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Influence of optical aberrations on the accuracy of an atomic gravimeter

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Abstract: We present numerical simulations of the impact of laser beam wavefront aberrations in cold atom interferometers. We demonstrate that to reach accuracy at the mrad level, simulations cannot be based on a description of the retroreflection optics only with low-order Zernike polynomials, as the results will then depend on the decomposition order and the decomposition technique chosen. Moreover, simulations with high-order Zernike polynomials or equivalently high spatial frequency components require the propagation of aberrations to be taken into account, rather than adding them to the ideally propagated beam. Finally, we examine the impact of the parameters of the atomic source and show that the use of delta-kicked atomic cloud would efficiently mitigate the impact of this systematic effect.

1. Introduction

Since the first realizations of a gyroscope [1] and a gravimeter [2] with atom interferometers, significant research efforts have been made to tailor these sensors for a variety of applications [3], and to improve both their sensitivity and accuracy [4]. Atomic interferometers allow to measure inertial quantities such as accelerations, like gravity, gravity gradients, and rotations, in laboratory setups [1, 2, 5–7], on dynamic platforms [8, 9] or on field [10, 11]. They allow for performing ultrasensitive tests of fundamental physics [12, 13] on the ground, and first cold atom experiments in space [14–16] are paving the way for ambitious missions operating these sensors onboard satellites [17–19].

Matter-wave interferometers consist in a series of coherent light pulses, separated by free evolution time, which split, deflect and finally recombine the atomic wavepackets. At each light-matter interaction, the phase of the light field is imprinted on the wavepacket. As times and laser frequencies are well defined, so does the scale factor of the interferometric phase. In addition, many of the systematic effects can be theoretically modeled and then suppressed thanks to sequences of measurements [5]. Among the remaining systematics, one of the most difficult to precisely evaluate is the one related to the wavefront aberrations of the lasers [4], which perturb the laser phases imprinted at the time of the pulses, depending on the position of the wavepacket in the light field, [5] and modify the trajectories of the atoms [20, 21]. The phase shift resulting from wavefront aberrations has been studied through different approaches in existing apparatus. For instance, the size of the detection [22] or the size of the Raman beams [20, 21, 23] have been modulated, as well as the temperature of the atomic cloud [24]. Moreover, it has been demonstrated that the bias caused by the introduction of a characterized optics could be either simulated and retrieved from the measured value [22] or corrected thanks to a deformable mirror [25]. This systematic effect will also be the subject of future studies for specifications in the context of state-of-the-art atom interferometers aboard space missions [17, 18].

In this paper, we demonstrate that to accurately calculate the phase bias to better than the mrad level, we cannot restrict the description of retro-reflecting optics to low order Zernike polynomials [26]. In addition, we show that considering aberrations described by high Zernike orders, or equivalently with high spatial frequencies, imposes to take their propagation into account. We apply these results to the concrete case of a gravimeter experiment [5] with

characterized, high-quality retro-reflecting mirrors.

2. Description of the gravimeter

The atom interferometer considered here is a gravimeter. It is a two-wave interferometer based on a $\frac{\pi}{2} - \pi - \frac{\pi}{2}$ sequence of stimulated Raman transitions separated by a free evolution time $T = 80$ ms. Thanks to a sequence of four measurements, most systematic shifts are eliminated [5], the remaining effects being the Coriolis phase shift, which can be evaluated by rotating the gravimeter of 180° or suppressed by compensating the Earth rotation [27], and the one resulting from wavefront aberrations. For free-falling atoms in the gravity field g and Raman counter-propagating laser fields aligned along the vertical axis with a linear sweep α of their angular frequency difference, the interferometer phase $\Delta\Phi$ is given by

$$\Delta\Phi = \phi_1 - 2\phi_2 + \phi_3 = (k_{\text{eff}}g - \alpha)T^2 + \Delta\varphi. \quad (1)$$

$k_{\text{eff}} \approx \frac{4\pi}{\lambda}$ is the effective wavevector of the Raman transition, ϕ_i is the phase difference of the laser beams at the position of the i^{th} Raman pulse, and $\Delta\varphi$ is the interferometer phase shift caused by wavefront aberrations. Since the sensitivity factor is $k_{\text{eff}}T^2 = 10^5 \text{ rad m}^{-1} \text{ s}^2$, a phase shift of 1 mrad corresponds to a bias of $10^{-8} \text{ m s}^{-2} = 1 \mu\text{Gal}$ in the measured gravity value. To assess the contribution of this effect and eventually subtract it from the experimental measurements, the numerical simulation presented thereafter is used.

