to note that for intensity interference to occur, the polarization of the beams must not be orthogonal. The bright regions will be brightest when the two beams lie along the same axis. The period of interference $\Lambda$ is found via Bragg's Law,

$$\Lambda = \frac{\lambda}{2 \sin \phi}. \quad (2.28)$$

Fig. 2.3(a) illustrates the geometry of the XY plane including the wave vectors and in Fig. 2.3(b) is the resultant one-dimensional interference pattern of bright and dark fringes. When one or more coherent beams interfere in a specifically-defined arrangement in photosensitive material, well-ordered two-dimensional surface patterns and three-dimensional volumetric patterns can result [26]. While the formation of all Bravais lattices via this technique is particularly important for the fabrication of photonic crystals, our interest is in the optical forces and torques that may be harnessed from these patterns.
2.2 An Introduction To Microfluidics

Any particle traveling through a viscous medium is acted upon by at least two forces, a driving force propelling it and a hydrodynamic drag force resisting it. As we will report in Chapter 3, the drag force is highly dependent upon the shape of the particle. To determine the drag force, we must know the boundary conditions of the environment. Once this is known, we can determine the balance of all forces present which reveals the motion of the particle. Unfortunately, this can become a challenging task—one faced by many in the world of microfluidics.

In terms of biological applications, devices incorporating microfluidics, such as lab-on-a-chip, offer distinct advantages such as shortened reaction times, smaller required reagent volumes, and portability. Specifically, analytical testing involving amplification of DNA in a microenvironment is beneficial due to lower required sample volumes and rapid temperature cycling [27]. Integrating fluorescence spectroscopy with microchannels allows for a highly efficient and portable system for measuring certain chemical concentrations [28]. Simply shrinking macroscale devices to a smaller size will not produce intuitive results—microscale physics must be understood beforehand.

While the terms flow, fluidics, hydrodynamics, and the like are used extensively when discussing macroscale and microscale fluidics, the physics of microfluidic environments are fundamentally different [6]. In this section we will summarize the important physical aspects of microfluidic environments.

2.2.1 Laminar Flow

The concept of laminar flow is crucial to the assumptions made in this dissertation. It may be described as a condition in which particle velocity within a fluid stream is not a random function of time, in sharp contrast to turbulent flow [29]. Within a microfluidic environment, flow is practically laminar at all times allowing for movement of fluid packets that stay intact and limited mixing between two neighboring streams (except by diffusion) [6].
2.2.2 The Reynolds Number

The Reynolds number, an important parameter in determining flow type, is a dimensionless ratio of the inertial forces to the viscous forces [5] and may be calculated by

$$R\# = \frac{s \cdot \nu / t + \nu^2 / d_h}{\eta \nu / d_h^2},$$

(2.29)

where $s$ is the fluid density, $\nu$ is the characteristic fluid velocity, $d_h$ is the hydraulic diameter over which changes in the fluid velocity occur, and $\eta$ is the fluid viscosity. The time, $t$, is a measure of how long the velocity vector of the fluid flow changes appreciably in amplitude or direction. Because $t \times \nu \sim d_h$, we may write the Reynolds number as

$$R\# = \frac{s \nu d_h}{\eta}.$$  

(2.30)

A laminar flow is characterized by $R\# < 2300$ and as turbulent when $R\# > 2300$ [6].

The low Reynolds number regime is generally entered when the bounding channel size of the fluid is below 100 $\mu m$ and fluid velocity is on the order of $1 - 100 \mu m/s$ [27]. It is here that $R\# \sim 1$ and the physics of the microscale become crucial: viscous forces dominate.
 inertial forces, turbulence is nonexistent, diffusion is necessary for mixing, and evaporation acts quickly on exposed liquid surfaces. The flow is dominated by the pressure in the channel assuming $v = 0$ at the walls. Although flow profiles are not a primary focus of this dissertation, it is important to be clear regarding the boundary conditions. We assume, as is customary and established [30], that there is no flow at the surface of a particle within the fluid. Such is termed “no-slip” boundary conditions.

2.2.3 Brownian Motion

The size of particles of interest in this dissertation range from just under a micrometer to hundreds of micrometers. In this range, particle Brownian motion caused by the thermal agitation of the solvent molecules can become significant. Brownian motion is a diffusive process with a diffusion coefficient written as $kT / \xi$, where $k$ is the Boltzmann constant, $T$ is the absolute temperature, and $\xi$ is the particle mobility. This leads to the diffusion coefficient of a sphere:

$$D = \frac{kT}{6 \pi \eta a}, \quad (2.31)$$

where $\eta$ is the viscosity of the suspending fluid and $a$ is the sphere’s radius.

Brownian motion is responsible for the near-constant flux of particles moving from a region of high concentration to a region of lower concentration in a fluid. This motion can be modeled by using stochastic differential equations known as Langevin equations [31]. For this dissertation, however, we make the following important assumption within our models: Brownian motion (and other stochastic forces) will time average to zero and we can neglect to consider it when determining particle motion.

2.3 The Design and Physics Of Optical Trapping

As we discussed in the introduction, the pioneering efforts in optical trapping were reported in the 1970s and 1980s by Arthur Ashkin [1–4]. The “levitation trap” was first [1] and was
soon followed by atom traps [8] and many other optical trapping techniques [9–12]. In this section, we will provide a brief description of the single optical trap, followed by an overview of recent work done in the field of optical manipulation.

2.3.1 The Single Optical Trap

In 1986, the seminal paper on “optical tweezers” was published [2] followed closely by works in which optical tweezers were used to manipulate biological particles [32,33]. Optical tweezers employ a strongly focused beam such that the axial gradient force is large enough to dominate the radiation pressure forces. Such occurs when the beam rapidly diverges from the focal point [15]. To achieve this, constructions often employ microscope objective lenses with high numerical apertures (N.A.) and corrected aberrations. If a sharp gradient does exist, the gradient force arises in the direction of the field gradient by means of a dipole moment within the particle, induced by the inhomogeneous electric field [22].

Ray optics can be used to describe the light scattering and momentum transfer associated with the particle being trapped. The electromagnetic energy stored in the fields scattered and absorbed by the object is minimized [14]. In Fig. 2.5, two rays of a highly focused beam are shown incident on a dielectric sphere. The sphere is assumed to be lossless and on the order of $10 \mu$m in size. A pair of rays, A and B, is incident on the particle about its center. The major momentum transfer from light to particle occurs due to multiple surface refractions, resulting in net trapping forces $F_A$ and $F_B$ directed down the beam axis toward the focus.

Three particle regimes exist: the subwavelength-scale Rayleigh regime where particle radius, $a$, is much smaller than the trapping laser wavelength, $\lambda$; the Mie regime, in which $a \gg \lambda$; and, albeit unfortunate for microscale particles such as polymers and mammalian cells, the regime in which $a$ is comparable to $\lambda$. The first two have been addressed several times within the literature as limiting cases for trapping force derivations owing to the simplicity of such.

In the Rayleigh regime, optical forces may be calculated by treating the trapped particle as
Figure 2.5: Spherical particle in a single optical trap.
a point dipole [22]. For a sphere of radius \(a\), the scattering force is

\[
F_{\text{scat}} = \frac{I_0 \sigma n_m}{c},
\]

(2.32)

where \(\sigma\), the scattering cross section of the sphere, is given by

\[
\sigma = \frac{128 \pi^5 a^6}{3 \lambda^4} \left( \frac{m^2 - 1}{m^2 + 2} \right)^2.
\]

(2.33)

The scattering force is in the incident light’s propagation direction and proportional to its intensity. The gradient force of the trap is

\[
F_{\text{grad}} = \frac{2 \pi \alpha c n_m^2}{m^2} \nabla I,
\]

(2.34)

where \(I\) is a given intensity profile and \(\alpha\), the polarizability of the sphere, is given in Eq. (3.3). It is important to notice here that the gradient force is proportional to the laser intensity gradient and the polarizability. Therefore, this force will increase as the focusing of the beam becomes tighter and/or as the particle radius increases. In addition, the gradient force points up the gradient when the particle index is greater than that of the medium \((m > 1)\) and points down the gradient when the reverse is true \((m < 1)\). For stable trapping to occur, \(F_{\text{grad}}\) must be greater than \(F_{\text{scat}}\).

When the particle’s radius is on the order of the trapping light’s wavelength \((a \sim \lambda)\), the previously described method is not applicable. Typically, electromagnetic theory from first principles must be applied, requiring more difficult derivations. This becomes a greater problem when we note that this limit \((0.1 \lambda - 10 \lambda)\) encompasses most particles useful for trapping including dielectric spheres used as manipulation handles and biological objects such as cells and bacteria [22]. The calculation of light scattering by particles—especially those devoid of symmetry—on the order of the wavelength may be done via the \(T\)-matrix method [34]. Using conservation laws, the incoming and outgoing fields may then be used to determine
forces, scattering matrices, momentum transfers, etc. Several methods involving a complete solution of Maxwell’s equations in order to find the net radiation force have been derived, including: describing the electromagnetic field of the incident beam using the complex-source-point method [35], using infinite surface integrals to determine the coefficients of the incident beam [36], and using finite surface integrals in order to describe an arbitrary incident beam [37].

It is most instructive now to discuss the series-form theoretical expressions for the net radiation force and torque for a specific spherical particle in an arbitrary beam as described in [38]. We will consider a particle in the size range of 1 to 10 \( \mu m \), a TEM\(_{00} \)-mode laser of beam waist \( \sim \) particle size and of wavelength \( \prec \) particle size. It is also important to note that our particles are homogeneous, dielectric spheres illuminated by a monochromatic electromagnetic beam.

Neglecting time dependence and assuming a steady-state, time-averaged condition, the net radiation force is

\[
F_{\text{rad}} = \oint \hat{n} \cdot \mathbf{T} dA,
\]

where the Maxwell stress tensor (MST) in vector form is best given by the Minkowski form in the case of steady-state optical conditions,

\[
\mathbf{T} = \epsilon \left( \mathbf{E} \cdot \mathbf{E}^* - \frac{1}{2} \mathbf{E}^2 \right) + \mu \left( \mathbf{H} \cdot \mathbf{H}^* - \frac{1}{2} \mathbf{H}^2 \right).
\]

\( \mathbf{T} \) (T) The net radiation torque is also found using the Maxwell stress tensor in vector format,

\[
\mathbf{M}_{\text{rad}} = -\oint \hat{n} \cdot (\mathbf{T} \times \mathbf{r}) dA.
\]

Solving these equations reveals a proportionality between the trapping force or torque and the power, i.e., increasing the power increases both the force and torque. Additional means of altering these parameters will be discussed within the context of our models to follow in Chapters 3 and 4.
2.3.2 Applications and Other Forms Of Optical Manipulation

The integration of microfluidics and optical manipulation methods results a field known as optofluidics. Such systems may employ light to move particles, hold particles, or probe particles. Whatever the application, optofluidic devices are quite prevalent and very customizable [39]. In this section, we review some of the applications of optical manipulation within the quickly-growing field of optofluidics.

One Beam, Many Traps

As discussed in Sec. 2.3.1, a strongly converging objective lens may be used to focus a laser beam, forming a trap at the focal plane. A diverging beam will focus downstream of the focal plane and a converging beam will focus upstream [15]. This single beam may then be translated, thus translating the trap. This process is easier when the objective input angle of the beam may be altered as illustrated in Fig. 2.6(a). With this system, tilting the mirror will sweep the trap along a plane within the sample stage. This allows for arrangements of multiple particles by pausing at each during the sweep.

![Figure 2.6: Creation of multiple trapping sites by: (a) mirror rotation, (b) beam diffraction via diffractive optical element(s).](image)
Optical manipulation goes well beyond the single trap. While manipulation of a particle in a single trap is a highly useful technique, combining several traps into a single system enables massively parallel operations, multi-dimensional traps, and highly ordered systems of particles—even with a single laser.

By introducing a diffraction grating or similar diffractive optical element (DOE) in the optical path prior to the objective lens, multiple trapping sites can be created simultaneously. As illustrated in Fig. 2.6(b), the angles of the beams output from the DOE are predictable making the array of trapping sites predictable as well. In this system, there is no need to move the mirror as the DOE controls all angles of beam travel. If a computer-generated hologram is used in place of the DOE, a specific and often more intricate pattern of trapping sites is created at the sample stage. Such a system is termed holographic optical tweezers (HOTs) [15]. HOTs are created by a computer program, can be implemented within liquid crystal displays (LCDs), allow for multiple trapping sites in multiple dimensions [40], and can be used for particle sorting [41]. A holographically-generated optical vortex, for example, may be used to trap low index particles [42].

Using an addressable liquid crystal spatial light modulator (SLM) in conjunction with three independent beams can further extend the abilities of HOTs. Such implementations are termed dynamic HOTs and are often able to be altered on-the-fly by an integrated computer program, limited only by the characteristics of the SLM (such as pixel size) and the time required to compute the hologram [22].

**Multiple Beams, Optical Landscapes**

We began our work in optical manipulation around the time that the Grier group described periodic, optical interference formed, potential energy patterns as optical landscapes [18, 43]. Such are usually created and defined via the interference of two or more coherent beams of light. Within this dissertation, the term *optical landscape* will refer to those periodic potential energy patterns defined exclusively via the interference of two or more coherent beams of light.
Our interest in a particle manipulation sense arises because large gradients exist within these landscapes and can be defined to impart specific translational—and in our case rotational—forces upon micro and nanoparticles.

The Grier group used a mathematical model to predict how spherical particles will behave in certain optical landscapes. Perhaps most importantly, they find that within a non-inertial fluid flow, particles can become “locked in” the landscape (i.e., trapped) based on optical parameters and particle size [18].

One of myriad advantages of using such a method is the highly predictable and controllable responses of the particles within the landscapes. By merely adjusting input power, flow velocity, or optical beam interference angle, to name a few, one can define which particles will be locked in and driven in a new direction and which will flow unaffected by the optical forces. Other researchers and modelers have also investigated particle behavior in periodic optical potential energy patterns as we discuss in the next section.

**Analytical Treatments**

Aside from the Grier group’s model for spherical motion in an optical landscape [18], other researchers have also developed models for describing particle behavior. Using a piecewise linear model, the motion of spheres has been described in multi-dimensional landscapes [44] while using a model balancing force and drag, the motion of red blood cells in an interference field has been described [12]. However, none of these models to date considers truly spheroidal particles and the inherent torque they experience in an optical landscape.

**Applications**

Optical manipulation may be implemented for a variety of applications and interrogations from sorting a heterogeneous mixture of particles to quantifying the optical forces and torques to massively parallel ordering of objects—similar or dissimilar. We highlight some of these many applications here,
• Particle Sorting

Various non-contact manipulation and sorting schemes exist. Sorting of colloidal microspheres on the order of 1.1 $\mu m$ to 3.2 $\mu m$ has been shown using line optical tweezers. The particles are driven past the tweezers by electrophoresis where larger particles are trapped because of the size difference [45]. The idea of sorting particles based on shape arises in [46]. The authors apply rigorous diffraction theory to the analysis of the optical force exerted by highly focused laser beams on elliptical nano and microcylinders. Most interestingly, they find a shape dependent response of such particles to the optical fields. Dielectrophoretic methods are also valuable and provide a fine comparison to purely optical sorting [47,48]. In fact, so many groups have been investigating particle sorting that whole reviews have been published on the various methods available for sorting [49,50] and general manipulation techniques [51].

• Particle Assembly

HOTs have been used in conjunction with SLMs for manipulation and assembly of semiconductor nanowires into two- and three-dimensional structures, facilitating the creation of larger systems [17]. Rotation of these objects has also been demonstrated, albeit by simply rotating the holographic plate. Three-dimensional arrangements of spheres and organic particles have been arranged in gelatin by means of HOTs [52]. This approach stalls the particles in their holographically-defined structure after the laser is switched off, allowing for study of inter-cellular proximity in cell differentiation.

• Biological Treatments

Other biological applications include in vitro control of DNA, molecular motors, and various other molecules. Typically, a spherical bead attached to the object in question is used as a handle controlled by the optical trap [53]. Other experiments include recording light scattering diagrams from single living cells within an optical trap in order to determine how cellular orientation exerts influence within the trap—an important step
in improving flow cytometry [54]. Cellular sorting has been shown effective within discrete optical traps [55], the motion of red blood cells within optical interference has been investigated [12], and several devices have been constructed that show the potential for biological particle sorting [49].
Chapter 3

A Form Factor Model Of Spheroidal Behavior Within Optical Landscapes

This chapter contains a preprint manuscript of work intended for publication in Physical Review E in the near future. Portions of this work have been presented at 4 individual professional conferences and the foundation was presented in the author’s Masters Thesis (see Sec. 1.3).

