Atomic diffraction in counter-propagating Gaussian pulses of laser light

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We present an analysis of atomic diffraction due to the interaction of an atomic beam with a pair of Gaussian light pulses. We derive a simple analytical expression for the populations in different diffraction orders. The validity of the obtained solution extends beyond the Raman-Nath regime, where the kinetic energy associated with different diffraction peaks is neglected, into the so-called channeling regime where accurate analytical expressions have not previously been available for the diffraction. Comparison with experimental results and exact numerical solutions demonstrate the validity of our analytical formula.

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I. INTRODUCTION

Diffraction of light and matter waves lies at the heart of a number of diagnostic measurement techniques in physics and engineering. Due to their internal level structure, atoms and molecules can be diffracted by resonant or near resonant laser beams \[1, 2, 3, 4, 5, 6\]. The field of atomic optics points to applications for high precision probing of inertial effects and fundamental physics \[7, 8, 9, 10\], as well as to the use of diffraction to diagnose single- and multi-particle properties of the atoms themselves in various physical settings \[11, 12, 13\]. The use of light induced potentials for structured deposition of atoms on surfaces has also been demonstrated \[14\]. By use of Laguerre-Gaussian laser beams, atomic diffraction was recently used to transfer not only linear but also angular momentum to an atomic gas \[15, 16\]. By tailoring the polarization and frequencies of light, it is possible to induce complicated multi-level dynamics with various potential applications \[17\]. For most species, using optical pumping and suitable polarization schemes, it is also possible to restrict the dynamics and to obtain a situation of effective propagation of a single component wave function in a single periodic potential \[17, 18\].

The coupling of atomic momentum components by absorption and stimulated emission events to a comb of other momentum states separated by twice the photon momentum cannot be solved analytically due to the non-commuting kinetic and potential energies. However, for two parameter regimes simple analytical solutions have been known for a long time. In the Raman-Nath regime of short pulse durations, the difference in kinetic energy of different momentum states is neglected and the coupling leads to an expansion with Bessel-function expression for different momentum component amplitudes \[17, 18\]. In the Bragg regime of long and weak pulses, kinetic energy must be strictly conserved by absorption and emission of an integer number of counter-propagating photon pairs, and the system reduces to an effective, analytically tractable, two-level system.

Atomic diffraction is applied extensively in experiments, and the need for numerical and analytical theoretical approaches beyond the range of validity of the Raman-Nath and the Bragg theoretical treatments, is explicitly expressed in the recent literature \[19, 20\]. Here we depart from the Raman-Nath approach, and suggest an analytical formula which extends into the channeling regime. Our analytical expression, includes effects due to the kinetic energy dispersion, and deploying numerical simulations we show that it extends the range of validity of the simple Raman-Nath approach into the channeling regime where both Raman-Nath and Bragg descriptions fail. In Section II, we introduce our analytical and improved approximate theories. In Sec. III we present numerical calculations and compare them to the different analytical approaches derived in the previous section, assessing their validity regime. Finally, Sec. IV concludes the paper with a discussion.

II. THEORY

We consider an atom with mass \(M\), two atomic levels with energy level separation \(\hbar \omega_0\), and dipole matrix element \(d\), interacting with two counter-propagating laser field pulses,

\[
\mathcal{E}(z,t) = \mathcal{E}_1(t-z/c)e^{i(kz-\omega t)} + \mathcal{E}_2(t+z/c)e^{-i(kz+\omega t)} + c.c. \tag{1}
\]

We imagine that the two pulses arrive at the origin, \(z = 0\), symmetrically from opposite directions. For realistic atomic and field parameters, the width of the atomic distribution around \(z = 0\) will be narrow compared to the spatial range of intensity variation of either light pulse and hence their interaction with the atoms is that of a standing wave with a time dependent strength. We assume that the atoms have initially a well defined momentum, \(p_0\), and we adiabatically eliminate the excited atomic state, which is off-resonance from the laser fields by an amount \(\Delta = \omega - \omega_0\), yielding the Schrödinger equation for the ground state wave function,
FIG. 1: (Color online) Diffraction patterns for various pulse durations, \( \tau \), as predicted by (a) the Raman-Nath solution Eq. (5), (b) its modified version, Eq. (6) and (c) the full numerical solution to the Eq. (2), plotted as functions of the momentum, \( p \). The color indicates the population intensity such that red corresponds to the maximum and dark blue to the minimum. Parameters are: \( q = 52.9 \) and \( p_0 = 20\hbar k \).