The simulation consists of a Riemann integral over the 5D phase space of the atomic cloud, with the initial distribution in longitudinal position disregarded. Assuming initial normal distributions in each dimension, we define the finite radius of the hyper-sphere on which to integrate by fixing the weight of the distribution that will be neglected. Choosing a weight of 0.25 % leads to a bias lower than $5 \times 10^{-2} \mu\text{Gal}$ in the simulations. The field amplitude corresponds to a Gaussian distribution of 12 mm waist. It is defined at the collimator output and propagated to the positions of the four laser pulses used in the experiment, one for the velocity selection and three for the Raman pulses, by solving the Helmholtz equation with Fourier transforms. These positions correspond to the classical path of the free-falling atoms despite the separation of the different momentum components of the wavepackets. This approximation is valid as long as the phase of the laser field evolves linearly along the separation distance, which is the case for low enough transverse spatial frequencies of the aberrations as shown below. The propagation length with the retro-reflection is roughly 1 m, thus the field is represented on a square grid with 84 mm sides and 2048 points along each transverse dimension to satisfy the sampling condition [28]. The transition probability is calculated for multiple sweep frequencies α , and eventually a fit with the function $P = P_m - \frac{C}{2} \cos(\Delta\Phi)$ allows to extract the interferometer phase bias (1) together with the contrast C and the mean value P_m of the transition probability. With the typical parameters chosen to run the simulations, the uncertainty obtained on the phase from the fit is typically $6 \times 10^{-3} \mu\text{Gal}$. Introducing deviations from the free falling trajectories due to extra-photon recoil [20] modify the results by quantities that are typically orders of magnitude smaller than the results without taking it into account, which is consistent with the typical size of the cloud, and the spatial frequencies and amplitudes of aberrations considered [21]. Hence, for simplicity and comparison with analytical models the results shown below do not take extra-photon recoil into account.

3. Mirror with an arbitrary surface

To our knowledge, most studies of the effect of laser wavefront distortions caused by retro-reflecting optics in atomic interferometers have used low-order Zernike polynomials to describe the wavefront aberrations [22, 24, 25], as these polynomials are generally used for this purpose in optics [29, 30] and in particular for the analysis of Shack-Hartmann sensor and optical

interferometers measurements. Though the contribution of high-order Zernike polynomials is not necessarily zero, even for large atomic clouds [5]. Moreover, propagation is usually not taken into account: aberrations are simply added to the wavefront of the propagated beam for the ideal case of a perfectly flat mirror [23, 24].

To examine the effect of each Zernike polynomial, we start by considering mirrors with an arbitrary surface defined by Zernike polynomials with rotational invariance Z_n^0 with n even, as in the case of an atomic cloud with the same symmetry property and coaxially centered, the contribution of the others Zernike polynomials is null. In Figure 1, the phase shift of the gravimeter is simulated with an atom source evaporatively cooled in a dipole trap, resulting in an atomic cloud of size of order of $\sigma_{x,y} = 10 \mu\text{m}$ and the possibility of adjusting the temperature [5, 24]. Irrespective of the index n of the Zernike polynomial, the amplitude of the aberration is set to $\frac{\lambda}{200}$. To consider only the impact of the mirror aberrations, the contribution due to the Gaussian field propagation, obtained with Z_0^0 , is subtracted. Finally, as the Zernike polynomials Z_n^0 have an overall factor $(-1)^{\frac{n}{2}}$, the absolute value of the phase shift is considered for simplicity.

