# Simulation of Atomic Dynamics in a Gaussian Optical Trap

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## Contents

# 1 Introduction

This document describes the numerical simulation of atomic motion in a Gaussian optical trap, focusing on the dynamics of cold atoms initially trapped in a magneto-optical trap (**MOT**) and subsequently guided towards a hollow core optical fiber, by an optical trap (modeled as a gaussian beam). The aim is to provide a **clear theoretical derivation**, describe the **dimensionless formulation**, and explain the **numerical integration scheme** used in the simulation.

# 2 Optical Potential

The optical potential experienced by an atom of mass $m$ in a Gaussian laser beam is given by:

$$U(\rho, z) = -U_0 \frac{w_0^2}{w(z)^2} \exp\left(-2\frac{\rho^2}{w(z)^2}\right), \tag{1}$$

where:

- $\rho$ is the *radial distance* from the beam axis,
- $z$ is the coordinate along the *beam axis*,
- $w_0$ is the *beam waist* at focus (i.e. at the fiber tip),
- $w(z) = w_0\sqrt{1 + (z/z_R)^2}$ is the *beam radius* along $z$,
- $z_R$ is the *Rayleigh range*,
- $U_0$ is the *trap depth* at the beam focus.

The **force** acting on the atom is derived from the potential:

$$\mathbf{F}(\rho, z) = -\nabla U(\rho, z), \tag{2}$$

and the corresponding **acceleration** is

$$\mathbf{a}(\rho, z) = \frac{\mathbf{F}(\rho, z)}{m}. \tag{3}$$

Formulating the problem in this way, we exploit the cylindrical symmetry of the system (i.e. the rotational symmetry about the axis of the fiber), getting rid of one coordinate, the azimuthal coordinate $\phi$.

# 3 Dimensionless Formulation (experiment-specific)

In this work the optical trap is generated by a *Nd:YAG* laser at wavelength $\lambda_{\mathrm{L}} = 1064\,\mathrm{nm}$ with optical power $P = 1\,\mathrm{W}$. The guiding element is a kagomé hollow-core fiber whose measured mode-field diameter (MFD) is $\mathrm{MFD} = 39\,\mu\mathrm{m}$. For a near-Gaussian guided mode we take the beam waist ($1/\mathrm{e}^2$ radius) as

$$w_0 \approx \frac{\mathrm{MFD}}{2} = 19.5\,\mu\mathrm{m}.$$

The Rayleigh range of the beam emerging from the fiber is

$$z_R = \frac{\pi w_0^2}{\lambda_{\mathrm{L}}} \approx \frac{\pi(19.5 \times 10^{-6}\,\mathrm{m})^2}{1064 \times 10^{-9}\,\mathrm{m}} \approx 1.12\,\mathrm{mm},$$

i.e. the longitudinal scale is on the order of millimetres for this large mode.

## Estimate of peak intensity and trap depth

For a Gaussian mode the on-axis peak intensity at the waist is

$$I_0 = \frac{2P}{\pi w_0^2}.$$

With the values above this yields

$$I_0 \approx \frac{2 \times 1\,\mathrm{W}}{\pi(19.5 \times 10^{-6}\,\mathrm{m})^2} \approx 1.67 \times 10^9\ \mathrm{W\,m^{-2}}.$$

Using a simple far-detuned two-level (scalar polarizability) approximation referenced to the $D_2$ line of $^{87}$Rb ($\lambda_0 \approx 780.24\,\mathrm{nm}$, natural linewidth $\Gamma/2\pi \approx 6.065\,\mathrm{MHz}$), the single-laser dipole potential at the focus can be estimated as

$$U_0 \simeq \left(\frac{3\pi c^2}{2\omega_0^3}\Gamma\right)\frac{1}{\Delta}\,I_0,$$

with $\Delta = \omega - \omega_0$ the angular frequency detuning. Evaluating this expression gives a trap depth magnitude of order

$$\frac{|U_0|}{k_B} \sim 2.2 \times 10^{-4}\,\mathrm{K} \approx 0.22\,\mathrm{mK}\ (\approx 220\,\mu\mathrm{K}),$$

(i.e. a few $10^2$ $\mu$K); the potential is negative for red detuning as used here. This estimate is adequate for order-of-magnitude scaling but should be refined with full multi-level polarizability for precise trap depths (see e.g. Refs. on atomic polarizability).