3.1 Abstract

Once optical trapping became an indispensable tool for mesoscale research, several works displaying and describing the abilities and nuances of the field entered publication. Colloidal particles of several shapes and sizes can now be selectively trapped, sorted and mixed within microfluidic systems under the influence of high-intensity optical fields. Few of these works, however, consider non-spherical particles and still fewer consider modeling and predicting particle behavior in the optical fields. In this vein, we have developed an order of magnitude model for the complete motion of optically-controlled spheroidal microparticles in a laminar flow. Our model conclusively shows that a particle’s shape has an exponential relationship to
its behavior and should be considered. In this work, we thoroughly develop our model and investigate its ability to predict particle behavior in periodic optical interference landscapes.

3.2 Introduction and Motivation

The advent of optical tweezers as a tool to selectively trap, sort, mix, align, and order mesoscale particles has ushered in a period of scientific advancement whose ultimate potential and impact has yet to be completely understood—especially on the analytical front. Several experimental examples, however, have been shown in recent decades [15, 49, 50, 56, 57]. Various means of affecting particles with dynamic control include holographic optical trapping [14, 58], optical interference landscapes [18, 43], optical conveyor belts [59], and multi-dimensional optical lattices [60]. These and similar methods provide the user reconfiguration and project-specific tailoring at a fraction of the time and cost as manipulation systems employing arrays of micro-machined obstacles [61] or even those using particle fluorescence for sorting [62]. Understanding of the physics that underlies particle motion in these systems and efforts at physical modeling are steadily advancing but must be carefully developed before optical trapping and manipulation is to reach wide applicability.

Many of the particles employed in optofluidic manipulation have shapes substantially similar to disks and rods (e.g., blood cells, nanowires), much of the theoretical work to date [18, 44, 63–65] focuses on spheres, ignoring ellipsoids in general. Notable rare exceptions include those that have explored the optical torques transferred to ellipsoids within gaussian intensity fields [66, 67] and those that have investigated non-spherical particle rotation due to inertial effects [68, 69].

In this work, analyze the influence of particle shape within periodic optical landscapes. We develop an order-of-magnitude description of the translation and rotation of generalized spheroidal particles within a microfluidic environment subject to intense optical fields. We show that the bright fringes and spots of interference landscapes give rise to highly selective trapping and influence of particles based on shape, size, and composition. Our findings differ
somewhat with previous theory [18], which can be attributed to our treatment of optically-induced force and the translational drag tensor. Additionally, as previously theorized [70] and demonstrated [71], we show that spheroidal particles will align in a lowest energy configuration when influenced by optical fields—a response dependent upon particle shape.

3.3 Hydrodynamics of Spheroids

3.3.1 Force and Torque Balance Equations

The force balance equation is derived from the Langevin equation of particle motion, previously solved in one-dimension considering stochastic processes [72] and in two-dimensions considering optical landscapes [18]. Similarly, the torque balance equation may be derived from first principles. By neglecting inertial effects (valid for laminar flows), we write the balance equations in terms of particle trajectory and orientation, respectively, as

\[
\begin{align*}
\vec{\xi} [\Omega] \frac{d\mathbf{r}}{dt} &= \mathbf{F} [\mathbf{r}, \Omega] + \mathbf{F}_0 + \mathbf{H}_T [t] \\
\vec{\gamma} [\Omega] \frac{d\mathbf{\Omega}}{dt} &= \mathbf{M} [\mathbf{r}, \Omega] + \mathbf{H}_R [t],
\end{align*}
\]  

(3.1a)  

(3.1b)

where \( \Omega \) is the particle orientation, \( \mathbf{F} [\mathbf{r}] \) and \( \mathbf{M} [\mathbf{r}] \) are the spatially-varying optical force and torque, \( \mathbf{F}_0 \) is the uniform flow force, and \( \mathbf{H}_T [t] \) and \( \mathbf{H}_R [t] \) describe stochastic processes (e.g. Brownian motion). We assume these relatively small stochastic forces average to zero within our characteristic time scale. Particle position is denoted by the vector, \( \mathbf{r} = (x, y, z)^T \). Due to laminar flow, no flow-induced torque is present for any particle type, i.e. there is no \( \mathbf{M}_0 \) term. Further discussion of the translational and rotational viscous drag coefficient tensors, \( \vec{\xi} \) and \( \vec{\gamma} \), is relegated to Appendix 3.6.1.

We define two coordinate axes systems as in Fig. 3.1: a local (prime) in which the primary semi-diameter \( (a) \) lies along the \( \hat{x}' \)-direction and the two equivalent semi-diameters \( (b, c) \) lie along the \( \hat{y}' \) - and \( \hat{z}' \) -directions; a global (non-prime) in which the orientation of the particle
Figure 3.1: Definition of ellipsoidal particle axes in the local (prime) and global (non-prime) coordinate systems.

may be any angle, $\Omega$. Both position vectors, $\mathbf{r}$ and $\mathbf{r}'$, are anchored at a shared origin. A prolate particle ($a > b = c$) is used for illustrative purposes though the system also applies to oblate ($a < b = c$) and spherical ($a = b = c$) particles.

### 3.3.2 Spheroidal Form Factor Definition

To discriminate among particle types, we employ the aspect ratio, a unitless parameter calculated by $b/a$ and hereafter referred to as $AR$. Values greater than one ($b > a$) represent prolate particles, values less than one ($b < a$) represent oblate particles, and a value of one ($b = a$) represents a spherical particle. In subsequent results, we specify an equivalent spherical radius shared by each particle and individual particle aspect ratios.

A key concept in our description is the three-dimensional form factor, an exponentially-varying representation of a particle whose influence extends beyond the hard particle boundary. A form factor was previously employed by Pelton and coworkers [18] and is a useful in deriving analytical solutions that are appreciably close to exact solutions. We write the form factor in the local coordinate system as

$$f[\mathbf{r}'] = a \sqrt[3]{abc} \exp \left( -\frac{x'^2}{2a^2} - \frac{y'^2}{2b^2} - \frac{z'^2}{2c^2} \right),$$

(3.2)
Figure 3.2: (a) Binary (hard particle) representation and (b) form factor representation of a prolate spheroid of major semi-diameter and of minor semi-diameter. The value varies from white (0) to black \((\alpha \sqrt{ab^2} \exp(-1.5))\)

where \(\alpha\) represents the matter-light interaction, or polarizability,

\[
\alpha = 2\pi \frac{\sqrt{\epsilon_m}}{c} \frac{\epsilon_m - \epsilon_p}{2\epsilon_m + \epsilon_p}, \tag{3.3}
\]

where \(c\) is the speed of light and \(\epsilon_m\) and \(\epsilon_p\) are the relative permittivities of the medium and the particle, respectively. For a spheroid with its major axis along \(x\), the minor axes are equivalent along \(y\) and \(z\) and, therefore, \(c = b\).

Fig. 3.2(a) is a two-dimensional binary representation of a prolate spheroid where \(a = 5\mu m\) and \(b = 2.5\mu m\). Fig. 3.2(b) is the form factor representation of the same particle (calculated assuming \(\epsilon_p = 2.10\) and \(\epsilon_m = 1.77\)). Even though the form factor particle is smoother and has a wider reach, it remains a fair and localized representation of the binary particle [18]. The form factor can also be written in the global coordinate system using the proper rotation matrix.
3.3.3 Force Scalar Potential

As previously developed [18], the optical force on a particle in an optical landscape can be written conveniently in terms of a scalar potential,

$$V[r, \Omega] = (f \circ I)[r, \Omega],$$  \hspace{1cm} (3.4)

where $f[r, \Omega]$ is the form factor and $I[r]$ is the optical landscape intensity. The net optical force $F[r]$ can be then expressed as a convolution:

$$F[r, \Omega] = -\nabla V[r, \Omega]$$

$$= - (f \circ \nabla I)[r, \Omega].$$ \hspace{1cm} (3.6)

In integral form over the three-dimensional particle, the net optical force is:

$$F[r, \Omega] = - \int f[r - \alpha, \Omega] \nabla I[\alpha] d^3 \rho,$$ \hspace{1cm} (3.7)

where $\alpha$ is the vector of integration. Informally, the particle’s size, shape, composition, position, and orientation alter features of the landscape.

Note that the Fourier convolution theorem enables us to express the scalar potential in terms of the Fourier transforms of $f$ and $I$,

$$V[r', \Omega] = \mathcal{F}^{-1}\{\tilde{f}[k'] \tilde{I}[k', \Omega]\}.$$ \hspace{1cm} (3.8)

Note that we have written the scalar potential in the local (prime) coordinate system for simplicity in the derivation. Rotation matrices may be applied as necessary to transition between coordinate systems. The form factor is independent of the landscape, and its Fourier transform
in the local coordinate system is straightforward:

\[
\tilde{f}[k'] = \iiint f[x', y', z'] \ast \exp(-2\pi i(k'_x x' + k'_y y' + k'_z z')) \, dk'
\]  
(3.9)

\[
\tilde{f}[k'] = 2\sqrt{2} \pi^{3/2} \alpha abc \sqrt{abc} \ast \exp(-2\pi^2(a^2 k'_x^2 + b^2 k'_y^2 + c^2 k'_z^2)).
\]  
(3.10)

Note that the function \( \tilde{I} \) in Eq. (3.8) may represent the Fourier transform of any arbitrary landscape, but must also be written in the local coordinate system.

### 3.3.4 Torque Vector Potential

Since our analysis explicitly involves spheroids, we must account for optically-induced torque (unlike the prior analysis on spheres [18]). In this section, we derive the vector potential for the torque, comparable to the scalar potential for the force. By definition, the net torque is the integral over all space of the infinitesimal moments defined by the cross product of the displacement vector \( \mathbf{r} \) and the infinitesimal force \( d\mathbf{F} \).

\[
M[r, \Omega] = \int (\mathbf{r} \times d\mathbf{F}) d^3 \rho,
\]  
(3.11)

where \( d\mathbf{F} \) is the integrand of Eq. (3.7). After some manipulation, this can be represented by a cross product of the particle’s position vector and the force field,

\[
M[r, \Omega] = r \times \nabla (f \circ I)[r, \Omega].
\]  
(3.12)

Using principles of vector calculus, we know that a cross product and a dot product can be interchanged without changing the result, leading to

\[
M[r, \Omega] = \nabla \times r (f \circ I)[r, \Omega].
\]  
(3.13)
Finally, using the associate property of convolution, we write the torque,

\[ \textbf{M}[\textbf{r}, \Omega] = \nabla \times (\textbf{r} f \odot I)[\textbf{r}, \Omega], \]  

(3.14)

in terms of a vector potential that we will represent as

\[ \textbf{A}[\textbf{r}, \Omega] = (\textbf{r} f \odot I)[\textbf{r}, \Omega]. \]  

(3.15)

It is useful here to write the vector potential in terms of the local coordinate system, \( \textbf{r}' \),

\[ \textbf{A}[^{\prime}\textbf{r}], \Omega] = \mathcal{F}^{-1}\tilde{\textbf{f}}[k][\tilde{I}[k'], \Omega]], \]  

(3.16)

where \( \tilde{\textbf{f}} \) is the Fourier transform of the vector \( \textbf{r}' \) and the form factor, \( f \). This vector potential and the associated torque, to our knowledge, is presented here for the first time in describing the response of non-symmetric microscale particles to potential energy landscapes. Its effect will be shown in the following analyses.

### 3.4 One-Dimensional Landscapes

The response of spheroidal particles to optical landscapes may be best understood from two perspectives: the net force and torque without flow (the “static” case), and the translation and rotation when flow is present (the “dynamic” case).

We begin our analysis by investigating particle interaction within a one-dimensional optical landscape that can be represented as a sinusoidal interference pattern of bright and dark fringes,

\[ I[x] = I_0 \left( 1 + \cos \left( \frac{2\pi}{\Lambda} x \right) \right), \]  

(3.17)

where \( \Lambda \) is the interference pitch. With the landscape and the form factor known, we can analytically determine both the scalar and vector potentials of Equs. (3.8) and (3.16) and then...
transform to the global coordinate system:

\[
V[r, \Omega] = 2\sqrt{2}\pi^{3/2} I_0 a b^2 \sqrt{ab^2} \left( 1 + \cos \left( \frac{2\pi}{\Lambda} x \right) \right) * \exp \left( -\frac{2\pi^2}{\Lambda^2} (a^2 \cos^2 \Omega + b^2 \sin^2 \Omega) \right) \tag{3.18}
\]

\[
A[r, \Omega] = \frac{2\sqrt{2}\pi^{5/2} I_0 a b^2 \sqrt{ab^2}}{\Lambda} \sin \left( \frac{2\pi}{\Lambda} x \right) * \exp \left( -\frac{2\pi^2}{\Lambda^2} (a^2 \cos^2 \Omega + b^2 \sin^2 \Omega) \right) \left[ \begin{array}{c}
  a^2 + b^2 + (a^2 - b^2) \cos 2\Omega \\
  (b^2 - a^2) \sin 2\Omega \\
  0
\end{array} \right] \tag{3.19}
\]

In the next section, we examine the relationship between the optically-induced force/-torque and particle shape, size, position, and orientation in this landscape in the static case. Following this, we examine the particle’s response in the dynamic case.

### 3.4.1 Static Analysis

Once the scalar potential, \( V[r, \Omega] \), of Eq. (3.18) is known, we can solve Eq. (3.5), the optically-induced force:

\[
F_x[r, \Omega] = I_0 \frac{2\pi}{\Lambda} \hat{f} \left[ \cos \Omega \hat{\Lambda}, \sin \Omega \hat{\Lambda}, 0 \right] \sin \left( \frac{2\pi}{\Lambda} x \right) \tag{3.20}
\]

As the landscape only varies in \( x \), the gradient results in a force only in \( x \). It is instructive at this point to observe how the \( F_x \) depends on the particle parameters, apart from the flow force and stochastic process in Eq. (3.1a).

The one-dimensional optical landscape generated with an electric field magnitude of 50V/\( \mu m \) is presented in Fig. 3.3(a) as optical intensity versus spatial position normalized to the interference pitch. A bright fringe exists at each maxima in the landscape (\( x/\Lambda = 0, 1 \)) and a dark fringe exists at each minima (\( x/\Lambda = 0.5 \)).
Fig. 3.3(b) shows the static forces on particles of varying aspect ratios at all positions within the landscape. Each particle’s semi-diameter of symmetry is oriented at $\Omega = 60^\circ$ and the normalized particle size ($a/\Lambda$) is $1/5$. As expected, a particle will be forced toward the nearest bright fringe, irrespective of its shape. The center of any fringe represents an equilibrium point—particles will experience a zero force.

Also apparent—quite notably—are the effects of shape. The magnitude of force experienced by a given particle at or near a “preferred” orientation ($90^\circ$ for prolate and $0^\circ$ for oblate particles) is generally greater for aspect ratios approaching 1 than for those far from 1. We conclude that, all else being equal, the optical landscape will act to draw a spherical or nearly spherical particle toward a fringe with greater force than it will, for example, an extremely prolate particle such as a long thin rod.

The normalized particle size also strongly influences the net optical force, as shown in Fig. 3.3(c). With a constant aspect ratio ($AR = 3$) and orientation ($\Omega = 60^\circ$), a particle will experience the greatest magnitude of force when its size is somewhat smaller than the interference pitch ($1/5$ to $1/3$ smaller in this case). The influence of the optically-induced force beyond this sweet-spot is dramatically reduced. Note that Eq. (3.20) can be used to directly find the grating period that leads to the maximum force for arbitrary particle parameters, potentially useful in experiment design.

It is important to note that as the particle volume becomes much larger or much smaller than the interference pitch, the optically-induced force becomes very small, nearing those of stochastic forces.

As the orientation of the particle changes in relation to the landscape, so too does the force. This effect is shown in Fig. 3.3(d), also for a prolate particle ($AR = 3$) at $a/\Lambda = 1/5$. The greatest force occurs as $\Omega$ approaches $90^\circ$ and the smallest force occurs when $\Omega$ approaches $0^\circ$. This arises from the form factor equation itself (Eq. (3.2)), and can be understood from the following: the prolate particle at $90^\circ$ experiences the peak of the force throughout its entire length (parallel to the fringe), whereas a prolate particle at $0^\circ$ experiences the highest force

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only in its center and a lower force at its extremes (perpendicular to the fringe).

Turning our attention to the static torque effects in the same one-dimensional landscape of Eq. (3.17), we again apply the form factor of Eq. (3.2) to solve for the optically-induced torque,

\[
M_z[r, \Omega] = 2I_0 \frac{\pi^2}{\Lambda^2} (b^2 - a^2) \sin 2\Omega \\
\times f \left[ \cos \frac{\Omega}{\Lambda}, \sin \frac{\Omega}{\Lambda}, 0 \right] \cos \left( \frac{2\pi}{\Lambda} x \right). \tag{3.21}
\]

To illustrate particle behavior, we present the one-dimensional landscape and the resultant optically-induced torques in Fig. 3.4. The landscape shown in Fig. 3.4(a) is the same optical landscape as in Fig. 3.3(a) with a electric field magnitude of 50 \text{V/\mu m}.