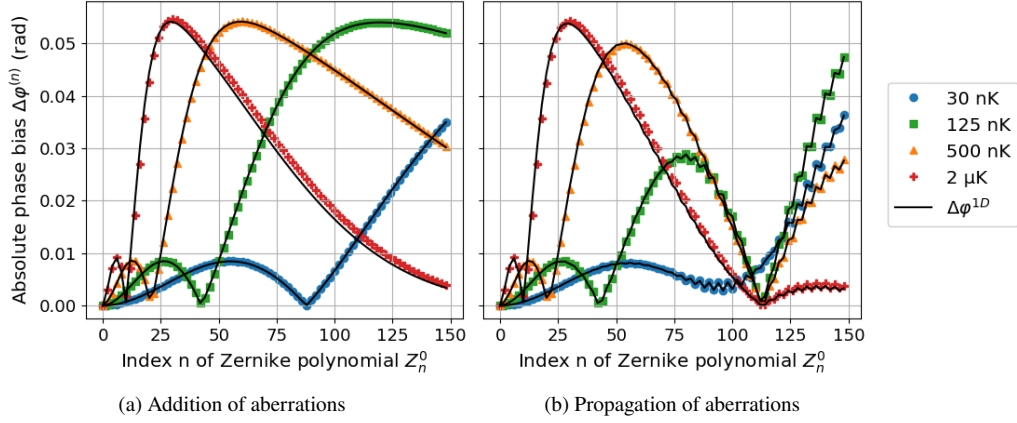


Fig. 1. Absolute phase bias caused by a mirror surface represented by a Zernike polynomial Z_n^0 on a $2R = 27 \text{ mm}$ diameter with an amplitude $\gamma = \frac{\lambda}{200}$, for an interferometer duration $2T = 160 \text{ ms}$, cloud size $\sigma_{x,y} = 10 \mu\text{m}$ and temperature $\Theta \in \{30, 125, 500, 2000\} \text{ nK}$. Markers corresponds to simulations where the aberrations have been: (a) added to the beam, (b) propagated with the beam. The continuous black lines $\Delta\phi^{1D}$ correspond to the 1D integral: (a) for addition (3), (b) for propagation (5) of the aberrations. Errorbars are smaller than the markers.

The simulations are carried out for a mirror of radius $R = 13.5 \text{ mm}$ and for different atomic cloud temperatures Θ from 30 nK to 2 μK . Firstly, mirror surface aberrations are added to the propagated field in the ideal case [23, 24], which corresponds to the markers in Figure 1a. These results show a maxima for high-order Zernike polynomials and are similar up to a temperature-dependent scaling factor on the Zernike index n , detailed hereafter. Secondly, the mirror aberrations are added to the field at the mirror position and then propagated, corresponding to the markers in Figure 1b. These second simulations exhibit significant differences at large Zernike orders when the ratio $\frac{(n+1)^2 \Delta z_{1,\text{mir}}}{k_{\text{eff}} R^2}$ starts to be of the order of 1, with $\Delta z_{1,\text{mir}}$ the distance between the mirror and the position of the first Raman pulse, as explained below. Considering that the atomic cloud is initially distributed according to a centered normal distribution of standard deviation $\sigma_{x,y}$ for its transverse position and according to a centered normal distribution of standard deviation $\sigma_v = \sqrt{\frac{k_B \Theta}{m_{\text{RB}}}}$ for its transverse velocity, the atomic distribution along the radial

coordinate ρ after a time t is given by

$$w(\rho, t) d\rho = \frac{\rho}{\sigma_\rho^2(t)} e^{-\frac{\rho^2}{2\sigma_\rho^2(t)}} d\rho \text{ with } \sigma_\rho^2(t) = \sigma_{xy}^2 + \sigma_v^2 t^2. \quad (2)$$

For a mirror of radius R with a surface described by the Zernike polynomial Z_n^0 of amplitude γ , in the case of added aberrations to an ideally propagated plane wave, the interferometric phase bias is

$$\Delta\varphi_{\text{add}}^{(n)} = \int \frac{4\pi\gamma}{\lambda} Z_n^0\left(\frac{\rho}{R}\right) [w(\rho, t_0) - 2w(\rho, t_0 + T) + w(\rho, t_0 + 2T)] d\rho. \quad (3)$$

t_0 is the time between the beginning of the free fall and the first Raman pulse. This model based on a 1D integral corresponds to the continuous black lines in Figure 1a and can be solved analytically by replacing the Zernike polynomial by its Bessel function approximation (A2)

$$\Delta\varphi_{\text{add}}^{(n)} \approx \frac{4\pi\gamma_n}{\lambda} e^{-\frac{\sigma_\rho^2(t_0)}{2\rho_n^2}} \left[1 - 2e^{-\frac{\sigma_v^2(T^2+2t_0T)}{2\rho_n^2}} + e^{-\frac{\sigma_v^2(4T^2+4t_0T)}{2\rho_n^2}} \right]. \quad (4)$$

