Insert title here

author1[†] and author2[‡]

†*university1*

‡ *school2*

E-mail:

Abstract

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1 Introduction

2 Methods

The goal of this work is to identify Zernike coefficients used to construct an incident beam profile designed to stabilize specific two-particle optical matter configurations. We learn these profiles in a two-stage optimization procedure. First, particle dynamics are performed to modulate the Zernike coefficients to achieve a target particle configuration in simulation. This step involves explicitly performing separate optical matter simulations for each trial set of Zernike coefficients to find a beam profile that drives two-particle systems into the target particle configuration. Second, the beam profiles learned from the particle dynamics stage are used as a starting point for a work-curve refinement stage. This step involves calculating work-curves for dimer separation and orientation to deepen the associated target minima relative to any other metastable states.

2.1 Optical Matter Simulation

To simulate optical matter systems we use the miepy and stokes libraries developed by John Parker.

2.2 CMAES

We use Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) as our optimization algorithm of choice. CMA-ES is a gradient-free algorithm for optimization of black-box functions in a continuous domain. Using CMA-ES we can optimize a set of Zernike coefficients as a continuous valued input that defines an incident beam profile to stabilize specific optical matter configurations. A CMA-ES implementation provided by the pycma Python library is used throughout this work using a population size of 100 and initial σ=XXX.

2.3 Step 1: Simulation Dynamics Optimization

The first step in our optimization procedure is to perform particle dynamics simulation to learn an approximate beam profiles capable of moving particles into a predefined target configuration. We attempt to stabilize particle configurations at integer optical binding separations along the y-axis. Simulations are performed by initializing particles at one optical binding separation beyond the intended target separation about the origin and at random orientations (angles). We elected to initialize particles at separations beyond the target separation as we found devising profiles that separate particles more challenging and sometimes not possible compared to learning profiles that ensure the particles come together – but not too far. This is also somewhat an arbitrary decision because the profiles learned from this step are eventually refined in the following step (Step 2).

For a given beam profile defined by the set of Zernike coefficients, we perform 12 separate simulations at random orientations. From each simulation we calculate the frame-by-frame average similarity of the instantaneous particle configuration observed in simulation to that of the predefined target particle configuration. The frame-by-frame averages for each simulation are then averaged for all 12 simulations performed at random orientations to yield a single scalar value fitness for the similarity of the particle configuration induced by the beam profile to that of the target particle configuration. To calculate the similarity of the instantaneous particle configuration to the target configuration we represent particle dimers using a vector representation similar to the permutation invariant vector (PIV) introduced by XXX [REF]. The instantaneous position of two particles in space is represented by a vector of pairwise distances between the particles and two ghost particles located at the origin and along the y-axis (Fig.XXX). The pairwise distances between the optical matter beads and sorted in the vector ensuring the representation remains invariant to the labeling of the particles. The L2 norm between the vector representation calculated for the target configuration and the particle position at each simulation frame defines the instantaneous similarity to the target configuration. This similarity is averaged over each frame and each independent simulation

to yield fitness score for the quality of a given beam profile defined by the set of Zernike coefficients. This fitness metric is used to define the loss function minimized by the CMA-ES algorithm as a function of the Zernike coefficients. Multiple CMA-ES optimizations are performed for a number of $\beta \in [0, 1]$ values, which controls the strengths assigned to the interactions between the optical matter beads and the ghost particles. Each CMA-ES instantiation is performed for 36 hours on XXX hardware, or until the calcaultion converges. The best beam profiles from each optimization are then evaluated post-hoc by ensuring the intended particle configuration are indeed stabilized in a test simulation, the best of these profiles for different β parameters are then passed as starting points for the work curve refinement optimization performed in Step 2.