Fig. 3.4(b) represents the torque on particles of varying aspect ratios at all positions within the landscape. Each particle’s semi-diameter of symmetry is oriented at \( \Omega = 60^\circ \) and the normalized grating length \( a/\Lambda = 1/5 \). Negative torques elicit clockwise particle rotation while positive torques evoke counter-clockwise particle rotation. Both act to align the particle in a minimum energy configuration. As expected, the torque on spheres at any location is zero. The torque on prolate particles (\( AR > 1 \)) at \( x/\Lambda = 0 \) is positive, causing a counter-clockwise rotation so that the symmetry axis of the particle aligns parallel to the bright fringe of the landscape. A similar situation occurs at \( x/\Lambda = 1 \), another bright fringe. At other positions the magnitude of the torque varies yet acts to rotate the particle into a stable minimum energy configuration, \( \Omega = 90^\circ \) or \( 0^\circ \). For oblate particles in the same position as prolate particles, the sign of the torque is reversed. This can be attributed to the means by which spheroids are described in space. At \( \Omega = 60^\circ \), a prolate particle exists in the first and third quadrants whereas an oblate particle exists in the second and fourth. In both cases, the torque acts to align the a particle’s largest axis parallel to bright fringes and perpendicular to dark fringes.

The optically-induced torque is highly sensitive to particle size. Fig. 3.4(c) shows the torque on a prolate particle (\( AR = 3 \)) at \( \Omega = 60^\circ \) as the particle size varies. As was the case for optically-induced force, particles somewhat smaller than the interference pitch experience the greatest effect. The sign of torque follows the same trend as in Fig. 3.4(b).
Figure 3.3: (a) One-dimensional optical landscape intensity variation and the optically-induced force (b) on particles of varying aspect ratios, (c) on prolate particles for varying normalized particle size, and (d) on prolate particles of varying orientation. Contour labels are shown in units of pN.
Finally, particle orientation has moderate influence on the optically-induced torque. As shown in Fig. 3.4(d), for the same particle as in Fig. 3.4(c), the greatest magnitude of torque occurs near $\Omega = 60^\circ$ and decreases for other orientations. When compared to Fig. 3.3(d), the maximum points of force and torque do not occur at the same orientations.

Eq. (3.21) reveals that optically-induced torque from optical landscapes acts on prolate and oblate particles in substantial and non-linear ways. Accurate modeling of non-spherical particles of nearly any shape and size must incorporate these aspects in order to fairly describe its response.

### 3.4.2 Dynamic Analysis

In order to predict how particles will behave over time in the one-dimensional optical landscape, we here employ the full hydrodynamic balance equations of (3.1a) and (3.1b), neglecting stochastic forces as discussed. The driving force ($F_0$) will be a microfluidic flow in a given direction with a constant velocity.

As described in the introduction, others have predicted and shown that particles of varying size and polarizability will behave differently from one another in a microfluidic flow within an optical landscape. We desire now to focus on how particles of varying shape will behave. We will demonstrate two important conclusions: (1) the path of particles through an optical landscape is highly sensitive to aspect ratio (i.e., shape), distinct from other parameters; and (2) particles will either be “locked-into” a fringe or be dispersed into a wide range of propagation directions, also highly sensitive to shape among other parameters.

To best analyze particle motion, we first determine if particles will traverse the landscape or be locked-into a fringe by defining a lock-in threshold,

\[
\cos \Theta \leq \eta_0 \left( \cos^2 \Omega + \frac{\tilde{\epsilon}_a \sin^2 \Omega}{\tilde{\epsilon}_b} \right) \exp \left( \frac{-\alpha^2 k_0^2}{2} \left( \cos^2 \Omega + \frac{\sin^2 \Omega}{AR^2} \right) \right),
\]

(3.22)
Figure 3.4: (a) One-dimensional optical landscape intensity variation and the optically-induced torque (b) on particles of varying aspect ratios, (c) on prolate particles for varying normalized particle size, and (d) on prolate particles of varying orientation. Contour labels are shown in units of $pN - \mu m$. 
with a normalized potential,
\[ \eta_0 = \sqrt{\frac{3\pi}{2}} \frac{3ak_0 I_0 |\alpha|}{v_0 \xi_a A R^{2/3}}, \]  
(3.23)

where \( k_0 = 2\pi/\Lambda \) and \( v_0 \) is the particle volume, \( 4/3\pi ab^2 \). Lock-in occurs when the right hand side of the threshold is greater or equal to the left hand side. With no optical landscape, \( \eta_0 \) is 0 and all particles will travel with the flow. With an optical landscape, particles will either be locked-into a fringe or will traverse the landscape at some predictable angle.

Looking carefully at this threshold, we note that it depends on \( \Omega \) at \( x = \Lambda/4 \). If we know this value, then we are able to exactly determine if a particle is locked-in. If we instead have a collection of particles with random orientations, then we can say the following: prolate lock-in is guaranteed when
\[ \cos \Theta \leq \eta_0 \xi_a \xi_b \exp \left( -\frac{a^2 k_0^2}{2AR^2} \right) \]  
(3.24)

and is possible for some orientations when
\[ \cos \Theta \leq \eta_0 \exp \left( -\frac{a^2 k_0^2}{2} \right), \]  
(3.25)

while oblate lock-in is guaranteed when
\[ \cos \Theta \leq \eta_0 \exp \left( -\frac{a^2 k_0^2}{2} \right) \]  
(3.26)

and is possible for some orientations when
\[ \cos \Theta \leq \eta_0 \xi_a \xi_b \exp \left( -\frac{a^2 k_0^2}{2AR^2} \right). \]  
(3.27)

With no dependence on orientation, the lock-in condition for spheres has a singular boundary. Lock-in will only occur when
\[ \cos \Theta \leq \eta_0 \exp \left( -\frac{a^2 k_0^2}{2} \right), \]  
(3.28)
Figure 3.5: Lock-in threshold condition versus intensity for different shapes. Flow angles may take on any value between 0 and 1 and examples are shown. Regions above the flow and between dashed and solid lines for a particular $AR$ represent possible lock-in for any orientation. The shaded region represents this condition for $AR = 1.3$ and $\Theta = 30^\circ$. Regions above the flow and the solid lines for a particular $AR$ represent guaranteed lock-in for any orientation. Spheres have only a guaranteed lock-in condition.

The trends of these cases against potential, $I_0$ are illustrated in Fig. 3.5 for three particle shapes and a chosen $\eta_0$. The trends among shape remain consistent as $\eta_0$ is altered.

We can also investigate the lock-in trends as the initial orientation of the particles varies for chosen $I_0$. This is illustrated in Fig. 3.6 for two spheroidal particles. These findings are consistent with the static case in that prolate particles at $\Omega = 90^\circ$ and oblate particles at $\Omega = 0^\circ$ are “easier” to trap (i.e., the lock-in threshold is lower) than are those same particles at other orientations. For example, with an electric field magnitude of $30V/\mu m$, the prolate particle ($AR = 1.3$) becomes locked-in as its initial orientation reaches approximately $\Omega = 70^\circ$. Also not surprisingly, as the electric field magnitude increases, particles become locked-in at less preferred orientations and, eventually, at any orientation.

We now turn our attention to the motion (translational and rotational) of particles in the optical landscape, specifically those that are not locked-in. Fig. 3.7(a) illustrates this in terms
Figure 3.6: Lock-in threshold condition versus initial orientation for different shapes. Flow angles may take on any value between 0 and 1 and examples are shown. The solid and dashed lines represent field magnitudes of $30V/\mu m$ and $50V/\mu m$, respectively.

of the relative spatial positions for various particle. For this case, the oblate particle quickly becomes locked-in while the sphere is alternatively influenced by the optically-induced force and flow force. The prolate particle is least affected by the landscape and travels closely with the microfluidic flow.

Figs. 3.7(b) and (c) illustrate the horizontal and vertical position of the same particles in time. As the landscape only varies in $x$ and, as discussed in the static section, only produces forces in $x$, each particle moves at the same rate in $y$.

Fig. 3.7(d) displays the change in orientation with time for each particle. The oblate particle quickly rotates to $\Omega = 0^\circ$ as it is locked-in at the first bright fringe. As discussed in the static analysis section, this is the lowest energy configuration angle for oblate particles. The prolate particle, on the other hand, experiences a periodic change in its orientation as it is alternatively drawn toward $\Omega = 90^\circ$ by each bright fringe and then back toward (and past) $\Omega = 40^\circ$ between bright fringes. As our model is that of a periodic system, such behavior is expected.
Figure 3.7: Dynamic motion of particles in a one-dimensional optical landscape (30 \( V/\mu m \), \( \Omega_0 = 40^\circ \), \( v_0 = 40\mu m/s \), \( \Theta = 35^\circ \), represented by the dashed line), (a) spatial position, (b) position along \( x \) in time, (c) position along \( y \) in time, and (d) orientation in time.
Figure 3.8: For a one-dimensional optical landscape ($v_0 = 90\mu m/s$, $\Theta = 30^\circ$, represented by the dashed line), steady state propagation angles and dispersion for different initial particle orientation. Dashed arrows represent increasing electric field strength. (a) and (c) represent $\Omega_0 = 0^\circ$ and (b) and (d) represent $\Omega_0 = 90^\circ$.

3.4.3 Steady-State Propagation Direction

Notable in Fig. 3.7(a) is the large separation among the particles’ travel directions. The applicability to microfluidic sorting is immediately apparent: by choosing parameters of the system (grating length, microfluidic flow rate and direction, etc.), the propagation direction of various particles within the system is altered. As such, the optofluidic system designer has many dials to tune in order to affect the behavior of the particles present within the microfluidic environment. In this section we will investigate the steady state propagation angles of particles in one-dimensional optical landscapes based on input conditions.

Illustrated in Fig. 3.8 is the steady state propagation angles and steady state dispersions versus aspect ratio for increasing electric field intensities represented by the dashed arrows.
Figure 3.9: For a one-dimensional optical landscape ($v_0 = 90 \mu m/s$, $\Theta = 30^\circ$, represented by the dotted line), steady state propagation angle versus initial particle orientation. Dashed lines represent $50V/\mu m$ and solid lines represent $62.5V/\mu m$.

Figs. (a) and (c) represent $\Omega_0 = 0^\circ$ and Figs. (b) and (d) represent $\Omega_0 = 90^\circ$. As we have already noted, an increase in the field strength leads to lock-in. An important conclusion from Fig. 3.8 is the large dispersion achievable among relatively large $AR$ ranges. For example, Fig. 3.8(d) illustrates that for the largest of the three electric field strengths, a sphere will be dispersed from both oblate and prolate particles with $AR$ just less than 1 and just greater than 1 by over 30 degrees. Furthermore, this result reveals the significance of initial particle orientation in the particle’s behavior. 

The results in Fig. 3.8 also reveals the significance of initial particle orientation in the particle’s behavior. To investigate this further, we show the steady state propagation angles for different particles based on their initial orientation, $\Omega_0$ in Fig. 3.9. The most notable conclusion here is that there are two regimes of $\Omega_0$ for each spheroid type: (1) angles very far—more than $80^\circ$—from the preferred orientation ($0^\circ$ for oblate and $90^\circ$ for prolate) and (2) all other angles.
3.5 Conclusions

We have described the complete motion of spheroidal microparticles in a microfluidic laminar flow influenced by optical interference landscapes. Our model implements optical force and torque balance equations, each of which is dependent upon a form factor description of the particle(s).

We have provided a three-dimensional form factor description of spheroidal particles and a full derivation of the optical torque and force balance equations that employ the particle form factor. To our knowledge, this is the first time both torque and force have been calculated for spheroidal particles in order to describe their complete behavior within optical landscapes. Implementation of our model has brought about the following conclusions concerning spheroidal particles within an optical landscape and microfluidic flow: (1) the steady state motion of the particles is exponentially sensitive to their shape; (2) a lock-in threshold can be calculated to determine if a given particle will be locked-in or traverse the landscape at some steady state angle; (3) the initial orientation of a spheroid upon entering an optical landscape may strongly influence its steady state motion; and (4) a large dispersion may be created among spheroids of relatively small AR range.

3.6 Appendix

3.6.1 Appendix A: The Viscous Drag Coefficients

The coefficient $\xi$ is generally a tensor describing the particle’s instantaneous viscous drag in a given axial direction. Considering a sphere with radius $a$ submerged in a microfluid of viscosity $\eta$, the viscous drag is scalar and widely represented by the Stokes formula, $\xi = 6\pi\eta a$. This coefficient has been developed [73] for spheroidal particles in the low Reynolds’s number regime by solving the Navier-Stoke’s equation. By assuming a no-slip and no-penetration
boundary condition at the fluid-particle interface, the drag coefficient may be expressed as

\[ \zeta = 6\pi \eta \vec{R}, \]

where \( \vec{R} \), a tensor of rank three with units of length, is the hydrodynamic “effective radius” of the spheroidal particle. We describe our adaptation of it in Appendix 3.6.2 which principally follows the prior derivation by Ambjörnsson and Apell [73].

Rotation transformations may be used to relate the effective radius tensor to the particle’s principal axis. Coordinate axes must be defined as in Fig. 3.1: the first is a local (prime) system in which the primary semi-diameter \((a \text{ or } a_z)\) lies along the \( \hat{x}' \)-direction and the two equivalent semi-diameters \((b, c \text{ or } a_y, a_z)\) lie along the \( \hat{y}' \)- and \( \hat{z}' \)-directions; the second is global (non-prime) in which the orientation of the particle may be any angle, \( \Omega \). Both position vectors, \( \vec{r} \) and \( \vec{r}' \), are anchored at a shared origin. A prolate particle is used for illustrative purposes.

The particle’s instantaneous drag response during rotational motion is described by the rotational viscous drag coefficient, \( \gamma \). The calculation of \( \gamma \) follows the Youngren and Acrivos model [74] summarized by Klüner and Dölle [75] and corrected by Sension and Hochstrasser [76]. The friction coefficients of an asymmetric ellipsoid rotating about principle axes \( i \) is given by

\[ \vec{\gamma} = V\eta \lambda_i, \]

where \( V \) is the particle volume and \( \lambda_i \) is a dimensionless friction factor determined through numerical solution of the Navier-Stokes equation [76].

3.6.2 Appendix B: Hydrodynamic Effective Radius

When the particle has a principal axis aligned in the \( \hat{u} \)-direction, the effective radius is given by

\[ \vec{R}_{uu} = \frac{1}{\pi} \frac{V}{Q + a_u^2 n_u}, \]

where \( n_u \) is...
where $V$ is the volume of the particle,

$$ V = \frac{4\pi}{3} a_x a_y a_z, \quad (3.32) $$

and $a_u$ is the principal radii along the direction of motion. For spheroids, $a_x = a_y$. Both $Q$ (particle symmetry factors) and $n_u$ (depolarization factors) vary in value depending on particle type.

The depolarization factors can be found for both the prolate and oblate cases [73]:

$$ n_x \mid_{prolate} = \frac{1 - e^2}{2e^3} \left[ \ln \left( \frac{1 + e}{1 - e} \right) - 2e \right] $$

$$ n_y, n_z \mid_{prolate} = \frac{1}{2} \left[ 1 - n_x \mid_{prolate} \right] \quad (3.33) $$

$$ n_x \mid_{oblate} = \frac{1 + q^2}{q^3} \left[ q - \arctan q \right] $$

$$ n_y, n_z \mid_{oblate} = \frac{1}{2} \left[ 1 - n_x \mid_{oblate} \right]. \quad (3.34) $$

where $e^2 = 1 - \frac{a_z^2}{a_x^2}$ and $q^2 = -e^2 \geq 0$. The $Q$ values also depend on particle symmetry in both the prolate and oblate cases:

$$ Q \mid_{prolate} = \frac{a_x^2}{2e} \ln \left( \frac{1 + e}{1 - e} \right) $$

$$ Q \mid_{oblate} = \frac{a_x^2}{q} \arctan q. \quad (3.35) $$

The effective radius tensor may now be constructed for any desired spheroidal particle.
Chapter 4

A $T$-Matrix Scattering Model Of Spheroidal Behavior Within Optical Radiation

This chapter contains a preprint manuscript of work intended for publication in Applied Optics in the near future. Portions of this work have been presented at 1 professional conference and published in its proceedings (see Sec. 1.3).

4.1 Abstract

Optical manipulation of nano- and micro-scale particles via optical tweezers and optical landscapes continues to be of great interest in several fields, reflected by the myriad experimental pursuits suggesting selective and parallel control over particles of anisotropic shape (blood cells, nanorods, etc.). Our work described here models the behavior of these particles within periodic optical intensity gradients by means of optical scattering principles and, specifically, the $T$-matrix method. Here we describe the salient features of our model for determining the behavior of dielectric, polarizable, mesoscale particles of anisotropic shape in arbitrary inten-
sity gradients. We investigate the forces and torques caused by periodic optical landscapes as well as torques induced by the polarization orientation of the electric field.