FIG. 2: (Color online) Diffraction intensities for a pulse duration \( \tau = 0.0375/\omega_r \) and intensity \( q = 52.9 \) in reduced units. The diffraction probabilities are shown as function of the final state momentum. Red diamonds, blue boxes and black bullets correspond to the frames (a), (b), and (c) in Fig. 1, respectively.

\[
\psi(z,t) \equiv a(z,t) \exp \left( i \frac{p_0 z}{\hbar} - i \frac{p_0^2 t}{2M\hbar} \right),
\]

\[
\frac{i\hbar}{\partial t} a(z,t) = \left( -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial z^2} + i\hbar \frac{p_0}{M} \frac{\partial}{\partial z} + V_{\text{ext}}(z,t) \right) a(z,t)
\]

where

\[
V_{\text{ext}}(z,t) = \frac{|d|^2}{\hbar \Delta} \left( |E_1(t-z/c)|^2 + |E_2(t+z/c)|^2 \right) + 2\text{Re}(E_1^*(t-z/c)E_2(t+z/c)e^{-2ikz})
\]

A. Neglecting the variation of the kinetic energy for different momentum states

Neglecting the second order spatial derivative in Eq. (2), it becomes solvable by straightforward integration \[21\]. We replace the assumed smooth position dependence of the amplitude, \( a(z,t) \), before the interaction with the laser field by a constant, arriving at the solution

\[
a(z,t) \propto \exp \left( \frac{i|d|^2}{\hbar^2 \Delta} \left( \int_{-\infty}^{t} |E_1|^2 \text{dt}' + \int_{-\infty}^{t} |E_2|^2 \text{dt}' \right) \right.
\]

\[
+ e^{i2k(p_0 t/M-z)} \int_{-\infty}^{t} |E_1|^2 |E_2|^2 e^{-i2kp_0 t/M} \text{dt}'
\]

\[
+ e^{-i2k(p_0 t/M-z)} \int_{-\infty}^{t} |E_1|^2 |E_2|^2 e^{i2kp_0 t/M} \text{dt}' \right)
\]

where we will assume real field amplitudes. Physically, neglecting the kinetic energy operator amounts to making the dynamics local in position involving only a position dependent phase factor. Assuming Gaussian pulses,
\[ E_{1,2}(t \pm z/c) = E_{1,2} \exp(- (t \pm z/c)^2/\tau^2), \]
the definite integrals in Eq. (4) can be evaluated at \( t = \infty \), i.e., after the pulse, and the exponential function can be expanded in the following series,

\[
a(z, t) = \sum_{m=-\infty}^{\infty} e^{im2k(z-p0t/M)} \times \\
i^m J_m \left( \frac{\sqrt{2\pi}|d|^2 E_1 E_2}{\hbar^2 \Delta} \tau e^{-2(z/c)^2} e^{-\left(\frac{m\hbar k\tau}{\Delta}\right)^2/2} \right). \tag{5}
\]

Note that this expression bears resemblance to the Raman-Nath solution obtained with constant laser amplitudes [17] [18]. However, the specific Gaussian shape and an exponential dependence on the duration parameter, \( \tau \), of the Bessel-function argument highlights certain specific physical properties of the diffraction process with Gaussian pulses. For all practical purposes, the position argument, \( z \), is much smaller than the pulse length \( c\tau \) and the first exponential term inside the Bessel-function will be replaced by unity in the following. An example of the results obtained from Eq. (5) for the momentum distribution, i.e., the absolute value of the square of the Bessel-functions evaluated for different diffraction orders, \( n \), are plotted in Fig. 1(a) as function of the final state momentum \( p = p_0 + 2n\hbar k \). Note the figure does not show the time dependent diffraction, but the asymptotic momentum distribution after the pulse, for different values of the pulse duration \( \tau \).

The Bessel-functions with \( m \neq 0 \) all vanish for vanishing arguments, and we see that both short (\( \tau \to 0 \)) and long (\( \tau \to \infty \)) pulses exclude diffraction to new momentum components. For short pulses of given strength, the explanation is that there is simply no time to significantly diffract the atoms, and the nearly vanishing \( \tau \) argument suppresses the higher order Bessel functions. For longer pulses the result can be ascribed to the exponential factor inside the Bessel-functions, which in turn reflects the lack of energy conservation in the diffraction process: In the rest frame of atoms moving at velocity \( p_0/M \), the photons in the counter-propagating light pulses are Doppler-shifted in frequency, causing an apparent change of 2\( \hbar k p_0/M \) in the field energy per absorption-emission cycle involving both beams. This is a violation of energy conservation, permitted because we consider a process of finite duration \( \tau \). Note that the process is suppressed by the exponential factor when the corresponding frequency mismatch exceeds \( \propto 1/\tau \), in support of our interpretation in terms of the energy-time Heisenberg uncertainty relation. Alternatively, the finite duration pulses may be thought of as (Gaussian) frequency distributions of light, and absorptions and emissions involving photons from the counter-propagating pulses may conserve field energy in the frame moving at \( p_0/M \), if the photons involved are at frequency components shifted by the amount \( \pm \hbar k p_0/M \) with respect to the field carrier frequency of the pulses. The field power at those frequencies is just given by the Gaussian factor, appearing inside the Bessel function arguments.

