GEOMETRIC OPTICS WITH ATOMIC BEAMS
SCATTERED BY A DETUNED STANDING LASER WAVE

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Abstract
We report on theoretical and numerical study of propagation of atomic beams crossing a detuned standing-wave laser beam in the geometric optics limit. The interplay between external and internal atomic degrees of freedom is used to manipulate the atomic motion along the optical axis by light. By adjusting the atom-laser detuning, we demonstrate how to focus, split and scatter atomic beams in a real experiment. The novel effect of chaotic scattering of atoms at a regular near-resonant standing wave is found numerically and explained qualitatively. Some applications of the effects found are discussed.

Keywords: atomic scattering, standing wave, optical nanolithography

1 Introduction
Manipulation of atoms by light becomes possible due to the dipole forces which are well described by the semiclassical model with quantum description of internal atomic transitions induced by a near resonant laser field and classical description of their center-of-mass motion [1]. For the first time, the ideas to trap and channel cold atoms with the help of standing laser waves (SLW) have been proposed by V. Letokhov and his co-workers [2–4]. The ability of a SLW to deflect, channel and split atomic beams [5,6] has been used for a variety of applications including atom microscopy, interferometry, isotope separation and optical lithography [6–9]. Lasers can be used to manipulate atomic trajectories to create atomic analogues of such familiar optical phenomena as focusing of light, beam splitting and light scattering. It is remarkable that now we are able to reverse the roles of light and matter from their familiar roles. The semiclassical description, used in this paper, is similar to the geometric optics limit in conventional optics. Atomic trajectories play the role of light rays with the SLW being a light mask.

In the present paper we intend to demonstrate theoretically and numerically that adjusting in an experiment only one parameter, the detuning between the frequencies of a working atomic transition and the SLW, one can explore a variety of the regimes of the atom-laser interaction to focus, split and scatter atomic beams. Near the atom-field resonance, where the interaction between the internal and external atomic degrees of freedom is intense, there is a possibility to create conditions for chaotic scattering of atoms [10–12] without any additional efforts like a SLW modulation. It becomes possible due to the peculiarities of the dipole force in a near-resonant optical lattice [13–16].
2 Focusing, splitting, bunching and scattering of atomic beams

2.1 Equations of motion

A beam of two-level atoms in the $z$ direction crosses a SLW laser field with optical axis in the $x$ direction. The laser beam has the Gaussian profile $\exp[-(z-z_0)^2/r^2]$ with $r$ being the $e^{-2}$ radius at the laser beam waist. The characteristic length of the atom-field interaction is supposed to be $\pm 1.5r$ because the light intensity at $z = \pm 1.5r$ is two orders of magnitude smaller than the peak value. The longitudinal velocity of atoms, $v_x$, is much larger than their transversal velocity $v_z$ and is supposed to be constant. Thus, the spatial laser profile may be replaced by the temporal one. The Hamiltonian of a two-level atom in the one-dimensional SLW can be written in the frame rotating with the angular laser frequency $\omega_f$ as follows:

$$
\hat{H} = \frac{P^2}{2m_a} + \hbar (\omega_a - \omega_f) \hat{\sigma}_z - \hbar \omega_0 \exp\left[-\left(t - \frac{3}{2} \sigma_t^2 / \sigma_r^2\right) \frac{\hat{\sigma}_- + \hat{\sigma}_+}{3} \cos k_f x_a - \frac{i \hbar \Gamma}{2} \hat{\sigma}_+ \hat{\sigma}_-,
$$

(1)

where $\hat{\sigma}_{\pm,z}$ are the Pauli operators for the internal atomic degrees of freedom, $X_a$ and $P$ are the classical atomic position and momentum, $\Gamma$, $\omega_a$, and $\Omega_0$ are the decay rate, the atomic transition and maximal Rabi frequencies, respectively. The simple wave function for the electronic degree of freedom is $|\Psi(t)\rangle = a(t)|2\rangle + b(t)|1\rangle$, where $a \equiv A + i \alpha$ and $b \equiv B + i \beta$ are the complex-valued probability amplitudes to find the atom in the excited, $|2\rangle$, and ground, $|1\rangle$, states, respectively.