4.2 Introduction and Motivation

Trapping and manipulation of nano- and micro-scale particles within a microfluidic environment continues to be of great interest to several scientific communities, including optofluidics and lab-on-a-chip designers who benefit from efficient mechanisms for sorting chemical and biological colloids. Broadly, there are two techniques for colloidal separation: extrinsic, requiring external identification of particles (e.g., fluorescence methods), and intrinsic, in which properties inherent to the particles themselves (e.g., size, refractive index) are exploited. Extrinsic methods can add time and cost to the design of new assays in addition to being invasive to the particles themselves. Leading the charge toward intrinsic-based techniques are dielectrophoretic (DEP) [48,77–80] and optical field [18,45,81–83] sorting systems. These incorporate continuous fluid flow and generally easy reconfiguration means for efficient particle sorting in theoretical terms, experimental observations, or both.

While the majority of these techniques and others like them consider spherical beads and mammillian cells as their particles of interest, they rely on properties such as surface conductance [48] or particle size [81, 83], often neglecting the shape of the particle.

Many analytical models and measurement schemes focus on single aspects of a system: periodic optical landscapes that exert optical forces on spherical particles [18,63,84], Gaussian intensity fields that transfer optical torques to ellipsoidal particles [67,70], etc. We submit that for the model to be complete, it must consider dielectric particles of arbitrary size, shape, and composition; it must address both optical forces and optical torques; and, when considering particle motion over time through a fluid, it must allow for an arbitrary fluid flow—all within the boundaries of optical trapping and microfluidic environments.

We have, therefore, developed and present here an order-of-magnitude analytical model of the response of isotropic dielectric particles of spheroidal shape in optical intensity fields.
Termed the $T$-matrix scattering model, or simply the $T$-matrix model, it is based on the linear scattering of the electric fields at the surfaces of the particles. We use the $T$-matrix method to calculate the amplitude scattering matrix in the far-field [85] thus allowing us to transform the incoming electric fields (incident plane waves) into the outgoing electric fields (scattered spherical waves). The Maxwell stress tensor (MST) is then employed around the particle to find the optically induced gradient forces (in-plane), scattering forces (out-of-plane), and torque. The incident fields we consider are primarily one- and two-dimensional periodic interference landscapes formed by simple holography. However, the generality of our model allows for a large range of incident radiation to be applied.

This work will provide a derivation of our $T$-matrix model and an analysis will be provided. We will show that our $T$-matrix model is capable of calculating the scattering forces as well as torques on particles of shape as induced by their angular separation from the incident electric field polarization orientation. We will show that these effects are significant and should be considered by any complete model.

### 4.3 The $T$-Matrix Model

The forces on our spheroidal particles within periodic optical interference patterns, or optical landscapes, include gradient forces, acting in the transverse plane, and scattering forces (radiation pressures) acting most appreciably in the direction of light propagation. We have developed here a model of particle motion accounting for both the gradient and scattering forces and polarization effects that arise from the polarization orientation of the electric field. The model is based on solving the Maxwell stress tensor (MST) using scattered electric fields in the far-field regime. Such fields may be found by employing the $T$-matrix method.

The $T$-matrix method has been effective in analyzing the forces and torques on particles suspended in a Gaussian optical trap [64,67,86] and has been well defined in more general terms [85,87] for analyzing far-field electromagnetic scattering. We employ it here in analyzing the forces and torques on isotropic, spheroidal particles within optical landscapes. The method
effectively provides exact solutions to Maxwell’s equations—necessary for accurate modeling of particles on the order of the illuminating wavelength—via expansion of the incident and scattered fields as vector spherical wave functions. The expansion coefficients of the scattered field are related to those of the incident field through a linear transformation matrix, i.e., the $T$-matrix.

Forces and torques on particles residing within the fields may then be found using the Maxwell stress tensor. We have chosen the $T$-matrix method for its flexibility in analyzing groups of particles, various media, and a large range of particle sizes. In addition, precision computer code for calculating the $T$-matrix itself is provided by Mishchenko et al [87].

4.3.1 Electric Fields, Particle Orientation, and the $T$-Matrix Method

We begin in the laboratory reference frame by defining the incident electric field with the time-harmonic factor, $\exp(-i\omega t)$ assumed and suppressed. Additionally, all magnetic fields are neglected as we will only consider non-magnetic particles. Following Escuti and Crawford [26], the $m$’th incident wave in phasor notation (Fig. 4.1(a)) is defined as

$$E_{m}^{\text{inc}}[r] = E_{m}^{\text{inc}} \exp(ik_{m} \cdot r + i\delta_{m})e_{m}, \quad (4.1)$$

where $E_{m}^{\text{inc}}$ is the real amplitude, $r = (x, y, z)'$ is the position vector connecting the origin of the laboratory reference frame to the observation point, $k_{m}$ is the propagation vector, and $\delta_{m}$ is the absolute phase. Note that the symbol ‘’ corresponds to the simple vector transpose. As will be convenient when describing our particles, we use the spherical coordinate system to express $k_{m}$ such that

$$k_{m} = \frac{2\pi}{\lambda} (\cos \phi_{m} \sin \theta_{m}, \sin \phi_{m} \sin \theta_{m}, \cos \theta_{m}), \quad (4.2)$$

where $\theta_{m}$ and $\phi_{m}$ are the polar and azimuthal angles, and $\lambda$ is the wavelength of the incident radiation. The polarization of the $m$’th wave can be described in terms of the orientation
and ellipticity angles, $\psi_m$ and $\chi_m$, as shown in Fig. 4.1(b) using the standard convention for handedness. The ranges of the polar, azimuth, orientation, and ellipticity angles are $0 \leq \theta \leq \pi$, $-\pi < \phi \leq \pi$, $0 \leq \psi < \pi$, and $-\pi/4 \leq \chi \leq \pi/4$. As per standard convention, $(\chi = 0, \psi = 0)$ corresponds to transverse-magnetic (TM) polarization and $(\chi = 0, \psi = \pi/2)$ corresponds to transverse-electric (TE) polarization. With polarization information, we can now define the spherical components of the $m$ incident electric fields in the laboratory reference frame interfering at the origin as

$$E_{m\theta}^{inc} = E_m^{inc} \exp(i\delta_m)(\cos \psi_m \cos \chi_m + i(-\sin \psi_m \sin \chi_m)) \quad (4.3a)$$

$$E_{m\phi}^{inc} = E_m^{inc} \exp(i\delta_m)(\sin \psi_m \cos \chi_m + i\cos \psi_m \sin \chi_m). \quad (4.3b)$$

Assuming linear boundary conditions on our particle, Maxwell’s equations allow us to express the scattered electric field linearly in the incident electric field. This is achieved via a $2 \times 2$ amplitude scattering matrix defined in the laboratory reference frame that transforms the electric field vector components of the incident wave into the corresponding components of the scattered wave. In the far-field region, when the observation point is a distance $R$ much
greater than \( \lambda / 2\pi \) away from the particle, the \( n' \)th scattered wave becomes spherical and may be written as [88]

\[
\begin{bmatrix}
E_{m\theta}^{\text{sc}} \\
E_{m\phi}^{\text{sc}}
\end{bmatrix}
= \frac{\exp(ikR)}{R} S \begin{bmatrix}
E_{m\theta}^{\text{inc}} \\
E_{m\phi}^{\text{inc}}
\end{bmatrix},
\]

(4.4)

where \( S \) represents the \( 2 \times 2 \) amplitude matrix. This amplitude matrix depends on the directions of the incident and scattered beams and on the size, morphology, and relative permittivity of the particle. Furthermore, since the particle must also exist in the laboratory reference frame, \( S \) will depend on the orientation of the particle. Because we will focus on rotationally symmetric particles, it will be easiest to align the axis of rotation along the \( \hat{z} \)-axis of a locally defined particle reference frame, transformed to the laboratory frame by the well-known Euler angles of rotation, \( \alpha \) and \( \beta \). Symmetry allows \( \gamma \) to be zero.

The calculation of \( S \) is performed primarily by the double precision \( T \)-matrix code for nonspherical particles in a fixed orientation from Mishchenko et al [87]. We have modified this code to provide a scattering matrix at any given number of points on a sphere surrounding the particle. Our general procedure for obtaining the scattered fields is as follows:

1. Define parameters of the particle such as Euler angles, dimensions, composition, shape, etc.

2. Describe a sphere with radius \( R \) such that \( kR >> 1 \), a criterion for far-field scattering. The sphere surrounds the particle and shares its origin. Using iterative functions of common computer programs, the surface of the sphere is then divided into \( n \) equal-surface-area segments having polar and azimuthal coordinates \( (\theta, \phi) \) centered at each segment. These define the points at which the scattering matrices will be calculated.

3. Define any number \( m \) of incident electric field vectors interfering at the laboratory frame origin using the coordinate system as defined in Fig. 4.1.

4. Using the \( T \)-matrix code, calculate the scattering matrix at each coordinate pair \( (\theta, \phi) \).
5. Transform the incident electric field vectors into \( m \) scattered electric field vectors at each of \( n \) points around the sphere using Eq. 4.4.

### 4.3.2 Force, Torque, and the Maxwell Stress Tensor

Once the scattered electric field vectors have been calculated around the particle, a simple superposition of the field vectors at each point must occur. This accounts for the interference that is created by the \( m \) incident beams interfering at the laboratory frame origin. This is done after calculation of the amplitude matrix and scattered field vectors merely for simplicity. To perform the component-wise summation of these vectors, we must first transform the scattered field vectors from spherical coordinates to cartesian using a \( 3 \times 2 \) transformation matrix as follows:

\[
E_{sca}^n [r] = \begin{bmatrix} 
E_{sca}^{nx} \\
E_{sca}^{ny} \\
E_{sca}^{nz} 
\end{bmatrix} = \begin{bmatrix} 
\cos \theta \cos \phi & -\sin \phi \\
\cos \theta \sin \phi & \cos \phi \\
-\sin \theta & 0 
\end{bmatrix} \begin{bmatrix} 
E_{sca}^{n\theta} \\
E_{sca}^{n\phi} 
\end{bmatrix}, \quad (4.5)
\]

where \( r = (x, y, z) \) and \((\theta, \phi)\) are the spherical coordinate components of the vector normal to the respective segment on the sphere. Superposition is performed via component-wise summation of all scattered electric field vectors.

As our goal is to use these fields to solve for the various forces and torques on our particle of interest, the full Maxwell stress tensor must be computed at at each of \( n \) points using the cartesian coordinate system. This involves writing the vector summation of the incident and scattered fields as \( E_{tot} \) and to then compute the MST at each of \( n \) points using the cartesian coordinate system. The MST is commonly represented by [64]

\[
\langle \rightarrow \leftarrow T_n [r] \rangle = \frac{\epsilon_m \epsilon_0}{2} \Re \left\{ E_{n}^{tot} [r] E_{n}^{tot*} [r] + \frac{1}{2} |E_{n}^{tot} [r]|^2 \rightarrow \leftarrow I \right\}, \quad (4.6)
\]

where \( \epsilon \epsilon^* \) is a dyadic product, \( \rightarrow \leftarrow I \) is the unit tensor, and angle brackets represent a time average of harmonic fields. Both the MST and the unit tensor are of rank two. The net force
on the particle can then be found by integrating the product of \( \langle \nabla \rangle \) and the unit vector at each of \( n \) points over the surface of the sphere enclosing the particle:

\[
F[r] = \int \langle \nabla n[r] \rangle \cdot \hat{n} dA,
\]

where \( \hat{n} \) is the unit vector on the sphere in cartesian coordinates and \( dA \) is the infinitesimal area which, in this case, is the area of each of \( n \) segments. Knowing the outgoing far-field scattered field components, we can write this force in terms of their complex amplitudes [86]

\[
F[r] = \frac{\varepsilon_m \varepsilon_0}{2} \int (E_{\phi}^{sca} E_{\phi}^{sca*} + E_{\theta}^{sca} E_{\theta}^{sca*}) \hat{n} dA,
\]

where the integrand is the rate of transfer of linear momentum per unit area. Similarly, the torque on the particle may be written in terms of the MST as

\[
M[r] = - \int r dA \cdot (\langle \nabla n[r] \rangle \times r),
\]

and in simplified fashion as

\[
M[r] = \frac{ic \varepsilon_m \varepsilon_0}{2\omega} \int (E_{\phi}^{sca} E_{\phi}^{sca*} - E_{\theta}^{sca} E_{\theta}^{sca*}) \hat{n} dA,
\]

where the integrand is the rate of angular momentum per unit area, \( c \) is the speed of light in a vacuum and \( \omega \) is the angular frequency. It is interesting to note that in the simplified equations for force and torque, only the scattered fields need to be considered, rather than the total fields as is the case with the full MST description. Part of this simplification arises from a consideration of the polarization changes—or the lack thereof—brought on by the particle. Both approaches are valid and our model implements the simplified equations.
4.4 Implementation of The T-Matrix Model

The following sections will explore the results of implementing the T-matrix model with spheroidal particles within plane wave radiation and optical landscapes. For consistency, some parameters are the same for all results. The relative refractive index is defined as

\[ n_r = \frac{n_p}{n_m}, \]  

(4.11)

where \( n_p \) and \( n_m \) are the refractive indices of the particle and of the medium, respectively. Throughout this work, we use \( n_r = 1.15 \) and we normalize results to the incident wavelength. An electric field magnitude of \( 10^6 \) V/m, roughly corresponding to an intensity magnitude of \( 10^9 \) W/m\(^2\), is employed in an effort to match probable laboratory laser systems. However, this could also be normalized out without adversely affecting trends within the results.

Our spheroid of interest is a prolate dielectric particle with rotational axis semi-diameter \( a \) equal to the radius of our sphere of interest and twice the length of the orthogonal axes’ semi-dimters \( b = c \). While its angle between the \( \hat{x} \)– and \( \hat{y} \)–axes may change according to the orientation angle \( \Omega \) corresponding to the Euler angle \( \alpha \), its rotational axis will always be in the \( \hat{x} – \hat{y} \) plane, achieved by Euler angle \( \beta = 90^\circ \). As polarization is important to this model, we follow the convention in Fig. 4.1(b) for linearly polarized light, setting \( \chi \) always to zero and \( \psi \) to \( 90^\circ \) (TE polarized) except where noted. For torque, we use the convention that a positive torque about the axis of propagation, the \( \hat{z} \)–axis, is in the clockwise direction when looking down the positive axis direction.

Finally, the reader should note that our model considers only plane waves in its current implementation. However, it is capable of any relevant input radiation described in terms of electric fields. For example, Gaussian beams could be considered by describing the incident radiation as a sum of several plane waves.
4.4.1 Single Plane Waves

Radiation consisting of a single plane wave propagating along the positive $\hat{z}$-axis is capable of transferring linear momentum to both spheres and non-spheres. This may also be referred to as radiation pressure. Eq. 4.8 allows for calculation of this force in terms of the scattered field. Due to the cross-sectional area and shape of various particles, total force may vary for the same incident field. Such a result is evident in Fig. 4.2(a) in which the scattering force on both a sphere and a prolate spheroid is plotted against the normalized size of the particle. The scattering force is roughly proportional to the cross-sectional area of the particle, $a^2$, as evident in this result.

Because the $T$-matrix model considers polarization, a single plane wave is also capable of transferring angular momentum to particles of anisotropic shape. Such a particle will align in a minimum energy configuration in an incident field. For a single plane wave, this is parallel to the orientation of the electric field polarization. Fig. 4.2(b) represents such a situation. The torque about the $\hat{z}$-axis on a prolate spheroid acts to align the rotational axis with the polarization direction. Due to symmetry, the total torque on a sphere is always zero.

The scattering force will remain appreciable for any number of incident beams or plane waves, always acting to “push” the particle in the direction of propagation. The impact of the polarization-induced torque will always be present but may be overcome by gradient forces acting orthogonal to the propagation direction as will become apparent in the following section.

4.4.2 Interference of Two Plane Waves (Optical Landscapes)

Radiation consisting of more than one plane wave propagating at some orientation $(\theta, \phi)$ as indicated in Fig. 4.2(a) will produce an interference pattern (optical landscape) with a period, $\Lambda$, in the plane orthogonal to the total vector direction of the incident waves. For our purposes, this period will be in the $\hat{x} - \hat{y}$ plane, parallel to the the rotational axis of the prolate particle. Because of its symmetry, the orientation with respect to a sphere is the same regardless of
Figure 4.2: Forces and Torques Produced by a Single Plane Wave. (a) Scattering force on a sphere and a prolate spheroid of varying size. (b) Torque on a prolate spheroid about the $\hat{z}$-axis. The torque acts to align the particle’s rotational axis with the orientation of the electric field polarization.

The 1D optical landscape created by two plane waves varies only in the $\hat{x}$-direction so that $I[x]$ is symmetrical in the $\hat{y}$-direction. Such is represented as

$$I[x] = I_0 \left(1 + \cos \left(\frac{2\pi}{\Lambda} x\right)\right). \tag{4.12}$$

The polar angle of the incident waves is related to the landscape period by

$$\theta = \sin^{-1}\left(\frac{\lambda}{2\Lambda}\right), \tag{4.13}$$

where $\lambda$ is the incident wavelength. We will consider only two incident plane waves where $\theta = \theta_1 = \theta_2$, $\phi_1 = 0^\circ$, and $\phi_2 = 180^\circ$, resulting in a one-dimensional optical landscape as described by Eq. (4.12). We will refer to the areas of constructive interference as bright fringes and to the converse areas as dark fringes. Our convention is such that a bright fringe will always occur at $x/\Lambda = 0$ and a dark fringe at $x/\Lambda = 1/2$.