$\gamma_n = (-1)^{\frac{n}{2}} \gamma$, $\rho_n = \frac{R}{n+1}$ is the characteristic length of the oscillation of the Zernike polynomial close to the center of the mirror. Neglecting the initial size σ_{xy} with respect to the expansion term $\sigma_v t_0$ in equation (4) results in an expression that depends on the product $(n+1)\sigma_v$, which explains the scaling feature in the index n with respect to temperature shown in Figure 1a. In addition, the averaging of the aberrations over the cloud efficiently suppresses spatial frequencies greater than the inverse of the atomic cloud size at the first Raman pulse $\frac{1}{\sigma_\rho(t_0)}$. When decreasing the temperature the bracketed term tends to zero, such that the unbiased g value is obtained [5]. Taking aberration propagation into account, the interferometric phase shift depends on the phase of $U(\rho, z_i)$ the complex amplitude of the laser field at the i^{th} Raman pulses

$$\Delta\varphi_{\text{prop}}^{(n)} = \int [\arg(U(\rho, z_1)) w(\rho, t_0) - 2\arg(U(\rho, z_2)) w(\rho, t_0 + T) + \arg(U(\rho, z_3)) w(\rho, t_0 + 2T)] d\rho - k_{\text{eff}} g T^2. \quad (5)$$

This model together with the approximation up to second order of the propagation of the aberrations presented in the **Appendix A: Propagation of aberrated beam**, corresponds to the black lines in Figure 1b. Using the first order correction (A3) of the propagation of the field with a Zernike wavefront aberration Z_n^0 and the same approximations as the ones leading to equation (4) results in

$$\Delta\varphi_{\text{prop}}^{(n)} \approx \frac{4\pi\gamma_n}{\lambda} e^{-\frac{\sigma_\rho^2(t_0)}{2\rho_n^2}} \left[\cos\left(\frac{\Delta z_{1,\text{mir}}}{k_{\text{eff}}\rho_n^2}\right) - 2\cos\left(\frac{\Delta z_{2,\text{mir}}}{k_{\text{eff}}\rho_n^2}\right) e^{-\frac{\sigma_v^2(T^2+2t_0T)}{2\rho_n^2}} + \cos\left(\frac{\Delta z_{3,\text{mir}}}{k_{\text{eff}}\rho_n^2}\right) e^{-\frac{\sigma_v^2(4T^2+4t_0T)}{2\rho_n^2}} \right]. \quad (6)$$

$\Delta z_{i,\text{mir}}$ is the distance between the position of the i^{th} Raman pulse and the mirror. This expression shows a characteristic variation length $l_n = k_{\text{eff}}\rho_n^2 = \frac{k_{\text{eff}}R^2}{(n+1)^2}$. Consequently, propagation is negligible when $n \ll \sqrt{\frac{2kR^2}{\Delta z_{1,\text{mir}}}}$, which corresponds in the gravimeter configuration to $n \ll 80$. Furthermore, as long as $n \ll \sqrt{\frac{2kR^2}{\Delta z}} \approx 1000$ corresponding to aberrations of typical variation

length of $\approx 10 \mu\text{m}$, where $\Delta z \approx 3 \text{ mm}$ is the maximal longitudinal separation of the atomic wavepackets, the distribution of the cloud's longitudinal position and the separation of the components of the wavepackets can be neglected. Finally, when decreasing the temperature, the expression in brackets in equation (6) does not generally becomes zero, unlike the case where aberrations are added (4). To reduce the bias on g , it is necessary either to obtain a better mirror with smaller aberrations of amplitude γ , or to use an atomic cloud with a larger initial size σ_{xy} which could be done through delta-kick collimation [31].

4. Specific mirror surface

We now examine the impact on the results, of the simulation of the propagation of the aberrations and of their representation on the Zernike polynomial basis, in the case of specific mirrors. For the sake of simplicity, we restrict the problem to the case where the mirror, the atomic cloud and the laser beams are coaxially centered. The mirrors surface have been analyzed using a Fizeau interferometer with a $77 \mu\text{m}$ resolution and are shown in Figure 2. They are characterized on the central disk of 5 mm radius by a typical peak-to-valley amplitude of $\approx 9 \text{ nm}$ and an RMS value of $\approx 1 \text{ nm}$. Simulations can be carried out directly using the raw mirror surface data, or the