In the semiclassical approximation, atom with quantized internal dynamics is treated as a point-like particle to be described by the Hamilton–Schrödinger equations of motion written for the real and imaginary parts of the probability amplitudes

$$
\dot{x} = \omega_x p, \quad \dot{p} = -2 \exp[-(\tau - \frac{3}{2} \sigma_x \sigma_f^2 / \sigma_r^2)] (AB + \alpha \beta) \sin x,
$$

$$
\dot{A} = \frac{1}{2} (\omega_r p^2 - \Delta) \alpha - \frac{1}{2} \gamma A - \exp[-(\tau - \frac{3}{2} \sigma_x \sigma_f^2 / \sigma_r^2)] \beta \cos x,
$$

$$
\dot{\alpha} = -\frac{1}{2} (\omega_r p^2 - \Delta) A - \frac{1}{2} \gamma \alpha + \exp[-(\tau - \frac{3}{2} \sigma_x \sigma_f^2 / \sigma_r^2)] B \cos x,
$$

$$
\dot{B} = \frac{1}{2} (\omega_r p^2 + \Delta) \beta - \exp[-(\tau - \frac{3}{2} \sigma_x \sigma_f^2 / \sigma_r^2)] \alpha \cos x,
$$

$$
\dot{\beta} = -\frac{1}{2} (\omega_r p^2 + \Delta) B + \exp[-(\tau - \frac{3}{2} \sigma_x \sigma_f^2 / \sigma_r^2)] A \cos x,
$$

(2)

where $x \equiv k_f X_a$ and $p \equiv P / h \omega_f$ are scaled atomic center-of-mass position and transversal momentum, respectively and dot denotes differentiation with respect to the dimensionless time $\tau \equiv \Omega_0 t$. The recoil frequency, $\omega_r \equiv h k_f^2 / m_a \Omega_0 \ll 1$, the atom-laser detuning, $\Delta \equiv (\omega_f - \omega_a) / \Omega_0$, the decay rate $\gamma = \Gamma / \Omega_0$, and the characteristic interaction time, $\sigma_r \equiv \gamma \Omega_0 / v_z$, are the control parameters.

Let us introduce instead of the complex-valued probability amplitudes $a$ and $b$ the following real-valued variables:

$$
u \equiv 2 \Re (ab^*), \quad v \equiv -2 \Im (ab^*), \quad z \equiv |a|^2 - |b|^2,
$$

(3)

where $u$ and $v$ are synchronized and quadrature components of the atomic electric dipole moment, respectively, and $z$ is the atomic population inversion. In the absence of any losses ($\gamma = 0$), Eqs. (2) can
be cast in the form

\[
\begin{align*}
\dot{x} &= \omega_r p, \\
\dot{p} &= -u \exp\left[-\left(\frac{3}{2} \frac{\tau}{\sigma} \right)^2\right] \sin x, \\
\dot{u} &= \Delta v, \\
\dot{v} &= -\Delta u + 2 \exp\left[-\left(\frac{3}{2} \frac{\tau}{\sigma} \right)^2\right] z \cos x, \\
\dot{z} &= -2 \exp\left[-\left(\frac{3}{2} \frac{\tau}{\sigma} \right)^2\right] v \cos x.
\end{align*}
\] (4)

The system (4) has two integrals of motion, namely, the total energy

\[
H \equiv \frac{\omega_r}{2} p^2 - u \cos x - \frac{\Delta}{2} z,
\] (5)

and the length of the Bloch vector, \(u^2 + v^2 + z^2 = 1\), whose conservation follows immediately from Eqs. (2).

Equations (4) constitute a nonlinear Hamiltonian autonomous system with two and a half degrees of freedom which, owing to the two integrals of motion, move on a three-dimensional hypersurface with a given energy value \(H\). In general, motion in a three-dimensional phase space in characterized by a positive Lyapunov exponent \(\lambda\), a negative exponent equal in magnitude to the positive one, and zero exponent [17]. The maximal Lyapunov exponent characterizes the mean rate of the exponential divergence of initially close trajectories and serves as a quantitative measure of dynamical chaos in the system. The values of the maximal Lyapunov exponent in dependence on the detuning, the recoil frequency and the initial atomic momentum have been computed in Refs. [14, 15].

There are different regimes of the center-of-mass motion along the SLW optical axis [12, 15]. In dependence on the initial conditions and the values of the control parameters, atoms may oscillate in a regular or a chaotic way in wells of the optical potential or move ballistically over its hills with regular or chaotic variations of their velocity. Chaotic motion with a positive value of the maximal Lyapunov exponent becomes possible in a narrow range of the detuning values, \(0 < |\Delta| < 1\) [15]. At \(\Delta = 0\), the synchronized electric-dipole component, \(u\), becomes a constant. That implies the additional integral of motion in the Hamiltonian version (4) of Eqs. (2) and the regular motion with zero maximal Lyapunov exponent. Far off the resonance, at \(|\Delta| > 1\), the motion is regular both in the trapping and ballistic modes.