The gradient forces experienced by a particle in this system are represented in Fig. 4.3. A
positive gradient will cause the particle to be drawn in the positive $\hat{x}$–direction. In general, we find that the gradient force will act to draw the particle toward the closest bright fringe as expected. A particle located at a bright fringe is in a minimum energy configuration and a stable equilibrium. A particle located at a dark fringe is in a non-stable equilibrium state and will be displaced by any perturbation.

We conclude from Fig. 4.3(a) that the greatest negative gradient force will occur at the midpoint between a bright and dark fringe for a particle semi-diameter between $a = \Lambda/2$ and $\Lambda/4$. As expected, for a particle placed to the positive side of a bright fringe, the gradient force on the particle will be toward the origin.

Fig. 4.3(b) is the gradient force on both particle types at the midpoint, $x/\Lambda = 1/4$, for varying particle sizes. When the particle is large relative to the period, several bright fringes are present within the dimension of the particle. The gradient force will still act in the direction of the nearest bright fringe, in this case the positive direction. However, when the particle is smaller than the period, the gradient force is restorative toward the origin. At large $a/\Lambda$, the intensity can be approximated as linear near the midpoint. As $a/\Lambda$ continues to decrease, the slope of the intensity decreases, resulting in a gradient force on the particle decreasing toward zero. Similar to the case of a single incident wave, the total force on the sphere is greater than on the prolate particle yet the trend is still present.

The scattering force is still present in our system regardless of the number of incident waves. In fact, the scattering force can be several orders of magnitude greater than the gradient force. This is evident in Fig. 4.4(a) in which the scattering force on a prolate particle varies between 100 – 1200 pN whereas, for the same system, the largest gradient force experienced is $\approx 100$ pN. This has important implications in an experimental setting in that the particles are more likely to be propelled in the direction of beam propagation than they are to be drawn toward bright fringes in the plane of the interference period. From our analysis, for certain particle sizes and aspect ratios, the scattering force must be counteracted or otherwise eliminated in order to manipulate particles in the optical landscape plane.
Figure 4.3: Gradient Force Induced by an Optical Landscape. (a) Contour plot of the gradient force on a prolate spheroid. Both the particle size and position are varied. (b) Gradient force on a sphere and a prolate spheroid. The position is set to $x/\Lambda = 1/4$, halfway between a bright and dark fringe.

Fig. 4.4(b) compares the scattering force on the two particle types. Most interesting to note is the intersection of scattering force magnitude on a prolate particle when $a \approx \Lambda$, regardless of the position. This occurs because in this case, the same number of bright fringes lies within the dimension of the particle, resulting in the same total scattering force. Increasing or decreasing the period will eliminate this condition. Also of note is that when the period becomes greater and much greater than the particle dimension for either particle, the scattering force remains constant at each position. While this was not true for the gradient force in the same situation (see Fig. 4.3(b)), the scattering force is not dependent on the intensity gradient between bright and dark fringes and, therefore, remains constant for a given electric field magnitude.

Two mechanisms of torque are present in optical landscapes: a gradient torque resulting from the intensity gradient across the particle, and a polarization-induced torque as discussed in Sec. 4.4.1. The total of these two torques is displayed in Fig. 4.5 for a prolate particle at position $x/\Lambda = 1/4$ and at two orientations measured from the positive $\hat{x}$-axis, $\Omega = 45^\circ$ and $\Omega = 60^\circ$. At small landscape periods, the gradient torque will dominate the characteristic
Figure 4.4: Scattering Force Induced by an Optical Landscape. (a) Contour plot of the scattering force on a prolate spheroid. Both the particle size and position are varied. (b) Scattering force on a sphere at $x/\Lambda = 0.25$ and on a prolate spheroid at various positions for various particle sizes.

as well as the magnitude of the total torque. As the landscape period becomes larger, the intensity gradient across the particle becomes smaller, and the polarization-induced torque will dominate. We note that the ratio between the total torques of the two orientations at small values of $a/\Lambda$ matches the ratio found in Fig. 4.2(b) for those same orientations. This is valid because for the optical landscape situation, TE polarization is used, meaning the parameter $\Omega$ is equal to the angle between the polarization orientation and the rotational axis of the particle. All applicable parameters are the same for these two situations. The only difference is that here, an optical landscape is present rather than a single beam.

### 4.5 Conclusions

Our analysis provides significant contributions in both theoretical and experimental study of spheroidal particles and their response in periodic optical fields. As mentioned in the Introduction, most theoretical models neglect to include shape and instead focus only on spheres. Spherical particles will not experience a torque and many “real-world” particles are not per-
Figure 4.5: Total torque induced by an optical landscape on a prolate spheroid. The variable $\Omega$ refers to the angle between the positive $\hat{x}$ -axis and the rotational axis of the particle.

fectly spherical. As such, the overall response of the typical non-spherical particle will differ (at times greatly) from that predicted for a sphere. Therefore, a complete model must include the effects of gradient torques and polarization-induced torques on non-spherical particles.
Chapter 5

Pathways To an Experimental Testbed

5.1 Towards an Optofluidic Designers Toolkit

We now change course from our analytical modeling work and enter the domain of experimental and observational optical manipulation. To this point, we have reported our contributions in modeling the interactions between asymmetric particles and periodic optical landscapes. The optofluidic system designer will continue to need more realistic and exact methods of forecasting the behavior of various particle types within these and similar periodic optical interference fields.

Beyond predictions, however, is the need for observation. To this end, we have laid the groundwork for a testbed of periodic optical interference landscape design and implementation. This chapter will report our development and validation of a customized optical trapping and manipulation apparatus and our design and fabrication of spheroidal particles. Our intent was to provide the pathway for a full-scale optical interference design system that, together with our analytical models, will equip the optofluidic system designer with the tools necessary to create and analyze microscale particle fractionation and manipulation techniques.

Such techniques have been experimentally investigated in recent years and the cases are quite varied [15]. Successful manipulation via periodic optical interference landscapes has
been demonstrated in multiple dimensions [89] while others have created arrays of optical
tweezers via holographic elements (e.g., spatial light modulators) to alter the path of many
particles traveling in a fluid flow [14, 43, 60]. Even non-Gaussian beams have been shown to
manipulate a few particles at a time in a static fluid [90]. Our landscapes of interest are, at their
core, quite simplistic as they are formed via simple holography—interference of two or more
beams as discussed in Section 2. The following section will report how we have leveraged this
simplicity in designing the optical interference apparatus.

The particles employed in many of the recently reported observational efforts are spheres
of various sizes and materials. Some of the biological experiments on optical fractionation
and manipulation use organic materials while some of the experiments concerned with nano-
and micro-scale assembly are conducted with rods and various other forms. We report here a
method of fabricating particles with highly-tunable sizes and aspect ratios, using basic litho-
graphic methods.

We stress here that it is not our intent to show multiple cases of particle manipulation
or fractionation but to provide the pathways and the tools necessary to do so—in effect, an
optofluidic designer’s toolkit. Our questions will be tested through designing and building an
experimental apparatus followed by proof-of-concept testing, thereby confirming our hypoth-
esis. Our resultant novel contributions that will be discussed in this section are: (1) the first
reported periodic optical interference landscape apparatus based on multi-beam optical inter-
ference alone that reasonably approximates the ideal optical landscape we have assumed, and
(2) a novel and comparatively straightforward method of designing and fabricating particles
with tunable sizes and aspect ratios.
5.2 Design and Fabrication Of a Custom Optical Manipulation Apparatus

We posed the question, *Can we experimentally implement a periodic optical landscape and microfluidic system that reasonably approximates the ideal periodic landscape assumed in Chapters 3 and 4.* We report here our successful efforts to answer this question positively. As discussed in Chapter 2, a periodic optical interference pattern can be formed by the interference of two or more beams of coherent light, i.e., laser beams. For two beams, the period (the spacing between successive bright fringes) is determined by selecting the proper polar angle, $\phi$, of each beam, as shown in Fig. 5.1(a) where $k_1$ and $k_2$ are the wavevectors. The equation determining the period, $\Lambda$, is the well-known diffraction grating equation:

$$\Lambda = \frac{\lambda}{2n_0 \sin \phi}$$  \hspace{1cm} (5.1)

where $\lambda$ is the wavelength of light and $n_0$ is the refractive index of the medium. As long as the beams share the same polarization, a periodic optical interference pattern, or optical landscape, is formed where the beams overlap as shown in Fig. 5.1(b). This optical landscape is the same that is considered in the one-dimensional cases described in the modeling work reported in Chapters 3 and 4. In an effort to address our questions, we have designed and built two separate approaches for creating a one-dimensional optical landscape, each based on Gaussian laser beam interference. Both designs may be expanded to support more than two beams and, thus, multi-dimensional landscapes.

As discussed in Chapter 2, an ideal wavelength range of light for interacting with biological particles (due to minimal absorbance) is in the infrared (IR). Because we intend our apparatus to be used for interrogating such particles, we have chosen to use a laser wavelength of 1064 nm. While this wavelength offers flexibility in terms of light-material interaction, it carries its own set of challenges such as being invisible to the naked human eye and generally requiring specialized IR optics and optical coatings for greatest efficiency. The former can be overcome
to some degree using frequency-doubling material such as the VIEW-IT® line of products from Kentek® for locating and aligning the beam.

5.2.1 Design One: A Traditional Holographic Approach

Layout and function

Perhaps the simplest method of creating an optical interference pattern is to interfere two coherent and similarly-polarized beams of light at specific incidence angles. Such is the idea behind our first design as illustrated in Fig. 5.2. Our laser of choice is a 1500 mW Compass™ Nd:YAG laser manufactured by Coherent®. Because the overall distance the light must travel in this scheme leads to significant divergence from this specific laser, a beam expander / spatial filter is employed to create a converging beam and to remove any aberrations in the beam.

We choose to use a polarizing cube beam splitter (PCBS) in this apparatus for flexibility in creating the optical landscape. The λ/2-waveplate on the incident face of the beam splitter can be used to dictate the relative powers in the two output beams. This is because the PCBS will evenly split unpolarized light into linear p- and s-polarized beams. If the incident radiation is linear—as the output of the laser is—then the ratio of the linear split will be determined by
Figure 5.2: Diagram of the two-beam holographic approach to forming one-dimensional optical landscapes. Wedge prisms dictate the interference angle and period, $\lambda/2$-waveplates adjust the polarization orientations, and the beam expander / spatial filter serves to create a converging, rather than a diverging, beam free of aberrations.
the polarization orientation, or in other words, the polarization orientation at the output of the \( \lambda/2 \)-waveplate.

After the beam is split, care must be taken to keep the path length of the two beams within the coherence length of the laser. For the Compass\textsuperscript{TM}, this is on the order of 2-3 cm. Because the PCBS outputs orthogonally polarized beams, additional \( \lambda/2 \)-waveplates are used for each beam to ensure the polarizations are made equivalent—a necessary condition for efficient optical interference. Another set of mirrors serves to adjust the path length of the beams and to direct them in parallel toward independent wedge prisms. Wedge prisms are essentially glass windows with a slight bevel, usually less than 5 degrees, on one face. The angle of these prisms relative to the beams determine the angles \( \phi \) of Fig. 5.1(a). We have found this method to be superior to adjusting the prior set of mirrors as doing such can also affect the path lengths of the beams.

After reflecting 90 degrees perpendicular to the table off of a mirror large enough for both beams to strike without clipping, the two beams enter a low-power objective (20X or less). We choose to use low-power objectives in order to maximize the area of the final optical landscape and, therefore, the area of particle-light interaction. With the proper adjustments, interference occurs at the sample stage within the fluid or microfluid of interest. A microscope with its own objective and a CCD camera is positioned over the sample area for viewing and recording.

**Analysis**

This initial iteration of our apparatus is, we believe, the first of its kind intended for optical trapping and manipulation by means simple optical interference to create optical landscapes. While it achieves its intended purpose, several drawbacks led us to consider an alternative approach: independent control of the beams may lead to unequal optical path lengths and unequal and difficult to control \( \phi \), a large footprint, and the need for a beam expander because of the long propagation distances. We expected that an advantage to this method would include the ability to use separate objectives for creating and viewing the optical landscape. However,
we ultimately determined that forcing two beams into the lower objective created additional 
degrees of freedom and, therefore, additional alignment difficulty. In an effort to overcome 
the limitations of this design, we developed an alternative approach based on a Michelson 
interferometer.

5.2.2 Design Two: A Michelson Interferometer Approach

Layout and Function

The well-known Michelson interferometer is a common interferometry configuration intended 
to produce an interference pattern by splitting a beam into two paths and then recombining 
them. Our second design for creating an optical landscape employs this approach in order to 
overcome the limitations of the first design. Our design is illustrated in Fig. 5.3 and uses the 
same laser as the previous design. Because this design minimizes the overall path length, we 
determined that a beam expander / spatial filter was unnecessary.

A non-polarizing cube beam splitter was chosen for this implementation to avoid the com-
plicity of polarization orientation adjustment at each face of the cube. Because the laser is 
linearly polarized, each beam retains its polarization orientation upon passing through the 
cube. The interference actually occurs inside the cube where the two beams recombine. The 
resultant interference pattern then propagates away from the cube as shown in Fig. 5.3. The 
period of the interference pattern is determined by the angles of the mirrors, M1 and M2 and 
by the relative angle of the cube beam splitter. To adjust the period slightly, the user needs 
only to rotate the beam splitter—no other optical adjustments are necessary. Larger period 
changes are best made by changing the orientations of M1 and M2.

The beam then strikes a hot mirror that allows visible light to pass but reflects light in the 
infrared region. Because this is an inverted microscope, we cannot use a standard mirror as 
this would block any light from traveling back down the microscope’s optical path to the CCD 
camera. After reflecting, the beam enters a low-power objective and is incident upon a sample 
on the sample stage. An integrated linear motion stage makes translation of the sample simple.
Figure 5.3: Diagram of the Michelson-interferometer approach to forming one-dimensional optical landscapes. The relative angles of the beam splitter and mirrors M1 and M2 dictate the final interference angle and period. An inverted microscope is chosen for simplicity in that the same objective is used for creating and viewing the optical landscape and its effects.
Because the objective is shared by both the optical landscape creation system and the viewing system, focus for both is always achieved at the objective’s focal point.

**Analysis**

This implementation of a custom optical trapping and manipulation system is one of the contributions of this dissertation. Our second implementation is a significant simplification over our first, allowing for easier changes to the period (single adjustment of the cube angle as opposed to adjustment of two wedge prisms), providing a shorter path length and a smaller footprint, and employing the utility of the inverted microscope.

Our models of Chapters 3 and 4 assume the optical landscapes are created by plane waves. In practice, we use Gaussian laser beams to create the landscapes. As such, the landscapes themselves are Gaussian in nature. This provides two main challenges: (1) the extent of particle influence of the landscapes is limited to the extent of the Gaussian beam; and (2) the optical intensity falls off in a Gaussian nature from the center of the landscape. Even with these challenges, our optical landscapes will still approximate those that we have modeled. By using low power objective lenses—as opposed to high power objectives—creates an optical landscape whose effective size is much greater than the sizes of the particles we are investigating. Therefore, our optical landscapes are reasonable approximations of those assumed in Chapters 3 and 4. To this point, we have answered or initial question positively in that we have built a system to approximate ideal periodic landscapes. However, confirmation of its utility is necessary to answer our next question. This is reported in the next section.

### 5.3 Optical Trapping and Manipulation Apparatus Operation

Our second question in terms of experimental pathways was: *Can this apparatus be shown to effectively lock-in or organize microscale particles within an optical landscape and a stationary microfluid?*. We now report on our answering of this question through employment of our Michelson interferometer-based apparatus.
5.3.1 Single Optical Trap

We will first test our apparatus by forming a single optical trap with our Michelson-interferometer approach, sometimes called optical tweezers. As this needs but one beam, M2 is blocked so as to minimize adjustments to the apparatus. For a sample, we used a 1.0 μm spherical polystyrene bead from Bangs Laboratories. The refractive index of this material is near 1.6, a value often considered in the simulations in Chapters 3 and 4. A dilute mixture was prepared in deionized water and a small quantity was placed on a glass microscope slide and covered with a glass cover slip, effectively creating a microfluidic environment.