B. Incorporation of the kinetic energy variation

After having presented the equation governing the diffraction within the Raman-Nath approximation, which does not take into account the energy difference between states with different momenta, it is natural to investigate if a simple modification of the final result may capture the characteristic features of the energy dispersion. To this purpose, we shall come back to our interpretation of the last exponential factor inside the Bessel function in Eq. (5). In the previous section we argued that this quantity expresses the mean change of field energy 2\( \hbar k p_0/M \) per absorption emission cycle, experienced by the moving atom due to the Doppler effect, and that it is appropriately measured relative to the frequency width of the light pulses due to their finite duration. For a Gaussian pulse, the frequency distribution is also Gaussian, hence the Gaussian dependence inside the Bessel function. Taking into account that the different momentum states have different kinetic energies, it is thus natural to suggest to apply the same argument as above but taking into account the change of field energy plus atomic kinetic energy. In the frame moving at velocity \( p_0/M \) the atom is initially at rest. Scattering process into the \( m \)th diffraction order by absorption and simulated emission of \( m \) photons propagating in opposite directions changes the field energy by an amount \( 2m\hbar k p_0/M \). Simultaneously atoms acquire a finite momentum kick of \( 2m\hbar k \) in the moving frame, and hence their final kinetic energy is \( 4m^2\hbar^2 k^2/2M \). The total energy defect per absorption-emission event is therefore \( 2\hbar k(p_0 + m\hbar k)/M \). Since the pulses have Gaussian frequency widths proportional to \( 1/\tau \), the atoms may interact with frequency components shifted by \( k(p_0 + m\hbar k)/M \) in order to conserve total (field plus atomic kinetic) energy. Motivated by the above analysis we thus suggest to replace \( p_0 \) in the exponential inside the Bessel-function in Eq. (5) by \( p_0 + m\hbar k \). This modification leads to the expression,

\[
b(z, t) = \sum_{m=-\infty}^{\infty} e^{im2k(z-p_0t/M)} \times \\
i^m J_m \left( \frac{\sqrt{2\pi}|d|^2 E_1 E_2}{\hbar^2 \Delta} \tau e^{-2(z/c)^2} e^{-\left(\frac{(p_0+m\hbar k)\tau}{\Delta}\right)^2/2} \right). \tag{6}
\]

for different diffraction orders, \( m \). The probability that an atom with initial momentum \( p_0 \) acquires the final momentum \( p_0 + 2m\hbar k \), is \( |J_m(f(p_0 + m\hbar k))|^2 \), with

\[
f(p) \equiv \frac{\sqrt{2\pi}|d|^2 E_1 E_2}{\hbar^2 \Delta} \tau e^{-\left(\frac{2\pi}{\hbar^2 \Delta}\right)^2}. \tag{7}
\]

The results of this modified version of the Raman-Nath approximation are shown in Fig. 1(b). We do not claim that such alteration is an exact result or even a systematic expansion in any small parameter, and although it is physically meaningful it must be justified a posteriori, for instance by comparison with an exact calculation. Such assessment will be made in the following section.
III. RESULTS

In the preceding section we have derived two different analytical solutions, which we shall now compare to the exact numerical solution of the problem.

A. Numerical solution

The full Schrödinger equation without omission of the second derivative term is amenable to numerical solution, and we have carried out such computations for a wide range of atomic and field parameters. Our numerical studies enable us to compare the predictions of the analytical approximations to the exact numerical solutions and assess their validity, and in particular, to investigate whether the modified form Eq. (6) represent an improvement over the Eq. (5) or not. To this end, we propagate wavefunctions, \( d(z, t) \), which interact with the Gaussian light pulses, in time from \( t = -2\tau \) to \( t = 2\tau \) according to the Eq. (2). The initial wave function represents a particle with a mean momentum, \( p = p_0 \), and is modelled as a Gaussian wave packet

\[
d(z, -\infty) = e^{-z^2/2\sigma^2}e^{ip_0 z/\hbar}
\]

where the waist, \( \sigma = 10/k \), is chosen wide enough that the momentum spread of the initial wave packet is narrow in comparison to the resulting momentum separation of adjacent diffraction orders.

For further convenience, following Ref. [19], we introduce dimensionless parameters for time and laser field intensity

\[
q = \left| \frac{d^2 E_1 E_2}{4\hbar^2 \omega_r \Delta} \right|; \quad \tau_r = \omega_r t
\]

where \( \omega_r = \hbar k^2/2M \) is the photon recoil frequency.