It is remarkable that there is a specific type of motion, chaotic walking in a deterministic optical potential, when atoms can change the direction of motion alternating between flying through the SLW and being trapped in its potential wells. We would like to stress that the local instability produces chaotic center-of-mass motion in a rigid SLW without any modulation of its parameters. Chaotic walking occurs due to the specific behavior of the Bloch-vector component of a moving atom \(u\) whose shallow oscillations between the SLW nodes are interrupted by sudden jumps with different amplitudes while atom crosses each node of the SLW [15]. It looks like a random like shots happened in a fully deterministic environment. It follows from the second equation in the set (4) that those jumps result in jumps of the atomic momentum while crossing a node of the SLW. If the value of the atomic energy is close to the separatrix one, the atom after the corresponding jump-like change in \(p\) can either overcome the potential barrier and leave a potential well or it will be trapped by the well, or it will move as before. The jump-like behavior of \(u\) is the ultimate reason of chaotic atomic walking along a rigid SW.

The total atomic energy (5) consists of the kinetic one, \(K = \omega_r p^2 / 2\), and the potential one, \(U = -u \cos x - z \Delta / 2\). The optical potential changes its depth in course of time. Averaging over fast oscillations of the internal atomic variables, we get the averaged potential \(\bar{U} = -\bar{u} \cos x - \bar{z} \Delta / 2\) that can be used to explain why atoms move in such or another way.
At small detunings $|\Delta| \ll 1$, the potential is approximately $U \simeq u \cos x$. If $K(\tau = 0) > |U_{\text{max}}| = 1$, then the atom will move ballistically. This occurs if the initial atomic momentum, $p_0$, satisfies to the condition $p_0 > \sqrt{2/\omega_r}$. If the initial conditions are chosen to give $0 \leq K(\tau = 0) + U(\tau = 0) \leq 1$, the corresponding atoms with $0 \lesssim p_0 \lesssim \sqrt{2/\omega_r}$ are expected to move chaotically at the appropriate values of $\Delta$.

2.2 Focusing and splitting

In this section we demonstrate how to focus and split atomic beams crossing a Gaussian laser beam by varying only one of the control parameters, the atom-field detuning $\Delta$. Firstly, we perform simulation with a negligible probability of spontaneous emission and solve the Hamiltonian equations of motion (4) at comparatively large value of the detuning, $\Delta = 1$. To be concrete we take as an example calcium atoms with the working intercombination transition $4^1S_0 \rightarrow 4^3P_1$ at $\lambda_a = 657.5$ nm, the recoil frequency $\nu_{\text{rec}} \simeq 10$ KHz, and the lifetime of the excited state $T_{\text{sp}} = 0.4$ ms. Taking the maximal Rabi frequency to be $\Omega_0/2\pi = 2 \cdot 10^7$ Hz, the radius of the laser beam $r = 0.3$ cm, and the mean longitudinal velocity $v_z = 10^3$ m/s, the interaction time is estimated to be 0.9 ms, longer than the atomic lifetime. The normalized recoil frequency is $\omega_r = 4\pi\nu_{\text{rec}}/\Omega_0 = 10^{-3}$ and the normalized characteristic time is $\sigma_\tau = 400$.

Trajectories for 50 calcium atoms to be prepared in the ground states ($u_0 = v_0 = 0$, $z_0 = -1$) with the same initial momentum, $p_0 = 10$, and initial positions in the range $-\pi/10 \leq x \leq \pi/10$ are shown in Fig. 1. In units of the optical wavelength, $X = x/2\pi$, this range is $-0.05 \leq X \leq 0.05$. The focusing occurs at those moments of time when the average transverse momentum in the atomic beam is approximately equal to zero. If one turns off the laser at one of these moments, it becomes possible to reduce the beam width practically in ten times. The reason of focusing is simple. It is well known [3] that at positive blue detunings atoms are attracted to the nodes of the SLW where the minima of the optical potential are situated at $\Delta > 0$. The first node the atoms reach at $p_0 > 0$ is situated at $X = 1/4$. The initial kinetic atomic energy, $K_0 = 0.05$, is not enough to overcome the potential barrier whose depth can be estimated to be $\simeq 0.35$ because the simulation gives $\bar{u} \simeq 0$ and $\bar{z} \simeq -0.7$. So, all the atoms in the beam oscillate in the first potential well in the $x$-direction around the first node. The initial width of the beam, $\delta X_0 = 0.1$, is gradually reduced because in course of time the atoms with initial negative positions catch up with the ones with positive $X_0$ near the first turning point where the average beam momentum is close to zero. The time interval of the atomic interaction with the SLW field is estimated to be $3\sigma_\tau = 1200$. So, the atoms leave the potential well after that time and move freely (see Fig. 1).