## Characteristic time scale

We define the characteristic time scale $\tau$ used to normalize temporal quantities as the typical radial oscillation timescale in the trap (harmonic approximation near the bottom):

$$\tau \equiv \sqrt{\frac{m w_0^2}{2|U_0|}}.$$

For $^{87}$Rb ($m \approx 1.443 \times 10^{-25}\,\mathrm{kg}$), the numbers above give

$$\tau \approx \sqrt{\frac{(1.443 \times 10^{-25}\,\mathrm{kg})\ (19.5 \times 10^{-6}\,\mathrm{m})^2}{2\ |U_0|}} \approx 9.6 \times 10^{-5}\,\mathrm{s} \approx 96\,\mu\mathrm{s}.$$

This is the order of magnitude of the radial oscillation period for atoms trapped near the beam center with the given parameters.

### Dimensionless variables and their numerical scales

We therefore adopt the dimensionless variables

$$\tilde{\rho} = \frac{\rho}{w_0}, \qquad \tilde{z} = \frac{z}{z_R}, \qquad \tilde{t} = \frac{t}{\tau}.$$

With the numerical values above:

- $w_0 = 19.5\,\mu\text{m}$ (sets radial scale);
- $z_R \approx 1.12\,\text{mm}$ (sets axial scale);
- $\tau \approx 96\,\mu\text{s}$ (sets time scale).

Using these scales the equations of motion are written in the unitless form

$$\frac{d^2\tilde{\rho}}{d\tilde{t}^2} = \tilde{a}_\rho(\tilde{\rho}, \tilde{z}), \qquad \frac{d^2\tilde{z}}{d\tilde{t}^2} = \tilde{a}_z(\tilde{\rho}, \tilde{z}),$$

where the dimensionless accelerations are obtained from the physical accelerations by

$$\tilde{a}_\rho = \frac{w_0}{\tau^2}\, a_\rho, \qquad \tilde{a}_z = \frac{z_R}{\tau^2}\, a_z,$$

with $a_\rho, a_z$ computed from the gradient of $U(\rho, z)$.

### Remarks and assumptions

- The trap depth estimate above uses a scalar, two-level, far-detuned approximation referenced to the $D_2$ line. For more accurate absolute $U_0$ values one should include the full atomic structure and sum over relevant transitions (or use measured polarizability data).
- The beam waist was taken as half the quoted MFD (i.e. MFD $\simeq 2\,w_0$), which is consistent with the common $1/e^2$ definition of Gaussian waist.
- Because $w_0$ is large (tens of $\mu$m) the Rayleigh range is comparatively long (millimetres). This implies the beam changes slowly over the MOT-fiber separation distances usually used (mm scale), and that axial variations of the beam must still be included in the acceleration.
- The numeric values above give natural dimensionless parameters $\tilde{\rho}, \tilde{z}, \tilde{t}$ of order unity for atoms within the MOT region; this improves numerical conditioning of the integrator.

# 4 Equations of Motion

The dimensionless **equations of motion** become:

$$\frac{d^2\tilde{\rho}}{d\tilde{t}^2} = \tilde{a}_\rho(\tilde{\rho}, \tilde{z}), \qquad \frac{d^2\tilde{z}}{d\tilde{t}^2} = \tilde{a}_z(\tilde{\rho}, \tilde{z}), \tag{4}$$

where $\tilde{a}_\rho$ and $\tilde{a}_z$ are the dimensionless radial and axial accelerations derived from the scaled potential.