The laser power was set at 218 mW and a single trap was formed at the focal point of the 20X objective and was manipulated as shown in Fig. 5.4. The progression from Fig. 5.4(a) through Fig. 5.4(c) shows a particle (indicated by the black arrow) attracted to the trap in image (a) and held in image (b). Because the focal point of the objective is not only the focal point for the optical trap but also the focal point for the camera on the microscope (an advantage of using an inverted microscope), the trapped particle is in focus. In image (c), the sample stage has been slightly translated but the particle stays in the same position. A second particle, indicated by the dashed arrow, is also being attracted to the trap and was itself trapped shortly thereafter. By creating a single optical trap, we have shown the first proof of concept of our apparatus. In order to fully answer our question, however, we must create a true optical landscape.

5.3.2 Optical Landscapes With Adjustable Period

We now turn our attention to implementing an optical landscape with our apparatus. Using a ThorLabs® beam profiler at the focal point of the objective, we can investigate and measure the period of our interference pattern. Fig. 5.5 presents two separate interference profiles, each with a different period. The variation was achieved simply by rotating the cube beam splitter with respect to mirrors M1 and M2. A period variation of 20μm in the first apparatus would have required fine tuning of two wedge prisms and the final mirror. The simplicity and utility
Figure 5.4: A single optical trap (a) attracts, (b) holds, and (c) translates the 1.0 $\mu$m diameter polystyrene sphere (indicated by the black arrow) in deionized water. The dashed arrow in (c) indicates a second particle being attracted to the trap.
Figure 5.5: Interference profiles created by our optical landscape apparatus along a single dimension. The variation in period is achieved simply by rotation of the cube beam splitter.

of our second apparatus is evident here.

Using the same particles, preparation scheme, and laser power as we did for the single optical trap, Fig. 5.6 presents particle response to an optical landscape with a period of roughly 10\(\mu m\). The time lapse from frame to frame is 5 seconds. The horizontal black lines approximately represent the bright fringes of the optical landscape. Over a short span of time, particles are attracted to and trapped within the bright fringes. The separation in frame (c) of the cluster of particles was caused by a low frequency vibration—a common occurrence not completely eliminated by our current infrastructure.

5.3.3 Analysis

At this point, we can say that our question has been answered positively—we have indeed created a system for forming optical landscapes that can be used to organize spheroidal microscale particles. The significance of these results should not be understated. Capturing and holding particles in traps and fringes as shown in Figs. 5.5 and 5.6 is a clear indication of our success and confirms that we have, in fact, designed and fabricated an apparatus capable of
Figure 5.6: Optical landscape with a period of 10 µm attracting and trapping 1.0 µm diameter polystyrene spheres. Time lapse between each frame is 5 seconds.
creating operational optical landscapes. Our contribution to the field of optical manipulation is an operational apparatus, shown to be effective in creating optical landscapes. Further uses of this system is discussed below. The total cost of the second system is less than $100,000 (U.S.) if all parts are purchased new.

5.4 Design and Fabrication Of Spheroidal Particles With Tunable Sizes and Aspect Ratios

5.4.1 Designing Spheroidal Particles

We suggested in earlier chapters that in general, experimental efforts employ spherical particles rather than particles with various aspect ratios. This is somewhat unfortunate as many “real-world” particles have aspect ratios not equal to one. Such was part of the motivation behind our modeling efforts. One reason spheres are ubiquitous in optical manipulation experiments is that they are easy to find and acquire. A second reason is that particles other than spheres are quite difficult to procure. To this end, we ask our third question: (3) Can close approximations of microscale spheroidal particles be designed and fabricated via photolithographic means and then also controlled with the apparatus? We answer this question by designing and fabricating particles with non-unity aspect ratios—prolate and oblate spheroids. The ability to easily and cost-effectively acquire spheroidal particles for testing and analysis of optofluidic designs will be a significantly useful tool.

5.4.2 Creating Spheroidal Particles

Our design methodology approximates spheroidal particles by a photolithographic process in which the aspect ratios of polymer particles may be approximated and quite easily adjusted to suit the needs of the user. We begin by creating a prolate particle outline in Agilent Technology’s Advanced Design System® (ADS). Fig. 5.7 shows a prolate particle with a 3:1 aspect ratio (6µm by 2µm).
Figure 5.7: Screen shot of a prolate particle drawn using Agilent Technologies Advanced Design System® (ADS).
This design is copied several times to create an array of particles for a photomask design. We then choose to outsource this portion of the process to a photomask fabrication company. A picture of a portion of a fabricated chrome photomask is presented in Fig. 5.8. The photomask is created such that the particle shapes are transparent and the remainder of the mask is opaque. This is necessary for the negative photoresist we will use in the next step.

The photolithographic process for preparing particles is outlined in Appendix A. The particles are formed from SU-8 epoxy-based negative photoresist, a viscous polymer that becomes very rigid and stable after proper processing. Its refractive index is near 1.6 in the infrared region, well suited for optical manipulation in microfluidic solvents such as water. Before being removed from their substrate, the hardened SU-8 prolate particles appear as those of Fig. 5.9.
5.4.3 Spheroidal Particles Behavior In the Optical Trapping and Manipulation Apparatus

As a final test of our optical manipulation apparatus, we employed the prolate particles described in the previous section. We again set up a one-dimensional optical landscape in order to investigate the behavior anticipated by our models of Chapters 3 and 4: that non-spherical particles will align themselves in a minimum energy configuration when exposed to an optical landscape. Fig. 5.10 shows the progression of the prolate particle. In frame (a), with an orientation highlighted by the dashed line, the prolate particle begins to be attracted toward the maximum energy portion of the optical landscape, represented by the dashed circle. In frame (b), the particle has begun to orient itself along the bright fringe of the landscape and within the maximum energy area. The bright fringe is horizontal in this image. In frame (c), the particle has rotated out of the plane to be in line with the propagation of the beam.

This exercise has achieved two goals: (1) it has confirmed our hypothesis that we can create
Figure 5.10: Prolate particle (a) being attracted to an optical landscape, (b) rotating as a result of the torque imposed by the landscape toward alignment with a bright fringe that is horizontal in the image, and (c) rotating out of plane toward alignment with the optical trap. The dashed line highlights the change in orientation. The dashed circle highlights the maximum energy area of the optical landscape.
particles with aspect ratios not equal to 1, thereby providing the novel contribution of simple spheroidal particle fabrication using SU-8; and (2) it has shown that spheroidal particles do align themselves in a minimum energy configuration as predicted by our analytical models.

5.5 Conclusion and Analysis

In sum, the optical manipulation apparatus we have described and demonstrated as well as the fabrication process for creating spheroidal particles are significant contributions to the field of optical trapping and manipulation and represent novel additions to an optofluidics toolkit. The apparatus and our optical modeling methods provide a pathway to achieving a complete optofluidics testbed.

Several challenges were encountered while implementing our optical manipulation apparatus. We overcame several of them and suggest means to overcome others in future iterations. Our first challenge was vibration within the system. Photonics and semiconductor researchers are well-aware that low frequency vibrations can prevent success. Our apparatus was constructed on an optical table supported by compressed air. This eliminated most, but not all, of the vibrations in our system. We determined, however, that the vibrations remaining were on a lower order than the period of the optical landscape but greater than observable Brownian motion. We concluded that the overall vibrations could be considered steady-state background that averaged to zero and would not adversely affect our experiments.

Working with IR light is a challenge as it is invisible to the human eye. We overcame this, as discussed above, by using IR viewing cards and by constructing the apparatus in a dark room. We suggest that designers of future iterations also take similar steps.

Finally, probably the largest challenge of this work was aligning and properly converging the beam(s). The second apparatus aided the latter challenge by reducing the path length of the beam, thereby minimizing the final spot size. Future iterations could employ a beam expander as our first apparatus did to control the divergence even further. Alignment of the beams was also aided by the second apparatus in that the number of optical elements was reduced and the path length of the two beams was made easier to adjust relative to one another. We fully
suggest that future iterations of optical landscape devices consider our approach.
Chapter 6

Graduate and Undergraduate Hands-On Education via Soft Electronics Lab Modules

This chapter contains a preprint manuscript of work submitted for publication in the American Journal of Physics. Portions of this work have been presented at 1 professional conference (see Sec. 1.3) at which peer reviewal of the manuscript publication was both positive and encouraging of continued development and dissemination.

6.1 Abstract

We have developed four laboratory teaching modules that offer hands-on experience with organic semiconductor devices and liquid crystal display technologies. This paper provides an overview of these modules: a liquid crystal display (LCD) pixel, an organic light-emitting diode (OLED) made from polymer materials, an organic photovoltaic (OPV) solar cell, and an organic thin-film transistor (OTFT). Through these hands-on lab activities, we aim to expand on traditional semiconductor device and optics education to address key concepts pertinent
to organic devices, including thin-film fabrication methods, electrical and optical characterization, charge injection and transport in organic materials, self-assembly, light emission/absorption/polarization, and basic molecular orbitals energy concepts. A comprehensive set of laboratory procedures has been prepared and the entire project has been designed with a low-cost approach so as to be implemented by most universities or similar institutions. Current versions of all modules and additional instructional material may be obtained at no cost online.

6.2 Introduction

Electrical and opto-electronic devices that depend on soft-condensed materials continue to attract significant research attention, and comprise the core technology of an increasing number of commercially-available consumer products including displays, lighting, flexible electronics, and renewable energy devices [91–93]. These we will term altogether "soft electronics". While these are arguably some of the most compelling devices for engineering and physics students (undergraduate and graduate), the electrical, optical, material, and device foundation for them is often found only in advanced graduate courses, if at all. However, because fabrication of soft electronic devices is simpler (less expensive and faster) than their traditional inorganic cousins, we endeavor to make them more accessible and understandable to a wider set of students (i.e., typically in electrical engineering, chemical engineering, materials science, and physics).

Our educational goals are both to explicitly study these devices themselves, and to study the essential and interdisciplinary electrical, optical, material, fabrication, and system principles. Our practical goals in developing these teaching modules were to create coherent instructional materials that offer the experience of building and characterizing soft electronic devices, which could be adopted and adapted with minimal investment of time and capital by interested educators nearly anywhere.

Our slate of laboratory modules includes the following: a single-pixel liquid crystal dis-
play (LCD), an organic light-emitting diode (OLED), an organic photovoltaic (OPV) solar cell, and a polymer organic thin-film transistor (OTFT). Within the modules, we have devised a method of layering cathodes without vacuum deposition and have developed procedures and infrastructure that ensures both safety and function without requiring dedicated environmental chambers. What follows is an overview of the fabrication processes, the academic value of each module as a stand-alone experiment, and the overall educational contribution to a companion undergraduate course in engineering or physics. Finally, we provide our analysis of the effectiveness of the modules and recommendations for employing them.

6.3 Background

All four modules are unified by soft-condensed-matter principles and share many overlapping application areas. As will become evident in the individual descriptions below, the fabrication and characterization of the devices also share many similarities. Before we delve into the specifics of each activity, it is important to gain an introductory understanding of the underlying principles of organic electronics and LCDs—principles that are made clear to the student by performing each activity.

Technical and fundamental topics central to soft electronics include partial order and self-assembly, carrier transport, photon generation and absorption, optics, chemistry, device properties, and fabrication processes. These topics represent several areas of scientific knowledge from physics to engineering to chemistry. As such, soft electronics is a challenging field requiring a significant breadth of knowledge not typically found in modern day scientists and engineers. We are attempting to fill this chasm by using hands-on activities to teach these important topics that may not otherwise be studied. It is our hope, in this article, that by briefly introducing some of the key concepts within each module, the reader will be better prepared to appreciate the value, potential, and limitations of the modules presented afterward.
6.3.1 Optics

Several fundamental optical principles are taught throughout our activities. For example, calculations of radiometric and photometric quantities such as irradiance and luminous flux are used to characterize the OLED output efficiency; learning to accurately read absorption spectra is crucial to appreciating the optical properties of the OPV device; and comprehending the various states of polarization (i.e., the direction and rotation of the electric field), the utility of polarizers (devices used to produce specific polarizations), and the effects of optical birefringence are necessary to explain the operation of LCD pixels. In addition, basic optical topics including the electromagnetic spectrum, Snell’s Law (to determine refraction of light across a material boundary), diffusion, transmission, absorption, luminescence, color, contrast, and the particle and wave natures of light provide background and depth to appreciating the modules. This list of topics can easily fill an introductory optics course but our modules approach them in such a way as to be directly applicable.

6.3.2 Partial-Order, Molecular Self-Assembly

Liquid crystal (LC) materials are composed of molecules with shape anisotropy that leads to both optical and electrical anisotropy, which make them functional for display applications. LCs by definition manifest mesophases (“in-between” phases) that constitute a genuine state of matter whose molecular properties share characteristics of both crystals and ordinary liquids. Like crystalline solids, liquid crystals have limited order (i.e., they exhibit orientational order but either no or partial positional order) [94] - known as partial-order. The geometry of a LC molecule is usually highly anisotropic—they can be four to six times longer than they are wide and are often modeled as rigid rods [95]. Several classes of LC phases exist, with the nematic phase being the simplest and most commonly employed for commercial displays. This phase possesses only orientational order along the long axes of the molecules with no positional or bond orientational order.

LC molecules do not, themselves, produce light. However, the transmission of light through
layers of LC molecules can be controlled. In addition to their geometrical anisotropy, nematic LCs also possess optical anisotropy, or birefringence, and dielectric anisotropy. This dielectric anisotropy causes specific alignment of the molecules when an electric field is applied across a layer. Light will preferentially travel along a specific path through the LC molecules depending upon the alignment. Light propagation—along with creation and absorption—in organic materials is a common theme among these modules and an important concept to understand. By performing the LCD pixel activity, the student will appreciate that unpolarized light passing through the layers of the LCD pixel can be selectively oriented to be transmitted or absorbed by varying the external electric field across the LC layer.

6.3.3 Organic Semiconductors

As previously mentioned, modern-day university students rarely receive instruction in organic electronic principles. Inorganic electronics, however, are ubiquitous in various engineering and physics curricula. Because we intend for these activities to be used across a broad range of disciplines, it is important to review the basics of inorganic semiconductors to get everyone on the same page. A semiconductor material (such as silicon) has an electrical conductivity less than a metal but greater than an insulator. The conductivity can be controlled by adding other elements to the material to create regions of excess electrons (n materials) or regions lacking electrons, also called holes (p materials). The building block of inorganic semiconductors devices is a material where both regions are present, the p-n junction. Several exciting events can occur at these junctions such as photon emission, photon absorption, and controlled current flow.

Our modules compare the analogous phenomena in organic semiconductors, in wherein p-n junctions do not generally form and are instead governed by charge injection and transport. For example, many polymer semiconductors are hydrocarbon molecules with conjugated bonds and delocalized pi-electron orbitals. Certain organic materials (e.g., phenylene-vinylene variants) are conductive in that charges can be injected and then transported across
the conjugated bonds, resulting in current flow. One of the most important parameters characterizing this transport is carrier mobility $\mu$, an inherent property of a material that is influenced not only by its chemistry but also by its fabrication [96]. Choice of organic materials for specific applications is highly dependent on this value and understanding its impact is paramount in soft electronics. Other organic materials have also been shown effective for soft electronic applications, including small molecules and sol-gels. While our devices employ polymers simply by choice and cost considerations, they could be re-designed around other organic materials.

6.3.4 Electroluminescence and Absorption

Organic materials can also be used to convert electrical current to light (OLEDs), to convert light to electrical current (OPVs), and to modulate electrical current to form a switch (OTFTs). OLEDs operate via electro-luminescence in a thin polymer film sandwiched between transparent electrodes. Injection of electrons and holes from the electrodes into the film results in radiative recombination of the carrier pairs and photon emission [96]. Similar to traditional, inorganic LEDs, OLEDs have a current-voltage characteristic that is highly non-linear. Students will fabricate an OLED and take data to produce this curve in addition to measuring performance in lumens per watt. In the process, students will recall that, in contrast to the valence and conduction band of inorganic semiconductors, organic semiconductors are characterized by a LUMO (lowest unoccupied molecular orbital) and a HOMO (highest occupied molecular orbital). It is the separation between these two that roughly determines the wavelength of the emitted light. OLEDs provide a great introduction to charge transport, organic material energy bands, and electro-luminescence—each of which is addressed in our OLED activity.

Electrical current can be generated due to incident light via the photovoltaic effect in OPVs [96]. The efficiency by which OPVs create current is much lower than conventional photovoltaics, but they are easy to fabricate and cost relatively little. Similar to OLEDs, OPVs consist of a thin film of organic material sandwiched between transparent electrodes. The
separation in the organic layer of the HOMO and LUMO is “tuned” to the wavelength of the incident radiation causing a charge carrier pair to be created and then transported to the electrodes—a process highly dependent upon the carrier mobility. OPVs enhance the introduction of charge transport as well as providing a foundation in optical absorption and organic device efficiencies.