In order to take into account spontaneous emission we use the standard stochastic wave-function technique [18,20] for solving Eqs. (2). The integration time is divided into a large number of small time intervals $\delta \tau$. At the end of the first interval, $\tau = \tau_1$, the probability of spontaneous emission, $s_1 = \gamma \delta \tau |a_{\tau_1}|^2 /(|a_{\tau_1}|^2 + |b_{\tau_1}|^2)$, is computed and compared with a random number, $\varepsilon$, from the interval $[0,1]$. If $s_1 < \varepsilon$, then one prolongs the integration but renormalizes the state vector in the end of the first interval at $\tau = \tau_1^+$: $a_{\tau_1^+} = a_{\tau_1} / \sqrt{|a_{\tau_1}|^2 + |b_{\tau_1}|^2}$ and $b_{\tau_1^+} = b_{\tau_1} / \sqrt{|a_{\tau_1}|^2 + |b_{\tau_1}|^2}$. If $s_1 \geq \varepsilon$, then the atom emits a spontaneous photon and jumps to the ground state at $\tau = \tau_1$ with $A_{\tau_1} = \alpha_{\tau_1} = \beta_{\tau_1} = 0$, $B_{\tau_1} = 1$. Its momentum in the $x$ direction changes for a random number from the interval $[0,1]$ due to the photon recoil effect, and the next time step commences.

We simulate lithium atoms with the relevant transition $2S_{1/2} \rightarrow 2P_{3/2}$, the corresponding wavelength $\lambda_a = 670.7$ nm, recoil frequency $\nu_{\text{rec}} = 63$ KHz, and the decay time $T_{\text{sp}} = 2.73 \cdot 10^{-8}$ s. With the maximal Rabi frequency $\Omega_0/2\pi \simeq 126$ MHz and the radius of the laser beam $r = 0.05$ cm one gets $\omega_r = 10^{-3}$,
Figure 1: (a) Focusing the atomic beam with a long lifetime of the excited state. (b) The effect of spontaneous emission on the focusing. The detuning is $\Delta = 1$ in both the cases. The atomic position $X$ is in units of the optical wavelength.

Figure 2: Splitting the atomic beam (a) without and (b) with spontaneous emission. The detuning is $\Delta = -1$.

$\sigma_r = 400$, and $\gamma = 0.05$. Trajectories for 50 spontaneously emitting atoms under the same conditions as in Fig. 1a are shown in Fig. 1b. As expected, spontaneous emission destroys in part the effect of focusing. However, the atoms move more or less coherently because spontaneous emission events are comparatively rare at $\Delta = 1$.

The other effect, we would like to demonstrate with atomic beams crossing the SLW, is a splitting of the beam. To do this one needs to choose such the value of the detuning in order that some atoms in the beam would be trapped in the first well of the optical potential but another ones could overcome the barrier and leave that well. It is possible to split atomic beams as at positive and negative values of the detuning. As an example, we demonstrate in Fig. 2 the effect of splitting at $\Delta = -1$ for atoms without and with spontaneous emission. It is seen that spontaneous emission changes slightly the effect because a few atoms may leave the potential wells due to random recoils.
The ability of blue and red detuned lasers to attract atoms to the nodes and antinodes of the SLW, respectively, can be used to create periodic structures composed of atoms deposited on substrates in the process of optical nanolithography [7–9]. To simulate a real experiment we consider a beam with $N_0 = 10^5$ calcium atoms with the initial Gaussian distribution (with the rms $\sigma_x = \sigma_p = 2$ and the average values $x_0 = 0$ and $p_0 = 10$) and compute their distribution against the SLW at a fixed moment of time $\tau = 1000$. The bunching of atoms at the SLW nodes at $\Delta = 1$ (blue detuning) is shown in Fig. 3a where the atomic density, $n = N(X)/N_0$, is plotted along the optical axis $X$ at $\tau = 1000$. The same effect, but with the atoms bunching around the SLW antinodes (red detuning, $\Delta = -0.2$), is shown in Fig. 3b. In both the cases we get a periodic atomic relief with the period $\lambda_f/2$ the width of which is restricted by the time the atoms interact with the Gaussian laser beam.