# 5 Numerical Integration: Verlet Method

The **Verlet algorithm** is used to integrate these equations, providing excellent energy conservation for conservative systems:

$$\tilde{\mathbf{x}}_{i+1} = 2\tilde{\mathbf{x}}_i - \tilde{\mathbf{x}}_{i-1} + \tilde{\mathbf{a}}_i(\Delta\tilde{t})^2, \tag{5}$$

with velocities estimated using a central difference:

$$\tilde{\mathbf{v}}_i = \frac{\tilde{\mathbf{x}}_{i+1} - \tilde{\mathbf{x}}_{i-1}}{2\Delta\tilde{t}}. \tag{6}$$

The first step is initialized using a Taylor expansion:

$$\tilde{\mathbf{x}}_1 = \tilde{\mathbf{x}}_0 + \tilde{\mathbf{v}}_0\Delta\tilde{t} + \frac{1}{2}\tilde{\mathbf{a}}_0(\Delta\tilde{t})^2. \tag{7}$$

# 6 Physical Interpretation

- $w_0$ sets the **radial length scale**.
- $z_R$ sets the **axial length scale**.
- $\tau$ sets the **natural timescale** of atomic motion.
- The dimensionless formulation allows the simulation to be **general for any atom species or beam parameters**.

# 7 References to Code

- `Verlet.py`: Implements the **dimensionless Verlet integrator** and data saving.
- `Dynamics.py`: Contains **acceleration functions** derived from the optical potential.
- `simulation.py`: Initializes atomic positions and velocities, calls the integrator, and stores results.
- `analysis.py`: Performs post-processing, including **fraction of atoms captured by the fiber**.

# 8 Conclusion

This document provides the **theoretical derivation**, **dimensionless rescaling**, and **numerical method** for simulating atomic motion in a Gaussian optical trap. The combination of a well-defined potential, dimensionless equations, and the Verlet integrator ensures **accurate, stable, and general simulations**, suitable for research in cold atom and photonics experiments.

# A Derivation of Dimensionless Equations of Motion

We start from the optical potential:

$$U(\rho, z) = -U_0 \frac{w_0^2}{w(z)^2} \exp\left(-2\frac{\rho^2}{w(z)^2}\right), \tag{8}$$

and the force on the atom:

$$F_\rho = -\frac{\partial U}{\partial \rho}, \quad F_z = -\frac{\partial U}{\partial z}. \tag{9}$$

Dividing by $m$ gives the accelerations:

$$a_\rho = \frac{F_\rho}{m}, \quad a_z = \frac{F_z}{m}. \tag{10}$$

Introduce dimensionless variables:

$$\tilde{\rho} = \frac{\rho}{w_0}, \quad \tilde{z} = \frac{z}{z_R}, \quad \tilde{t} = \frac{t}{\tau}, \quad \tau = \sqrt{\frac{m w_0^2}{2U_0}}. \tag{11}$$

Then

$$\frac{d^2\tilde{\rho}}{d\tilde{t}^2} = \frac{w_0}{\tau^2} a_\rho = \tilde{a}_\rho(\tilde{\rho}, \tilde{z}), \tag{12}$$

$$\frac{d^2\tilde{z}}{d\tilde{t}^2} = \frac{z_R}{\tau^2} a_z = \tilde{a}_z(\tilde{\rho}, \tilde{z}). \tag{13}$$

The resulting equations are now **unitless** and can be numerically integrated using the Verlet method, capturing the correct dynamics independent of absolute physical units.

# B Explicit form of the accelerations

In this appendix we provide the explicit analytic expressions for the radial and axial accelerations used in the simulation. We start from the optical potential (as in the main text)

$$U(\rho, z) = -U_0 \frac{w_0^2}{w(z)^2} \exp\Big(-2\frac{\rho^2}{w(z)^2}\Big), \qquad w(z) = w_0\sqrt{1 + \Big(\frac{z}{z_R}\Big)^2}.$$

It is convenient to define the *dimensionless potential*

$$V(\tilde{\rho}, \tilde{z}) \equiv \frac{U(\rho, z)}{U_0} = -\frac{1}{\widetilde{w}(\tilde{z})^2} \exp\Big(-2\frac{\tilde{\rho}^2}{\widetilde{w}(\tilde{z})^2}\Big), \qquad \widetilde{w}(\tilde{z}) \equiv \sqrt{1 + \tilde{z}^2},$$

where $\tilde{\rho} = \rho/w_0$ and $\tilde{z} = z/z_R$ as in the main text.