6.3.5 Charge Injection and Transport

Shifting from optical to electrical principles, the OTFT provides a distinct opportunity to compare and contrast organic and inorganic devices. The OTFT, an organic film-based version of a field-effect transistor, allows for current modification between the source and drain electrodes through a low electric field produced by a third electrode, the gate. The OTFT is created as an organic sandwich structure whose performance can be roughly approximated by the drain current in the saturation region [97],

\[ I_{D,sat} = \frac{W}{2L} C_{ox} \mu_{sat} (V_G - V_T)^2, \]  

where \( W \) is the source-drain channel width, \( L \) is the channel length, \( C_{ox} \) is the capacitance of the insulator per unit area, \( V_G \) is the gate voltage, and \( V_T \) is the threshold voltage. The carrier mobility in the saturation region, \( \mu_{sat} \), and the carrier mobility in general, is affected by the junction formed between the metal and the semiconductor. A potential barrier naturally exists at this interface that prevents charge carriers from freely passing. An applied bias can make this barrier appear lower from the semiconductor side, or it can make it appear higher. The applied bias does not change the barrier height from the metal side. Such an interface is a Schottky barrier and is found in almost all metal-semiconductor junctions. In order to increase the performance of OTFTs, designers employ various strategies to make these interfaces Ohmic—a condition in which conduction of carriers in both directions is equal. OTFTs enhance characterization skills, convey the advantages and disadvantages of implementing organic materials, and introduce solid state physics.
6.3.6 Laboratory Infrastructure and Considerations

Each of our modules can be created in a standard laboratory environment in about an hour—a cleanroom and expensive fabrication equipment are not necessary. A properly equipped soft electronics laboratory will consist of four independent stations: material preparation (where the instructor will prepare all materials prior to each lab session), substrate preparation and assembly (where students will clean components and fabricate devices), spin casting and annealing (where students will operate in a fume-evacuation area), and device characterization (where students will have access to common bench-top testing equipment). Ideally, all materials will be prepared prior to the student participation since extra safety precautions must be observed. Complete manuals for each module are available on our companion website [98]. Each manual contains a relevant technology primer with references, student procedures, and an instructors section in which preparation directions and suggested suppliers are provided. We note that a certain level of safety should be observed at all times and the instructor will be assumed to have taken appropriate measures to ensure the safety of all participants.

6.4 Module One: LCD Pixel

As the modern university student no doubt knows, life would be quite different without the convenience of high-resolution smartphone displays, laptops, and high-definition televisions. Each of these devices and many others incorporate some form of liquid crystal display. Understanding the science of these devices can provide useful technical insight into our ever-advancing world. The first lab module, therefore, directs the student to fabricate his or her own single-pixel LCD.

In the process, topics such as LC chemistry, physical optics, and light measurement techniques are explored. Specifically, this module enables the student to explain how a particular liquid crystal would respond to an applied electric field, calculate and measure the transmittance of polarized and unpolarized light through a polarizer, calculate and measure the thresh-
old voltage of a particular LCD, and employ a spectrometer and photodetector for photonic characterization.

The vast majority of devices employing LCs operate by manipulating the polarization state of light. The unpolarized light from a fluorescent or LED backlight is first polarized and then passes through the LC layer established between two substrates with transparent conducting electrodes (usually Indium-Tin-Oxide (ITO)). Based on the orientation of the LC molecules at the surfaces, those in the bulk will configure into a lowest energy state. The birefringence of the molecules selectively orients the light polarization. An external voltage applied across the cell can alter the molecular configuration (and thereby the polarization state of incident light), thereby electrically modulating light intensity.

It is important to understand how the optical properties of the LCD pixel change when a voltage is applied across the LC cell. Until the applied voltage reaches a certain threshold \(V_{th}\), there is no change in the transmittance \(T\) of the light through the cell. Beyond this, \(T\) decreases and approaches a minimum. The threshold voltage is related to the LC material parameters and determines not only the operating voltage of the pixel but usually also the switching time—the speed at which the device can switch between the “On” and “Off” states. Transmittance \(T\) of light through a 90 degree twisted LC cell between crossed polarizers, can be obtained analytically by [24]:

\[
T = \frac{1}{2} \left( 1 - \sin^2 \left( \frac{\pi}{2} \sqrt{1 + u^2} \right) \right),
\]

Here \(u = 2\Delta n d/\lambda\), where \(\Delta n\) is the birefringence of the liquid crystal material, \(d\) is the cell thickness, and \(\lambda\) is the wavelength of operation. The cell thickness is an important parameter for proper LC director field rotation.

The LCD pixel in this module employs a twisted nematic (TN) structure where the LC is arranged in a twist deformation [95]. The LC we chose is MLC-6080 from Merck. An alignment polymer (polyvinyl alcohol, Sigma-Aldrich) on glass substrates dictates the LC molecule
Figure 6.1: LCD Pixel Module: (a) device cross-section fabricated by students; and (b) example opto-electronic response to white light from a flashlight.

orientation at the surfaces. Crossed polarizers enclose the substrates resulting in a “Normally Bright” display mode where light is passed in the “Off” state and blocked in the “On” state. A cross-section of the LCD pixel is shown in Fig. 6.1(a).

The students determine the best thickness based on the given conditions and use that information to construct their cells and then physically measure the cell thickness via spectrometry. Figure 6.1(b) shows the measured voltage response of the transmittance from a student-constructed pixel. Using data collection and calculations, the students will find a threshold voltage on the order of $V = 1.5$ Volts, switch-on and switch-off times of approximately 6 ms
and 55 ms, respectively.

### 6.5 Module Two: Organic LED

Several cutting-edge applications such as ultra-thin and flexible displays, roll-to-roll processing, and inexpensive lighting mean that the up-and-coming physicist or engineer would do well to be familiar with the science of OLEDs. The first practical OLEDs were reported in 1987 and employed a small organic molecule as the light-emission layer [99]. Sharing the same physical operation [100], polymer OLEDs were reported later and have since surpassed small molecule OLEDs in performance and efficiency. As opposed to inorganic LEDs, all device layers of OLEDs can be processed in solution and coated with economically-attractive techniques. Moreover, the interfaces between the layers do not have to be structurally regular at the atomic level. A decade ago, high performance OLEDs rivaled the efficiency of conventional incandescent filament lamps [101] and continue to make impressive progress [102]. In this module, the student will fabricate his or her own polymer OLED, learning aspects of polymer science, photonics, electro-optics, electro-luminescence, and organic device lifetime along the way.

The basic operation of a OLED has similarities to that of an inorganic LED, but is based on molecular electroluminescence (EL) [99]. In simple terms, electrons from the cathode and holes from the anode are injected into the light-emitting polymer layer where they recombine and release energy as a photon, a process known as radiative recombination. The wavelength of the emitted radiation generally depends on the applied voltage, the band gap ($E_g$) of the polymer semiconductor—defined as the energy difference between the HOMO and LUMO levels, and the HOMO energy of the hole transport layer.

The current density in an OLED may be approximated by [103],

$$ J = \frac{9\varepsilon \varepsilon_0 \mu V^2}{8L^3}, $$

(6.3)
Figure 6.2: OLED Module: (a) device cross-section fabricated by students; (b) example current density versus applied voltage characteristic; and (c) example emitted optical power versus applied voltage characteristic.
where $\epsilon$ is the relative dielectric constant, $\epsilon_0$ is the dielectric constant, $\mu$ is the carrier mobility, $V$ is the applied voltage, and $L$ is the thickness of the light-emitting layer. In order to achieve emission, a minimum voltage must be applied, termed the turn-on voltage of the OLED. It must be large enough for the electrons and holes to overcome the barriers of the LUMO and HOMO energy levels. The electrical characterization of an OLED is similar to that of an inorganic LED in that a minimum turn-on voltage must be reached for light emission to occur. Once this voltage is exceeded, the current density roughly follows the square law relation of the current density.

The OLED in this module employs two polymer layers, a hole-transporting layer (HTL), poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS), and an electron-transporting/light-emitting layer (ETL/LTL), poly[2-methoxy-5-(2’-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV), both from Sigma-Aldrich. A small amount of GaIn (Sigma-Aldrich), a eutectic alloy that is liquid at room temperature and low work-function, acts as the cathode. A cross-section of the device is shown in Fig. 6.2(a). For MEH-PPV, the energy difference between the HOMO energy of the HTL and the LUMO energy of the ETL is $\sim 2.3$ eV, corresponding to an emission wavelength of 540 nm, the red-orange region.

Student-obtained current density data is shown in Fig. 6.2(b). The emitted optical power for the same OLED is shown in Fig. 6.2(c). From this data, the turn-on voltage can be ascertained by extrapolating the linear area of the current density plot to the $x$-axis at approximately 3 V. Evident in both plots is the breakdown of the device at 15 V when both current density and optical power fall drastically. This likely occurs from a short between the two electrodes from debris or a defect in the polymer film and often occurs at higher voltages. Students will calculate both photometric and radiometric parameters: radiant flux, radiance, luminous flux, and luminance. Based on the measurements taken, students will calculate the luminous efficiency and external quantum efficiency (EQE) of their devices. Values of the EQE range from somewhat less than 1% to greater than 5%. This value is very dependent upon the measurement techniques, e.g., the correspondence between the center of the cathode and the center.
of the optical power meter, the preparation of the MEH-PPV material, and the quality of the polymer films.

6.6 Module Three: Organic Photovoltaic Solar Cell

Photovoltaic (PV) devices, specifically inorganic and organic solar cells, have experienced a surge in growth over recent years and are becoming one of the strongest contenders for cheap, scalable, and efficient renewable energies [104]. PV devices are unique among renewable energy sources in that they require no generators, are customizable by the end-users, are flexible in terms of fabrication, and scalable in terms of electrical power supply. Their downside is higher cost when compared to fossil fuels and other renewable resources. OPV devices promise to close this gap by decreasing production costs and increasing efficiencies. As a relatively young technology, this is an ideal time and field for which engineering and physics students can be prepared.

The family of OPVs include solid-state bulk-heterojunction devices (BHJs), dye-sensitized nanostructured oxide solar cells (DSSCs), and organic-inorganic composite devices [105]. These and other current OPV technologies present several advantages beyond lower production costs including flexible substrates, continuous printing processes (e.g. inkjet), and easy integration into other commercial devices. Efficiency and lifetime, however, must both be improved in order to make OPVs competitive with inorganic technologies on the performance front. For example, recent organic solar cells have shown efficiencies on the order of 5% as compared to 20% – 40% for inorganic solar cells [105].

A BHJ solar cell based on a conjugated polymer as the donor and a fullerene as the acceptor forms the basis of this lab module. Students will become familiar with power generation and charge transport in a laboratory setting, as opposed to abstract textbook examples as is often the case with undergraduate education. This module affords an opportunity to fabricate a working solar cell and to physically measure its power density and efficiencies all while learning more about polymer science, transmission spectra, and solar absorption.
Figure 6.3: OPV Module: (a) device cross-section fabricated by students; (b) example optical absorption spectrum showing high absorption in the short wavelength portion of the visible range; (c) example current density characteristic under two illumination densities; (d) example power density characteristic under two illumination densities.
An OPV cell can take on a bi-layer configuration. The photoactive region of such devices absorbs photons and then separates the resulting exciton and transports the electrons and holes to their respective electrodes, thereby creating current [106]. A conjugated polymer (the acceptor) and a fullerene material (the donor) can be utilized to perform the charge transport. Electrical characterization is similar to that of an inorganic solar cell. For example, performance is measured under illumination and consists of parameters extracted from a current density plot. A power density plot allows the devices to be characterized based on efficiencies. Using the incident radiometric power density, $P_{OPT}$, and the output electrical power density, $P_{ELEC}$, the overall efficiency can be roughly estimated. Finally, the quantum yield, or external quantum efficiency is the ratio of externally created charges per second to incident photons per second.

Our hole transporter, i.e. the acceptor, is the conjugated polymer poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-p-phenylene vinylene] (MDMO-PPV) from Sigma-Aldrich. Our fullerene-based material, i.e. the donor, is methano[60]fullerene [6,6]-phenyl C61 butyric acid methyl ester (PCBM) from Sigma-Aldrich. PCBM is responsible for transporting electrons to the cathode. To increase the exciton creation area, PCBM and MDMO-PPV are mixed into a single solution. PEDOT:PSS is employed as a hole transport layer in order to ease injection of holes from the anode by lowering the intrinsic energy barrier between ITO and the donor material. The GaIn again acts as the cathode. A cross-section of the OPV is shown in Fig. 6.3(a).

Students first acquire an absorption spectrum of the polymer layer as shown in Fig. 6.3(b). This shows that absorption is highest in the near-UV region of the electromagnetic spectrum—reasonable for a photovoltaic cell designed for solar absorption. Students will have the opportunity to gather current density data from their own solar cells and form such a plot as shown in Fig. 6.3(c) for two illumination power densities. The two illumination power densities shown in the figure correspond to a Maglite® LED flashlight mounted at two different distances from the OPV. Values were calculated using a standard power meter. Students will also be able to create a power density plot as in Fig. 6.3(d) leading to approximate overall
efficiency values on the order of 0.3%.

6.7 Module Four: Organic Thin Film Transistor

In the past decade, OTFT research has seen a surge due to a rising consumer demand for smaller, cheaper, and more portable electronics. Applications such as electronic-paper, flexible displays, and large-area transistor printing have promised to meet such demands. The first OTFTs could not approach the mobility of inorganic TFTs produced from amorphous silicon. In a span of fewer than fifteen years, however, discovery of better materials and device structures have brought OTFT devices into direct competition with their inorganic brethren [91]. With consumers unlikely to request bulkier or less portable electronic devices anytime soon, this is a perfect time for resourceful scientists to be familiar with OTFTs. This module addresses concepts such as transistor device physics [97], charge transport, and carrier mobility along with concepts not typically encountered in an undergraduate curriculum including polymer science and the operation of organic transistor devices that rely on charge injection [107].

Organic material categories exhibiting semiconducting properties include polymers and small molecules [108]. Charge transport (i.e. conductance) in these materials is due to the \( \pi \)-orbital overlap of neighboring molecules [107]. This overlap is enhanced—and mobility is improved—through self-assembly and ordering. Additionally, these materials exhibit great mechanical properties such as flexibility, toughness, and the ability to be processed in solution at low temperatures, resulting in new manufacturing processes such as roll-to-roll and ink jet printing.

Unlike a metal-insulator-semiconductor field-effect transistor (MISFET), an OTFT does not contain p-n junctions or even a bulk region. Instead, the metal electrodes easily inject charge into the semiconductor meaning the operation of the device, i.e. the regime in which current enhancement is appreciable, occurs in accumulation, not in inversion. Current in an OTFT arises from two processes: a bulk current that is present even without an applied gate voltage
Figure 6.4: OTFT Module: (a) device cross-section fabricated by students; (b) overall and magnified interdigitated source-drain electrode pattern; (c) example drain current versus drain voltage characteristic for several gate voltages; (d) example drain current and square root of drain current versus gate voltage characteristics.
and a field-effect current that increases as a potential appears on the gate electrode, causing accumulation of carriers in the semiconductor. Because of this, an n-channel OTFT contains an n-type semiconductor and a p-channel OTFT contains a p-type semiconductor. Characterization of an OTFT and its operating regimes is similar to that of a MISFET in that the important measurements concern the drain current.

A cross-section of the OTFT is shown in Fig. 6.4(a). The organic semiconductor, regioregular poly(3-hexylthiophene) (P3HT) from Sigma-Aldrich, is separated from the gate electrode, by a solution-processable [109] polymer insulator, poly(4-vinylphenol) (PVP), also from Sigma-Aldrich. An interdigitated pattern of ITO, shown in Fig. 6.4(b), forms the source and drain electrodes.

Figure 6.4 presents the key characteristic curves (drain current vs drain voltage and gate voltage) for a student-fabricated OTFT with a grounded source electrode. A transition in the current as it approaches the saturation regime becomes more pronounced with increasing gate voltage, $V_g$. Additionally, the application of negative drain and gate voltages and a resultant negative drain current reveals this to be a p-channel device, i.e. holes are the charge carriers. Figure 6.4(d) presents drain current and square root of drain current versus gate voltage for the same OTFT. Students will use collected data such as this to estimate the threshold voltage ($\sim -10$ V), the ratio of $I_{on}/I_{off}$ ($\sim$2-4 orders of magnitude), and the carrier mobility for their individual devices.

### 6.8 Assessment and Conclusions

While the selection of the devices in our four modules was straightforward, choosing the proper materials and designing the fabrication methods proved to be demanding and rife with challenges. Aside from producing modules of foremost educational value, our goals were to keep set-up and fabrication costs down, to keep device construction times low, to keep device performance and efficiency high, and to eliminate low-value tasks. We will now provide a few examples of our approach and experiences.
Our initial choice for LCD pixel alignment material (a commercial polyimide material from Brewer Science) was expensive but easy to prepare. In an effort to reduce the cost, we tested several other suitable polymer materials and chose polyvinyl alcohol as the best replacement. Similar efforts were extended with many of the other materials in these modules. While literature exists for research-grade devices, often times the materials used are relatively expensive in appreciable quantities. As such, our devices make compromises between high-quality performance and cost. The exception, for now, is the C61 material used for the OPV—a necessary yet expensive material.