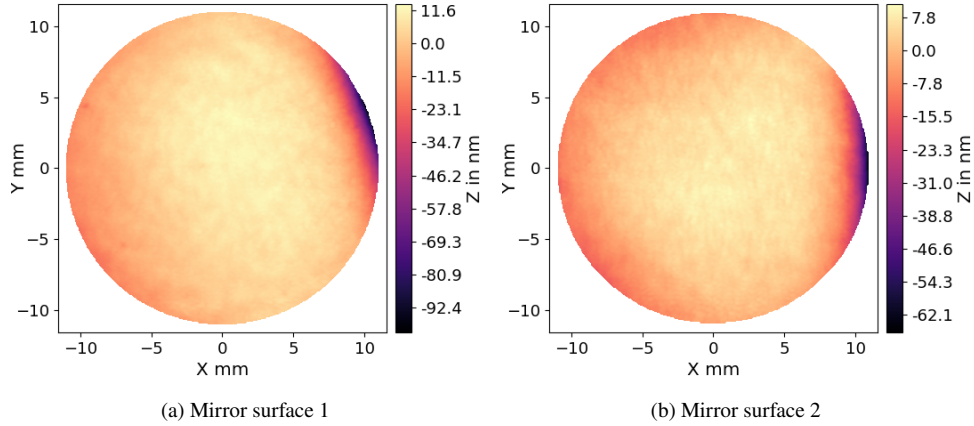


Fig. 2. Available mirrors surface truncated at 22 mm diameter and corrected of piston and tilt terms. On the central 5 mm radius disk: (a) mirror surface 1, peak-to-valley amplitude of 9.5 nm and RMS value of 1.5 nm, (b) mirror surface 2 and peak-to-valley amplitude of 9.2 nm, RMS value of 1.1 nm.

mirror surface can be decomposed on the basis of the Zernike polynomials. The usual method for performing such a decomposition is based on a least mean squares regression, which will be referred as *LSQR* in the following. However, as the Zernike polynomials form an orthogonal family on a reference disk, the decomposition can also be performed by a scalar product consisting of an integration over this disk. Using the mirror surface 1 in Figure 2a, simulation with the raw data yields a gravity bias $\Delta g_{\text{prop}}^{\text{Raw}} = -8.042(5) \mu\text{Gal}$ ($1 \mu\text{Gal} = 10^{-8} \text{ m s}^{-2}$), represented by the red line in Figure 3a. The mirror surface is decomposed over an increasing number of Zernike polynomials corresponding to the abscissa [32] and gravimeter simulations are performed with these decomposed surfaces, both for the least mean squares technique (solid blue squares) and for the scalar product (orange circles) decomposition. In addition, approximate results (green crosses) labeled *ID Integral*, are obtained using the coefficients of the scalar product decomposition together with the integral (5) and the propagation approximation outlined in the **Appendix A: Propagation of aberrated beam**. The simulations resulting from the decomposition show several μGal of difference with the one based on the raw data at low decomposition order