The physical accelerations are

$$a_\rho(\rho, z) = -\frac{1}{m}\frac{\partial U}{\partial \rho}, \qquad a_z(\rho, z) = -\frac{1}{m}\frac{\partial U}{\partial z}.$$

Using the chain rules $\partial/\partial\rho = (1/w_0)\partial/\partial\tilde{\rho}$ and $\partial/\partial z = (1/z_R)\partial/\partial\tilde{z}$, these can be expressed in terms of derivatives of $V$:

$$a_\rho(\rho, z) = -\frac{U_0}{m w_0}\frac{\partial V}{\partial \tilde{\rho}}, \qquad a_z(\rho, z) = -\frac{U_0}{m z_R}\frac{\partial V}{\partial \tilde{z}}.$$

In the dimensionless time $\tilde{t} = t/\tau$ with $\tau$ defined in the main text, the dimensionless accelerations used by the integrator are

$$\tilde{a}_\rho \equiv \frac{w_0}{\tau^2}\, a_\rho = -\frac{U_0}{m\tau^2}\,\frac{\partial V}{\partial \tilde{\rho}}, \qquad \tilde{a}_z \equiv \frac{z_R}{\tau^2}\, a_z = -\frac{U_0}{m\tau^2}\,\frac{\partial V}{\partial \tilde{z}}. \tag{14}$$

Hence the whole spatial dependence is contained in the derivatives of $V$, while the global multiplicative factor $C \equiv \dfrac{U_0}{m\tau^2}$ depends on the chosen scaling.

## Derivation step-by-step

It is convenient to introduce the auxiliary function (this is the same `beta` function defined in the code):

$$\beta(\tilde{z}) \;\equiv\; \frac{1}{1+\tilde{z}^2} \qquad \Longrightarrow \qquad \frac{d\beta}{d\tilde{z}} \equiv \beta'(\tilde{z}) = -2\tilde{z}\,\beta(\tilde{z})^2.$$

With this definition the dimensionless potential (Appendix A) reads

$$V(\tilde{\rho},\tilde{z}) = -\beta(\tilde{z})\,\exp\!\big(-2\,\beta(\tilde{z})\,\tilde{\rho}^2\big),$$

and its derivatives assume the compact forms

$$\frac{\partial V}{\partial \tilde{\rho}}(\tilde{\rho},\tilde{z}) = 4\,\beta(\tilde{z})^2\,\tilde{\rho}\,\exp\!\big(-2\,\beta(\tilde{z})\,\tilde{\rho}^2\big), \tag{15}$$

$$\frac{\partial V}{\partial \tilde{z}}(\tilde{\rho},\tilde{z}) = \beta'(\tilde{z})\,\big(2\,\beta(\tilde{z})\,\tilde{\rho}^2 - 1\big)\,\exp\!\big(-2\,\beta(\tilde{z})\,\tilde{\rho}^2\big). \tag{16}$$

Recalling the multiplicative prefactor $C \equiv U_0/(m\tau^2)$ (see Eq. (14)) the dimensionless accelerations used by the integrator can be written very compactly as

$$\boxed{\tilde{a}_\rho(\tilde{\rho},\tilde{z}) = -\,C\;4\,\beta(\tilde{z})^2\,\tilde{\rho}\;\exp\!\big(-2\,\beta(\tilde{z})\,\tilde{\rho}^2\big)} \tag{17}$$

$$\boxed{\tilde{a}_z(\tilde{\rho},\tilde{z}) = -\,C\;\beta'(\tilde{z})\;\big(2\,\beta(\tilde{z})\,\tilde{\rho}^2 - 1\big)\;\exp\!\big(-2\,\beta(\tilde{z})\,\tilde{\rho}^2\big)} \tag{18}$$

These expressions are algebraically identical to the expanded formulas presented earlier, but the $\beta$-form is more compact and numerically convenient: the code can compute $\beta(\tilde{z})$ once per time-step and reuse it for both radial and axial components.