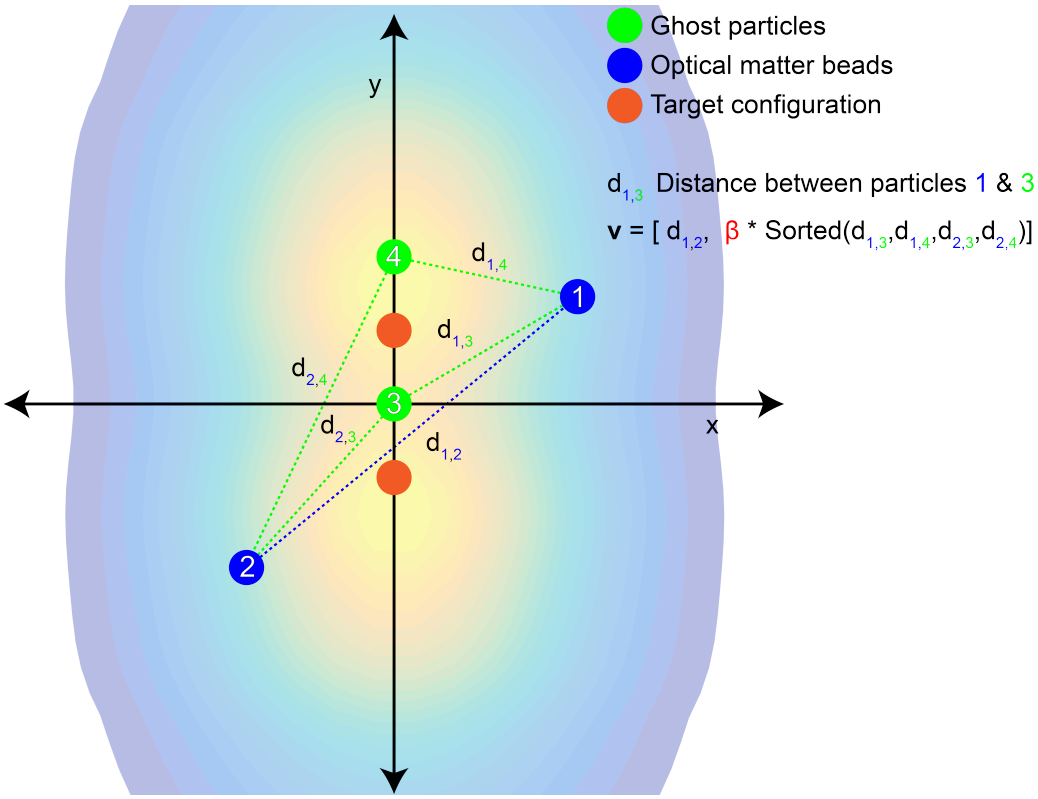

Figure 1

2.4 Step 2: Work-curve Refinement Optimization

Using the beam profiles learned from the simulation dynamics optimization in Step 1 as starting points, we perform a secondary optimization over the calculated radial and angular work curves to further stabilize the desired particle separation and orientation. This optimization step is significantly cheaper to execute and allows us to learn beam profiles at different beam widths than those originally obtained by the particle dynamics simulation. During this step we can also apply an L2 regularization weight on the Zernike coefficients to decrease the overall magnitude of the Zernike coefficients to help make them more experimentally manageable.

Given a beam profile defined by a set of Zernike coefficients, we calculate a radial work and an angular work curve of the particle pair (Fig. XXX). The radial work curve is defined along the path specified by separating the particles about the origin along the y-axis from a separation of XXX to XXX. The angular work curve is calculated via the circular path where the particles begin at the target separation about the origin aligned along the x-axis and rotate 180 degrees counterclockwise. The component of the loss from the angular work curve is calculated as the difference in the work at the target orientation and the global minima. The loss component from the radial work curve is calculated following the flow presented in XXX, effectively attempting to maximize the difference between the minima at the target separation and the most competitive secondary minima. These two losses are balanced by a parameter α. A third component of the loss involves an L2 norm weight decay on the Zernike coefficients scaled by a parameter λ. The optimization is carried out until convergence where the best performing set of Zernike coefficients are then used as the final beam profile that stabilizes the intended target particle configuration.

The radial work curve loss component is calculated according to the following procedure. First the radial work curve is calculated along the path of pulling the particles apart starting from a separation of 150 nm (twice an individual particle radius) to the target distance + three optical bindings (i.e. if the target distance is at the 2nd optical binding the radial

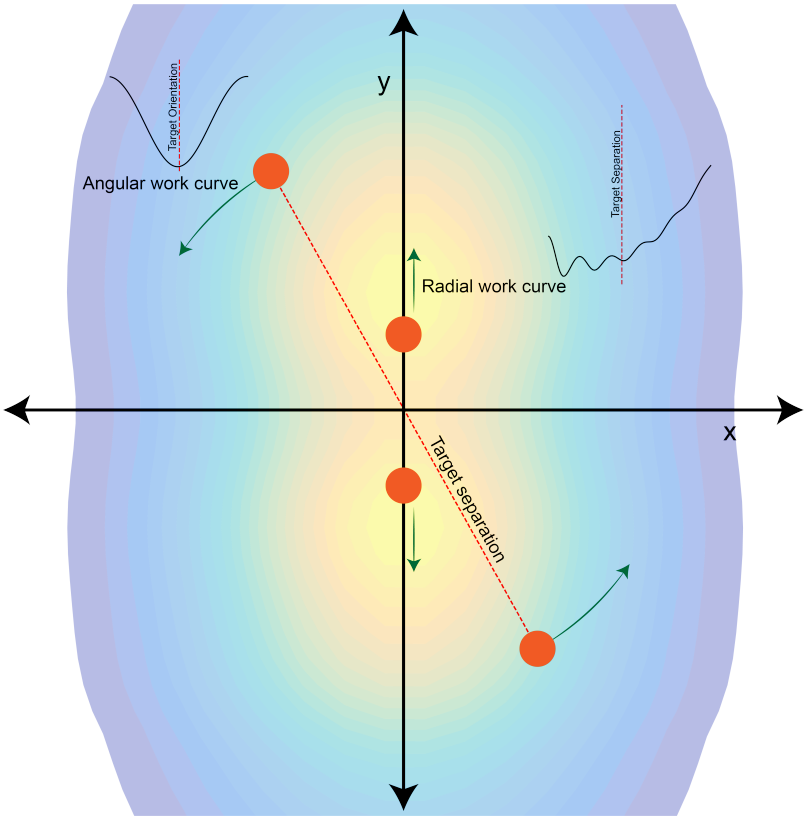

Figure 2

work curve is taken out to the $2 + 3 = 5$th optical binding separation). Local minima from this radial work curve are then identified using scipy's argrelextrema function. If there does not exist a local minima between half an optical binding greater than the target separation $(+\frac{a_0}{2})$ and a quarter of an optical binding less than the target separation $(-\frac{a_0}{4})$, the radial work curve loss is calcaulted as the difference in work at the global minima of the work curve and the work at the target separation. If a minima does exist in this range of separations, but there also exits a global minima in the work curve that is less than the work at the target minima, the radial work curve loss is calculated as the work at the target minima minus the work at the global minima. If the work at the target minima is also the global minima of the work curve, the radial work curve loss is then the work at the target minima minus the work at the 2nd lowest local minima. If the local minima near the target separation is the only local minima, and there are no other local minima throughout the radial work curve, but the global minima of the work curve has a lower work value than the target local minima,

the loss is the work at the target minima minus the loss at the global minima. Finally, if the work at the target minmima is also the global minima, and there are no other local minima present, the loss is calculated as the work at the target minima minus the work value at the global maximum.

3 Results and Discussion

4 Conclusions

Data Availability

Acknowledgments

Supporting Information

References

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