We originally fabricated each device (save for the LCD pixel) in a nitrogen-rich glovebox significantly deprived of water vapor and oxygen. This decision was based on prevailing literature showing that such methods greatly increase yield, lifetime, and device performance. Quickly, however, we realized that getting students comfortable using a glovebox so that four devices can be fabricated consumed too much time and resulted in poor student performance. After analyzing our method, we determined that using the nitrogen-rich environment did not significantly improve device performance and that lifetime of the devices was not important in a two to three hour lab activity. While we still use and strongly recommend a fume hood (ductless and custom-built, in our case) for filtration of hazardous fumes, we no longer find it necessary to provide a nitrogen flow or even to use specially-designed glovebox gloves. This has improved student performance and morale without negatively impacting device functionality.

By far, the most challenging portions of designing each of these activities has been development of the fabrication processes and preparation of the organic materials. Several cathode materials and application methods were attempted before reaching the GaIn eutectic alloy. In kind, several solvents and mixing processes were attempted and debugged before determining that the ones currently in use are the best choices.
6.9 Acknowledgments

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Chapter 7

Conclusions and Suggested Work

7.1 Summary Of Contributions

This dissertation has reported on several unique and valuable contributions to the research field of optofluidics and to the educational field of soft electronics. As was said in the introduction, light can be harnessed for an endless number of applications on both the macro- and micro-scales. Without the pioneering work of Ashkin, Chu, MacDonald, Grier, and countless others, optical manipulation would certainly not exist in its current form. We submit that our contributions have added value to the overall research community and provide abilities to better understand and and more effectively harness light for optical manipulation in theory and in practice.

7.1.1 Correlating a Particle’s Shape and Behavior In an Optical Landscape

Previous research into optical manipulation has been focused on phenomena visible in a microscope. We have reported on our development of a quantifiable analysis of these phenomena by means of a form factor model of spheroidal particle motion in periodic optical interference landscapes in Chapter 3. Our question was as follows: Does the shape of microscale particles have an appreciable and quantifiable impact on their motion within a spatially periodic optical potential?
We addressed this question by developing an analytical description of particle response to optical landscapes using optical force and optical torque balance equations. These equations are dependent upon a particle’s form factor, an exponentially-varying analytical representation of a particle whose influence extends beyond the hard particle boundary. Our form factor takes into account a particle’s size, shape, and electrical permittivity as well as the electrical permittivity of the medium. The form factor is used to calculate the force scalar potential and torque vector potential for a given optical landscape.

The analysis in Chapter 3 reports many interesting results in both a static and a dynamic analysis. Based on that analysis, the overwhelming answer to the question posed is Yes, shape does indeed have a quantifiable impact on a particle’s motion in an optical landscape. In fact, the relationship between shape and the optically induced force and torque is exponential as described by the particle form factor. One of our conclusions exemplifies this: a large dispersion may be created among spheroids in an optical flow with a relatively small range of aspect ratios. The impact of this finding should be emphasized: a collection of particles will all traverse an optical landscape differently based directly on their respective sizes, refractive indices, and shapes, sometimes with a high degree of dispersion. Our form factor description allows for predicting a spheroidal particle’s motion in an optical landscape and represents a novel contribution to the field.

Chapter 3 also quantified a lock-in threshold that will determine if a given particle will become trapped (or locked-in) within the bright fringes of the optical landscape or if it will travel through the landscape at some other angle. This threshold quantification is also an original contribution that can easily be employed to determine the relationship between the potential of the optical landscape and the expected behavior of the particles within it. Finally, our analysis also determined that a particle’s orientation upon entering the optical landscape can have a major impact on the steady state direction it travels, further illustrating the appreciable effects of particle shape in these systems.
7.1.2 The Effect Of Scattering Forces and Electrical Polarization On Spheroidal Particles

After analyzing our form factor method, we questioned whether or not the scattering forces and the electric field polarization had an appreciable effect on the motion of particles in optical landscapes. As such, we asked the following questions: (1) Is it reasonable to assume that the scattering forces imposed on both spherical and non-spherical particles by an optical landscape can be neglected? (2) Under what conditions does the torque produced by the optical gradient force on prolate and oblate particles overwhelm the torque caused by the electric field?

In Chapter 4, we addressed these questions by designing a new model, one capable of quantifying both the scattering forces and the electric field polarization effects. Using the $T$-matrix scattering approach, we have been able to answer both of these questions. We have concluded that as the particle size gets larger, the scattering forces become greater and very quickly rise above an order of magnitude larger than the gradient forces of the optical landscape. This finding answers our first question in a positive fashion but with a stipulation: it is reasonable to neglect the scattering forces imposed on spherical and non-spherical particles when the particle size is small relative to the optical period of the landscape. Our contribution concerning this finding is a quantification of such conditions as reported in Chapter 4.

The second question was also addressed by the $T$-matrix scattering model. We have concluded that the condition necessary for the torque produced by the optical gradient force to overwhelm the torque caused by the electric field is related to the normalized size of the particle (i.e., the size of the particle with respect to the period of the optical landscape). The effects of the electric field polarization induced torque are greatest when the period of the optical landscape is large compared to the particle size, $a/\Lambda >> 1/2$. Below this condition, the optically induced torque dominates whereas above this condition, the electric field polarization induced torque dominates and becomes the only torque present as $a/\Lambda >> 1/2$. 

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7.1.3 Implementation Of an Optical Landscape Apparatus and Pathways To an Optofluidics Testbed

We reported on our experimental pathways in Chapter 5. Our questions were as follows: (1) Can we experimentally implement a periodic optical landscape and microfluidic system that reasonably approximates the ideal periodic landscape assumed in Chapters 3 and 4? (2) Can this apparatus be shown to effectively lock-in or organize microscale particles within an optical landscape and a stationary microfluid? (3) Can close approximations of microscale spheroidal particles be designed and fabricated via photolithographic means and then also controlled with the apparatus?

We addressed the first two questions first by designing and constructing a custom optical manipulation apparatus with the intent of forming periodic optical interference landscapes and then testing the apparatus with microscale particles. Two were constructed. The first was based on interference of two Gaussian beams from an infrared laser. We believe this to be the first design of its kind to create optical landscapes from multi-beam interference. Drawbacks of this first system led us to implement a second. Based on a Michelson interferometer construct, our second apparatus improved on the first with a smaller footprint, smaller laser path length, and simpler adjustment of the landscape period.

To prove that our design was functional, we created and demonstrated both a single optical trap and an optical landscape with an adjustable period. By doing so, we have positively answered our first two questions in that we have indeed created a system for forming optical landscapes that can be used to organize spheroidal microscale particles. Showing that we can control such particles indicates the operation and success of our apparatus.

We addressed the third question by fabricating approximations of spheroidal particles by means of a photolithographic process. The 3 : 1 aspect ratio particles were formed of SU-8 epoxy and tested within our apparatus and a microfluidic environment. We showed that the particles were attracted to and rotated within the landscape, answering our third question positively.

Our experimental work has provided the pathway to a complete optofluidic testbed, capa-
ble of creating and implementing optical landscapes with adjustable periods and capable of analyzing the behavior of fabricated spheroidal particles.

7.1.4 Creating a Teaching Laboratory On Soft Electronics

We reported on our creation of a hands-on teaching laboratory in Chapter 6. Our question was: *Can a hands-on teaching laboratory on organic electronics and liquid crystal displays be developed that effectively teaches their operational principles, fundamentals, and practical aspects of fabrication, within a reasonable budget and broadly accessible way?*

We addressed this question first by developing four hands-on laboratory teaching modules on organic electronics and liquid crystal displays, i.e., Soft Electronics. These modules offer hands-on experience with the following: a liquid crystal display (LCD) pixel, an organic light-emitting diode (OLED), an organic photovoltaic (OPV) solar cell, and an organic thin-film transistor (OTFT). The successful creation of these modules was the first step in answering our question affirmatively.

We then addressed the question by evaluating student feedback and analyzing student performance while teaching these laboratory modules during three separate semesters at NCSU. All four devices were continually fabricated with great success and high yield by both undergraduate and graduate students. In the process, these students were exposed to key concepts pertinent to organic devices, including thin-film fabrication methods, electrical/optical characterization, charge injection/transport in organic materials, self-assembly, light emission/absorption/polarization, and basic molecular orbitals energy concepts. Student feedback and performance has been positive. Those students who struggled to fabricate working devices still marveled at the simplicity of the design and the instructional hands-on approach.

This effort has been achieved using a reasonable budget and has been experienced by students from all manners of engineering, physics, chemistry, and materials. *We believe this effort has been a fantastic success and that it has positively answered the guiding question.* We look forward to sharing the modules with other schools and universities in the near future.
We gratefully acknowledge the Preparing the Professoriate Program for this opportunity, encouraging the author to work in a mentor-protege relationship with Dr. M.J. Escuti over the course of several semesters. In terms of providing a broadened experience to the Ph.D. program, this effort has allowed the author to engage collegiate students on a teaching level and has provided valuable experience in course and laboratory formation and professorial preparation. The effort has been an invaluable experience and novel contributions have been exchanged: we have created a highly educational and novel approach to teaching Soft Electronics while NCSU has provided the invaluable service of instructional education.

7.2 Suggestions For Future Work

In this section we briefly summarize our suggestions for using our work and for taking advantage of our contributions.

7.2.1 Analytic Description Of Steady State Particle Direction In an Optical Landscape

In Chapter 3, we detailed our contributions in terms of modeling the motion of spheroidal particles in optical landscapes via a form factor method. We illustrated the various paths a particle might travel within these landscapes and concluded that while the path may be stair-shaped or otherwise, each particle reaches a steady state motion and, therefore, a steady-state direction. We suggest that an analytic description of this direction be developed. This will lead to a more useful interpretation of the model for the optofluidics system designer.

This description is likely determined by the relationship between the force and torque balance equations, two differential equations coupled through the particle’s orientation, \( \Omega \). One approach is to determine the maximum and minimum propagation angles achieved each period by the particle and then use the average of those angles as an effective \( \Omega \) allowing the differential equations to be de-coupled and solved.
7.2.2 Multi-Dimensional Optical Landscape Modeling

Our models have considered one dimensional sinusoidal optical landscapes. However, the use of such landscapes was a research decision and not a restriction. Future work could explore the use of other landscapes in multiple dimensions as our models are capable of employing them. The flexibility of our models in this sense leaves open the door to many future research directions as well as applications. Furthermore, those that use our models are not restricted to the particle types we chose. We designed the models to be very general and they can describe the motion of non-spheroidal particles as well, as long as the particles can be mathematically described in the three dimensional cartesian coordinate system.

7.2.3 Enhancing and Implementing the Optical Manipulation Apparatus

The optical manipulation apparatus we have described and demonstrated as well as the fabrication process for creating spheroidal particles are significant contributions to the field of optical trapping and manipulation and represent novel additions to an optofluidics toolkit. The apparatus and our optical modeling methods provide a pathway to achieving a complete optofluidics testbed. In this section we will suggest means of enhancing this toolkit further through experiment and observation.

Multi-Dimensional Optical Landscapes

To create multi-dimensional landscapes, i.e. those that vary in more than one linear direction, more than two beams are required. Here we suggest a method for creating such landscapes, thereby enhancing and expanding the optofluidics testbed.

The cartoon in Fig. 7.1 depicts a three-beam interference set-up similar in design and function to the two-beam apparatus demonstrated previously. The output of an infrared laser is split into three separate beams, each with individual polarization control via waveplates. The interference pattern is determined by selecting the proper polar angle, $\phi$, as shown in Fig. 5.1(a). Additionally, by employing half- and/or quarter-waveplates, we have control over
Figure 7.1: Experimental set-up employing three-beam interference to create an optical interference landscape. [Courtesy of C. van Hesch]

the polarization state of each beam and, as a result, the polarization state of the interference pattern (Fig. 5.1(b)). Following the waveplates, the beams pass through wedge prisms used to set the polar angle which, for two beams, determines the grating period. The beams next enter a pair of opposing corner cube prisms (right angle prisms for two beams). These are in place to control the plane of interference by simply adjusting the spacing between their flat faces. Finally, the beams are directed upward through the particles contained in a microfluidic sample chamber and into a microscope used for imaging. The optical landscape is formed at the intersection of the beams.

**Dynamic Particle Manipulation In Microfluids**

As we have discussed in the Introduction and elsewhere, many research groups have reported on optical trapping and manipulation via assorted methods. Our apparatus is likewise fully capable of optical trapping and manipulation. We suggest that future work with our system consider dynamic particle manipulation to further progress the pathway to a complete optofluidics testbed.
Dynamic manipulation can be investigated using microfluidic devices, such as the one shown in Fig. 7.2. The microfluidic cell is actually a series of channels on the order of hundreds of micrometers tall and wide and several millimeters in length. They are formed via “soft lithography”, i.e., creation of a polydimethylsiloxane (PDMS) structure using a mold composed of patterned photoresistive material. PDMS, also used as a stamp resin in a similar manner, is desirable as it is inert, optically clear, and can be made hydrophilic or hydrophobic. The advantage to using such cells is that the flow velocity can be well controlled and the height and width can be finely tuned to correspond with the optical landscape.

**Improving the Apparatus**

As is usually the case with experimental devices, improvement can always be made. Future iterations of our Michelson interferometer based apparatus—perhaps in moving the laboratory prototype device toward a commercial version—can take advantage of the challenges we encountered and overcame by avoiding them up front. While the period of the optical landscape can be finely tuned, the current version of the apparatus does not have a quantifiable method for “tuning” a particular period. Employing computer-controlled micrometers on the beam splitter stage and the mirror mounts could greatly improve the system, making it easier for the user to choose the exact period.

The position of the hot mirror within the inverted microscope makes it difficult to finely
tune the incidence angle of the beam with respect to the objective. Improving this setup either with commercial parts from the microscope manufacturer or with customized optics would greatly improve the overall setup.

As our $T$-matrix modeling approach revealed, particles experience a greater scattering force as they become larger. In order to use a wide range of particle sizes in our system, we suggest that a future iteration employ a mechanism for counteracting this scattering force. This could be an identical objective incident $180^\circ$ from the incidence direction of the interfering beams. Of course the optical path length would need to be designed such that additional interference is not created while an opposing scattering force is provided, thereby allowing the gradient forces within the landscape to dominate the particles’ motion as dictated by our form factor model. One group has shown that by employing counter-propagating optical tweezers, the optical scattering force can be counteracted to hold high refractive index particles otherwise unable to be trapped [110].

Our final suggestion for future work concerns moving our prototype apparatus into the commercial world. Doing this will likely require the suggestions above but also a reduction in the overall footprint, the integration of a high frame rate camera, the use of laser line optics throughout, and computer controlled optic mounts and sample stage. Many researchers have shown systems capable of optical manipulation as we have discussed. Ours is truly a game changer in its optical flexibility (many types of landscapes with variable periods can be formed), sample flexibility (we have shown how to fabricate spheroidal particles for interrogation and have shown that our apparatus can control them), and cost (the major components are the laser and the microscope). Our design does not require any spatial light modulators or other customized equipment and can be built and made operation on a reasonable budget.

In conclusion, we have had great success in our experimental objectives and have been the pioneers in laying a sturdy pathway for future research.
REFERENCES


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Appendix A

Spheroidal Particle Fabrication

What follows is our recipe for fabricating spheroidal particles from SU-8 photoresist (Microchem). It assumes a photomask has already been designed as described in Sec. 5.4.2.

A.1 Prepare and Coat Substrate

1. Clean a 1 square inch glass substrate in an Ozone cleaning chamber;

2. Place substrate in spin-caster;

3. Dispense enough OmniCoat\textsuperscript{TM} (Microchem) onto substrate to completely cover the substrate;

4. Spin at 3000 rpm and 300 rpm/s for 30 seconds;

5. Bake at 200\textdegree C for 60 seconds;

6. Repeat steps 3-5 twice more (results in 100 nm thickness of OmniCoat, which will act as a release layer for the SU-8);

7. Dispense enough SU-8 photoresist (Microchem) onto substrate to completely cover the substrate;
8. Spin at 1200 rpm and 300 rpm/s for 30 seconds (results in a 2μm thickness of SU-8);

9. Bake at 95°C for 90 seconds.

A.2 Exposure

1. Place chrome mask in MA6 machine;

2. Expose substrate (exposure time = exposure dose / measured intensity);


A.3 Develop

1. Prepare a glass vial of PGMEA (Sigma-Aldrich) large enough to submerge the entire substrate;

2. Immerse substrate in PGMEA for 5 seconds;

3. Remove substrate and immediately coat with IPA (Sigma-Aldrich) and allow to dry (white film may appear);

4. Repeat steps 2 and 3 until no white film appears;

5. Particles should be visible at this point in an optical microscope;

6. Hard-bake at 200°C for 600 seconds.

A.4 Liftoff

1. Submerge substrate into a fresh glass vial of PGMEA;

2. Place vial into a heated (60°C) ultrasonic bath for 60 minutes;

3. Remove substrate transfer particles to another container or use within the PGMEA.