## Numeric evaluation for the experimental parameters

Using the experimental values adopted in Section 3:

$$\lambda_{\mathrm{L}} = 1064\,\mathrm{nm}, \quad P = 1\,\mathrm{W}, \quad \mathrm{MFD} = 39\,\mu\mathrm{m}, \qquad w_0 = 19.5\,\mu\mathrm{m},$$

and the trap-depth order-of-magnitude estimate $|U_0|/k_B \approx 2.2\times10^{-4}\,\mathrm{K}$ (see Section 3), the characteristic time and numeric prefactor evaluate approximately to

$$\tau \approx 9.5\times10^{-5}\,\mathrm{s}, \qquad C = \frac{U_0}{m\tau^2} \approx 2.33\times10^{6}.$$

Therefore, with these experimental choices the dimensionless accelerations (**??**)–(**??**) become numerically:

$$\tilde{a}_\rho(\tilde{\rho},\tilde{z}) \approx -2.33\times10^{6}\;\frac{4\tilde{\rho}}{(1+\tilde{z}^2)^2}\;\exp\!\Big(-\frac{2\tilde{\rho}^2}{1+\tilde{z}^2}\Big),$$

$$\tilde{a}_z(\tilde{\rho},\tilde{z}) \approx -2.33\times10^{6}\;\frac{2\tilde{z}(\tilde{z}^2+1-2\tilde{\rho}^2)}{(1+\tilde{z}^2)^3}\;\exp\!\Big(-\frac{2\tilde{\rho}^2}{1+\tilde{z}^2}\Big).$$

### Remarks on implementation

- The code implements the accelerations in the dimensionless form shown above (the integrator expects $\tilde{a}_\rho, \tilde{a}_z$ evaluated at the current $\tilde{\rho}, \tilde{z}$). Using the dimensionless expressions avoids repeated conversions and keeps the integrator inputs numerically well-scaled.
- The exponential factor ensures the force decays rapidly away from the beam axis; the axial derivative contains the geometric term $(\tilde{z}^2 + 1 - 2\tilde{\rho}^2)$ which accounts for the change of waist with $\tilde{z}$.
- In the code a logical mask (update = z > 0) is applied to freeze the motion when atoms reach the fiber plane (captured atoms), which is why the accelerations are multiplied by that conditional in the integrator loop.
- For high-precision work replace the scalar two-level estimate of $U_0$ used above with the full multi-level polarizability at $\lambda_{\mathrm{L}}$ (see main text remarks); this modifies the numerical value of $C$ but not the functional dependence on $\tilde{\rho}, \tilde{z}$.

# C Mode Field Diameters of Common Hollow-Core Fibers

The choice of $w_0$ in the dimensionless model is linked to the optical mode-field diameter (MFD) of the guiding fiber. Hollow-core fiber (HCF) designs such as photonic bandgap, kagome, and anti-resonant fibers offer different MFDs depending on guiding mechanisms and core geometry. Table 1 below summarizes representative MFD ranges based on published literature:

| **Fiber type** | **Guiding mechanism** | **Typical MFD ($\mu$m)** |
|---|---|---|
| Photonic Bandgap HCF | Photonic bandgap | 5–10 |
| Kagome HCF | Inhibited coupling | 20–50 |
| Negative Curvature HCF | Inhibited coupling | 30–60 |
| Anti-Resonant HCF | Anti-resonant reflection | 25–50 |
| HC-PCF (mixed guidance) | Hybrid photonic crystal | 5–15 |

Table 1: Representative mode-field diameters (MFD) of different hollow-core fiber designs used in cold-atom and nonlinear optics experiments. Values are approximate and depend on core geometry and wavelength [1, 2].

For example, kagome-style hollow-core anti-resonant fibers demonstrate low attenuation near 1 µm wavelength and support large mode diameters (tens of $\mu$m), advantageous for coupling high-power beams and reducing intensity-related heating [1]. The MFD ranges given here help determine the physical $w_0$ used for normalization in the simulation.

# References

[1] N. V. Wheeler *et al.*, "Low-loss Kagome hollow-core fibers operating from the near- to the mid-IR," *Opt. Lett.*, vol. 42, no. 13, pp. 2571–2574, 2017.

[2] G. J. Pearce *et al.*, "Models for guidance in kagome-structured hollow-core photonic crystal fibers," *Opt. Express*, vol. 15, no. 20, pp. 12680–12691, 2007.