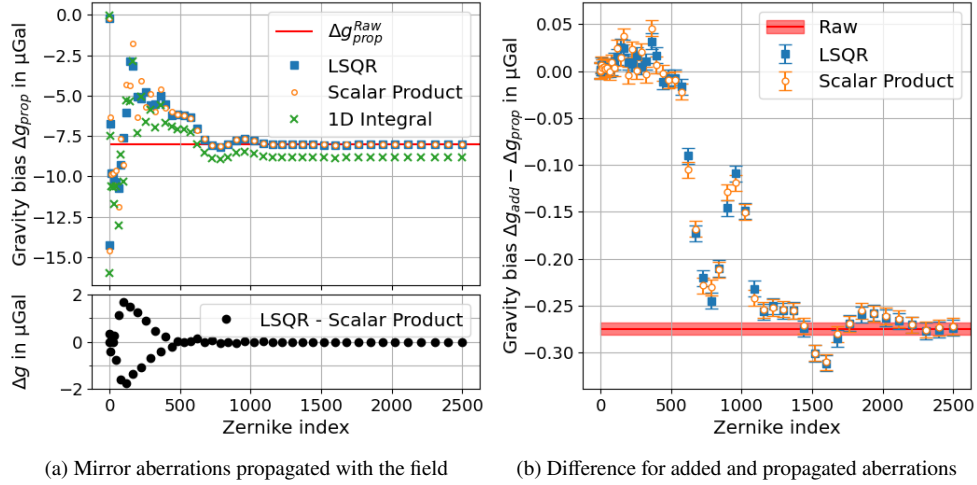


Fig. 3. Simulation of the gravimeter with the mirror surface 1 shown Figure 2a, for $T = 80$ ms, $\sigma_{xy} = 300$ μm and a temperature $\Theta = 2$ μK . The simulations are done for a decomposition of the mirror surface, either with least mean square *LSQR* or the *scalar product*, on a growing family of Zernike polynomials, (a) with propagation of the aberrations (errorbars are smaller than the markers). (b) Difference with the case of added aberrations to ideally propagated beam. The analytical points are derived from the 1D integrals (3)-5) with the coefficients obtained from the integral decomposition of the mirror surface. The Zernike indexing scheme ISO-14999 is used [32] and simulation points correspond to rotational invariant Zernike polynomials.

and converge to Δg_{prop}^{Raw} when considering sufficiently high-order Zernike polynomials, with the exception of the values resulting from the approximations for propagation and 1D integral, which converge to a difference of $-0.794(5)$ μGal . The difference between the results of the two decomposition methods: *LSQR* and the scalar product, is highlighted at the bottom of Figure 3a and reaches the μGal level for low-order decomposition. Eventually, the simulations were run a second time with the addition of the aberrations to the ideally propagated beam, with the raw data and both decomposition methods, the difference with the previous results that take propagation into account is shown in Figure 3b. For both methods there is initially no significant difference for decomposition on low-order Zernike polynomials, though the differences converge to that obtained with the use of the raw data: $-0.274(7)$ μGal .

Thus, to simulate the gravimeter to the μGal level, describing optical aberrations with low-order Zernike polynomials is not sufficient, as the result depends on the decomposition order considered and on the decomposition technique used. It is necessary either to consider high-order Zernike decomposition, or to use raw data with sufficiently high resolution, which is determined by the initial size of the cloud and its expansion length through the interferometer, and hence the propagation of the aberrations during laser beam propagation.

5. Dependence on the atomic cloud initial position

To compare simulations with experimental results, the initial preparation of the atomic cloud can be modified, for instance a dipole trap can be used after the magneto-optical trap (MOT) and molasses sequence to lower the initial cloud temperature [24], and delta-kick collimation technique could be used to obtain a larger cloud with a lower expansion temperature [31]. However, it is also important to be able to position the atomic cloud relative to the mirror and laser beams, as the spatial dependence of the bias can be significant, as shown below. For sake of

simplicity, the mirror and laser beams are considered to be coaxially centered and only the initial mean position of the atomic cloud is modified. In Figure 4, simulations are carried out for the same interferometer sequence with an interval between Raman pulses of 80 ms and for different configurations of the initial atomic cloud: (4a) in a MOT with a temperature of $\Theta = 2 \mu\text{K}$ and an initial size of $\sigma_{xy} = 300 \mu\text{m}$, (4b) in a dipole trap with a temperature of $\Theta = 30 \text{ nK}$ and an initial size of $\sigma_{xy} = 10 \mu\text{m}$, (4c) for a delta-kicked cloud with a temperature of $\Theta = 5 \text{ nK}$ and an initial size of $\sigma_{xy} = 200 \mu\text{m}$.