The problem we consider resembles the scattering process with particles entering an interaction region along completely regular trajectories and leaving it along asymptotically regular trajectories. It is known from many studies in celestial mechanics, fluid dynamics and other disciplines that under certain conditions the motion inside the interaction region may have features that are typical for dynamical chaos, (homoclinic and heteroclinic tangles, fractals, strange invariant sets, positive finite-time Lyapunov exponents, etc.) although the particle’s trajectories are not chaotic in a rigorous sense because chaos is strictly defined as an irregular motion over infinite time. It has been found [21–24] that transient Hamiltonian chaos in the interaction region occurs due to existence of, at least, one nonattractive chaotic invariant set consisting of an infinite number of localized unstable periodic orbits and aperiodic orbits. This set possesses stable and unstable manifolds extending in the phase space into the regions of regular motion. The particles with the initial positions close to the stable manifold follow the chaotic-set trajectories for a comparatively long time, then deviate from them, and leave the interaction region along the unstable manifold. It is the common mechanism of chaotic scattering that in our problem causes the chaotic walking of atoms along the SLW.

In Fig. 4a we show the atomic position distribution at $\tau = 1000$ in the regime of the chaotic scattering at $\Delta = 0.2$ with $10^5$ calcium atoms. This plot should be compared with Fig. 3a where the atomic position

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{The effect of bunching of $10^5$ calcium atoms around (a) the SLW nodes (blue detuning, $\Delta = 1$) and (b) the antinodes (red detuning, $\Delta = -0.2$). The plot of atomic density $n = N(X)/N_0$ at the fixed moment of time $\tau = 1000$.}
\end{figure}
Figure 4: The distributions of $10^5$ calcium atoms at $\tau = 1000$ in (a) the real and (b) momentum space under the conditions of chaotic scattering at $\Delta = 0.2$.

Figure 5: Comparison of the distributions of $10^5$ calcium atoms at $\tau = 1000$ over the phase plane in the regimes of (a) chaotic ($\Delta = 0.2$) and (b) regular scattering ($\Delta = -0.2$).
distribution is shown for regularly scattered atoms at $\Delta = 1$. First of all, the distribution of chaotically scattered atoms has a prominent pedestal and is much broader. Moreover, it has no such a periodic structure as shown in Fig. 3a. Only the peaks around the first two SLW nodes are prominent in Fig. 4a. The atomic position distribution in the momentum space in Fig. 4b is much broader than the one for regularly scattered atoms at $\Delta = 1$ (not shown). Thus, we predict that under the conditions of chaotic scattering there should appear less contrast and more broadened atomic reliefs as compared to the case of regular scattering because a large number of atoms are expected to be deposited between the nodes as a result of chaotic walking along the SLW axis. The effect is expected to be more prominent under the coherent evolution but it seems to be observable with spontaneously emitting atoms as well. The difference between chaotic and regular scattering of atoms at a rigid SLW is especially prominent on the corresponding phase space portraits shown in Fig. 5 where positions and momenta of $10^5$ calcium atoms are plotted at the fixed time moment.

4 Conclusion

We have simulated some geometric optics effects with atomic beams crossing a SLW in the limit of long relaxation time and with spontaneous emission taken into account. Trajectories of spontaneously emitting atoms have been simulated with the help of the standard stochastic wave-function technique \[15\-20\]. It has been shown that by adjusting the detuning it is possible to focus, split and scatter atoms. The effects have been explained by a coupling between external and internal atomic degrees of freedom. The depth of the optical potential depends on the sign and value of the detuning. Varying $\Delta$, one can create conditions for focusing, splitting and bunching the atoms. It is remarkable that near the atom-field resonance we have found the new type of atomic diffraction at a SLW without any modulation of its parameters that can be observed in real experiments. That would be the prove of existence of the novel type of atomic motion, chaotic walking in a deterministic environment. The effects found could be used in optical nanolithography to fabricate complex atomic structures on substrates.

We predict that experiments on the scattering of atomic beams at a SLW can directly image chaotic walking of atoms along the SLW. In a real experiment the final spatial distribution can be recorded via fluorescence or absorption imaging on a CCD, commonly used methods in atom optics experiments yielding information on the number of atoms and the cloud’s spatial size. The other possibility is a nanofabrication where the atoms after the interaction with the SLW are deposited on a silicon substrate in a high vacuum chamber. In this case the spatial distribution can be analyzed with an atomic force microscope. As to the momentum distribution, it can be measured, for example, by a time-of-flight technique \[25\]. The modern tools of atom optics enable to create narrow initial atomic distributions in position and momentum, reduce coupling to the environment and technical noise, create one-dimensional optical potentials, and to measure spatial and momentum distributions with high sensitivity and accuracy.

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