B. Comparison of different analytical solutions

In Fig. 1(a)-(c), we have plotted the diffraction patterns for a range of pulse durations, \( \tau \), as functions of the momentum, \( p \) for two different approximations and the exact solution to the diffraction problem, respectively. We obtain the diffraction peak intensities as a square modulus of the Fourier transformed wave functions. Note that the ‘onion shape’ does not show the momentum distribution as a function of time, instead, each horizontal cut through the figure indicates the asymptotic momentum distribution after a pulse of the given duration. The pulse parameters for all of the frames are \( q = 52.9 \) and \( p_0 = 20\hbar k \). The modified Raman-Nath solution, shown in Fig. 1(b), is observed to be in an excellent agreement with the exact numerical solution, Fig. 1(c), for these parameters.

To obtain better quantitative feeling for the quality of the equation (6), we plot the diffraction pattern for a single pulse duration, \( \tau = 0.0375/\omega_r \), as shown in Fig. 2. Here the red diamonds, blue boxes and black bullets correspond to the values shown in the frames (a), (b), and (c) in Fig. 1, respectively. From this graph, it is clear that our modified solution still works excellently in the
FIG. 5: (Color online) Pulse duration versus intensity diagram for atomic diffraction dividing the parameter space in three distinctively different regimes. Black bullets correspond to the experiments in Ref. [19]. Triangles joined by a line correspond to the modified Raman-Nath solution in Fig. 1(b) and the boxes joined by a line are from Fig. 3. Dashed line marks the region where the modified Raman-Nath formula loses its validity.

regime where the Raman-Nath approximation fails.

C. Validity assessment and relation to experiments

We have also compared our modified Raman-Nath prediction, Eq. (6), with the actual experiment as reported in Ref. [19] in addition to the full numerical solution. In the experiment, the smooth-shaped pulse was varied as $\cos^2(\alpha t)$ which is well approximated by our Gaussian shaped pulse and allows a direct comparison. With parameters corresponding to the experiment, $q = 3.5$, $\tau_r = [0, 1.5]$ and $p_0 = \hbar k$, Fig. 3 shows our prediction while Fig. 4 is the corresponding numerical solution. Comparison between these and the experimental result presented in [19], we observe all of them to be in fair agreement for short pulse durations, i.e., in the Raman-Nath regime. For longer pulse durations, both experiment and numerical solution exhibits Bragg-like channeling behavior with an associated Rabi cycling. Such long-time behavior for these parameters cannot be reproduced by our analytical formulas. This may be because the experiment is carried out with parameters very far from the Raman-Nath regime. The experiment is in fact not that far from the Bragg regime, where we know that a correct treatment of the kinetic energy is crucial.

Figure 5 is in parts reproduced from Ref. [19] and summarizes the applicability of various approximations on the $(\tau_r, q)$ parameter space. In the spirit of Ref. [19], the region boundaries are defined by $\tau_r = 1/2\sqrt{2q}$ and $q = 1$. Black dots mark the experiments as in Ref. [19]. The upper horizontal line connecting triangle symbols corresponds to the results shown in Fig. 1(b) and the lower line connecting square symbols depicts the parameters used in Fig. 3. The dashed part of the lower line indicates that Eq. (6) fails for these parameters, deep into the channeling regime. However, it is clear that the validity of our analytical solution enters the previously unknown channeling territory. It is also worth noting that for the case of high intensity (high $q$ value), demonstrated in Fig. 1, our expression maintains its validity for all pulse durations, $\tau$, since the diffraction process itself is confined to relatively short times.

IV. DISCUSSION

We have presented an analytical solution to a problem of atomic diffraction from a pulsed time-dependent light grating for the so called Raman-Nath regime where the kinetic energy of the atoms participating in the diffraction process may be neglected. We have extended this approximation by including certain aspects of the kinetic energy in the diffraction process and we have proposed a phenomenological improvement to this solution which is based on physically motivated arguments. Through a comparison with an exact numerical solution of the Schrödinger equation, it is shown that our modification extends the validity regime of the parameter space of the analytical solution from the Raman-Nath into the channeling regime. Qualitatively the modification predicts the asymmetry due to the Doppler effect in the diffraction pattern. The proposed analytical formula is compared with available numerical results and is found to be in good agreement even fairly deep in the channeling regime of strong and long interactions. Although, containing certain elements of Bragg diffraction, the proposed equation is not, however, capable of predicting correctly the effective two-state Rabi cycling between momentum states $\pm p_0$. Exploration of the channeling regime from the Bragg-formalism seems a promising avenue for attempts to provide good analytical expressions for atomic diffraction closer to the Bragg regime. Together with the present work, this may perhaps exhaust the full parameter range with good analytical approximations for the atomic diffraction.

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