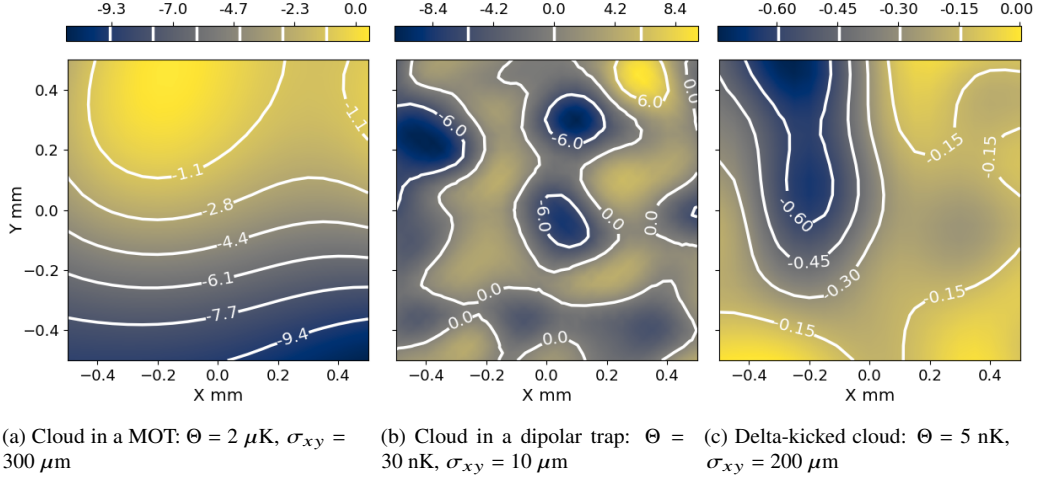


Fig. 4. Simulation of the gravimeter bias in μGal with the mirror surface 2 represented in Figure 2b, for an interferometer duration $2T = 160 \text{ ms}$. The initial mean position of the atomic cloud is changed over an area $[-500 \mu\text{m}, 500 \mu\text{m}] \times [-500 \mu\text{m}, 500 \mu\text{m}]$ and for three different initial configurations of the atomic cloud.

For the cloud in the MOT or delta-kick configuration in Figures 4a and 4c, the typical variation lengths correspond to the initial cloud size, which is larger than the $77 \mu\text{m}$ mirror surface resolution. Though, in the dipole trap configuration in Figure 4b, where the cloud size at the first Raman pulse is roughly $30 \mu\text{m}$, the typical variation length is close to the mirror resolution. In the latter case, simulation results are limited by the initial resolution of the mirror surface data.

While the MOT configuration in Figure 4a has a gravity bias gradient of $\approx 10 \mu\text{Gal mm}^{-1}$ at the center of the zone of interest, the area for $-500 \mu\text{m} \leq x \leq 500 \mu\text{m}$ and $200 \mu\text{m} \leq y \leq 500 \mu\text{m}$ exhibits a typical gradient of $\approx 1 \mu\text{Gal mm}^{-1}$ which would enhance the stability of the apparatus with respect to intensity fluctuations of the MOT laser beams that cause fluctuations in initial position [5]. Finally, in the delta-kicked cloud configuration of Figure 4c, the gradient is at maximum of the order of $\approx 1 \mu\text{Gal mm}^{-1}$ on the overall represented area, and the gravity bias is closer to the ideal case of the Gaussian beam reflected on a perfectly flat mirror, which yields a bias of $-0.21(1) \mu\text{Gal}$. This result is consistent with equation (6), as the dependence of the interferometric phase shift over the initial size is a Gaussian function, increasing the size of the source should result in bias closer to the ideal case.

6. Conclusion

In this paper, we show that to simulate the effect of wavefront aberrations in a cold-atom gravimeter at the mrad level, it is not sufficient to represent the wavefront aberrations of the retro-reflecting optics with low-order Zernike polynomials, as this will lead to errors at the mrad order depending on the decomposition order and the decomposition method chosen. In addition, for the distance considered between the retro-reflecting optics and the positions of the Raman

pulses, and the spatial frequencies of the aberrations considered, it is necessary to take into account the propagation of the aberrations and not simply add them to the beam propagated in the ideal case. The study of the dependence of the bias on the initial position of the atomic clouds shows that it would be necessary in a MOT configuration to be able to position the cloud relative to the mirror and laser beams with an accuracy of the order of $100 \mu\text{m}$ to reach the mrad level. Eventually, the use of a delta-kicked atomic source could reduce both the interferometer phase shift caused by wavefront aberrations and the sensitivity associated with the initial position of the atomic cloud, as the resulting bias is closer to the ideal case of a beam reflected on a flawless mirror.

This simulation is not exhaustive and focuses on the effect of wavefront aberrations, it could be developed in order to take into account additional features, such as the Coriolis effect and the two-photon light shift which are the next largest contributors to the inaccuracy budget [5, 24], as well as the residual differential light shift caused by the intensity fluctuations resulting from the propagation of the aberrations. Moreover, the characterization of the beam at the collimator output and of the different optics on the beam path, together with the use of an atomic distribution and detection response closer to experimental conditions [33], could improve the accuracy of this simulation. In addition, our simulations are based on data acquired with a Fizeau interferometer with a spatial resolution limited to $77 \mu\text{m}$. Accounting for higher spatial frequency components, which will have an impact in the case of a cloud with a typical size of tens of μm , would require to consider the longitudinal distribution of the cloud and to calculate the field along this longitudinal direction instead of simply using the mean position of the classical path.

Thanks to these simulations and their future comparisons with the experiment, we hope to be able to improve the characterization of our device and determine the targeted correction at the μGal level. More generally, the evaluation of wavefront aberrations will also be necessary to achieve better accuracy and complement the error budget of other atom interferometry inertial sensors, such as the ones embarked in space missions, which target beyond state-of-the-art performances.

Appendix A: Propagation of aberrated beam

The radial part of Zernike polynomials are specific cases of Jacobi polynomials [30]

$$R_n^m(x) = (-1)^{\frac{n-m}{2}} x^m P_{\frac{n-m}{2}}^{(m,0)}(1-2x^2) \text{ with } |x| \leq 1. \quad (\text{A1})$$

Using the Jacobi polynomials convergence property [34] and for $|x| \ll 1$ the radial Zernike polynomials can be approximated by a Bessel function

$$R_n^m(x) \approx (-1)^{\frac{n-m}{2}} \frac{\left(\frac{n+m}{2}\right)!}{\left(\frac{n-m}{2}\right)! \left(\frac{n+1}{2}\right)^m} J_m((n+1)x). \quad (\text{A2})$$

Considering a beam with Gaussian amplitude and a wavefront described by a Zernike polynomial with its radial part replaced by the Bessel approximation (A2), would lead to first order in amplitude of wavefront aberration to a generalized Bessel Gauss expression [35]. To have an analytical expression up to second order, a beam with a flat intensity and a wavefront described by a Zernike polynomial with rotational invariance is considered

$$\begin{aligned} U(\rho, 0) &= A e^{i\alpha Z_n^0\left(\frac{\rho}{R}\right)} \approx A e^{i\alpha_n J_0\left(\frac{\rho}{\rho_n}\right)} \\ &\approx A \left\{ 1 + i\alpha_n J_0\left(\frac{\rho}{\rho_n}\right) - \frac{\alpha_n^2}{2} J_0^2\left(\frac{\rho}{\rho_n}\right) \right\} \end{aligned} \quad (\text{A3})$$

With $\rho_n = \frac{R}{n+1}$. The first two terms can be propagated by solving the paraxial equation using the closure relation $\int_0^\infty u J_0(au) J_0(bu) du = \frac{\delta(a=b)}{a}$ and the Hankel transform. Eventually, using a continuity argument at $z = 0$, the Bessel function is replaced by the initial Zernike polynomial

$$U^{(1)}(\rho, z) = A e^{-ikz} \left\{ 1 + i\alpha e^{i\frac{z}{2k\rho_n^2}} Z_n^0\left(\frac{\rho}{R}\right) \right\}. \quad (\text{A4})$$

To treat the second order term of expression (A3), the integral of the triple product of 0th order Bessel function [36] is used

$$\int_0^\infty \rho J_0(a\rho) J_0(b\rho) J_0(c\rho) d\rho = \frac{1}{2\pi\Delta} \delta_{\Delta>0} \quad (\text{A5})$$

$$\Delta^2 = s(s-a)(s-b)(s-c) \text{ with } s = \frac{1}{2}(a+b+c).$$

Then performing a change of variable $u = \arcsin\left(\frac{K}{2\rho_n}\right)$, with K the coordinate in reciprocal space, the propagated expression of the second order term is derived using the integral $\int_0^{\frac{\pi}{2}} J_0(2\gamma \sin\theta) \cos(2\mu\theta) = \frac{\pi}{2} J_\mu^2(\gamma)$ [37],

$$U^{(2)}(\rho, z) = -\frac{\alpha^2}{2} A e^{-ikz} e^{i\frac{z}{k\rho_n^2}} \times \left\{ J_0\left(\frac{z}{k\rho_n^2}\right) J_0^2\left(\frac{\rho}{\rho_n}\right) \right. \\ \left. + 2 \sum_{p=1}^{\infty} (-1)^p J_{2p}\left(\frac{z}{k\rho_n^2}\right) J_{2p}^2\left(\frac{\rho}{\rho_n}\right) \right. \\ \left. - 2i \sum_{p=0}^{\infty} (-1)^p J_{2p+1}\left(\frac{z}{k\rho_n^2}\right) J_{2p+1}^2\left(\frac{\rho}{\rho_n}\right) \right\}. \quad (\text{A6})$$

Again, by continuity at $z = 0$, the Bessel function $J_0\left(\frac{\rho}{\rho_n}\right)$ can be replaced by the initial Zernike polynomial $Z_n^0\left(\frac{\rho}{R}\right)$.

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