Atomic diffraction from nanostructured optical potentials

G. Lévêque, C. Meier, R. Mathevet, C. Robilliard, J. Weiner
Laboratoire de Collisions, Agrégats et Réactivité
UMR 5589 du CNRS et l’Université Paul Sabatier
Institut de Recherche sur les Systèmes Atomiques et Moléculaires Complexes
Université Paul Sabatier
31062 Toulouse Cedex 4 France

C. Girard
Centre d’Elaboration de Matériaux et d’Etudes Structurales
29, rue Jeanne Marvig, BP 4347
31055 Toulouse Cedex 4 France

J. C. Weeber
Laboratoire de Physique de l’Université de Bourgogne
9 avenue A. Savary, F-21078
Dijon, France
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We develop a versatile theoretical approach to the study of ultracold atom diffractive scattering from light-field gratings by combining calculations of the optical near field generated by evanescent waves close to the surface of periodic nanostructured arrays together with advanced atom wavepacket propagation techniques. Nanometric 1-D and 2-D arrays with subwavelength periodicity deposited on a transparent surface and optically coupled to an evanescent wave source exhibit intensity and polarisation gradients on the length scale of the object and can produce strong near-field periodic modulation in the optical potential above the structure. As a specific and experimentally practical example we calculate the diffraction of cold Cs atoms dropped onto a periodic optical potential crafted from a 2-D nanostructure array. For an "out of plane" configuration we calculate a wide diffraction angle (≃ 2 degrees) and about 60% of the initial atom flux in diffraction orders ±1, an encouraging result for future experiments.

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I. INTRODUCTION

The prospect of manipulating neutral atoms and molecules by light forces acting at nanometer scale lengths offers fascinating but experimentally challenging possibilities in many areas of atomic physics. Atom optics [1], atom nanolithography [2, 3], and atom interferometry [4] are prime examples. The use of high-refractive-index dielectric or metallic nanometric objects to produce subwavelength localized light field distributions [5, 6, 7] raises the possibility of "integrated atom optics" in which atoms or molecules can be confined, guided or diffracted above nanostructured surfaces fabricated to a designed shape [8, 9]. Tailoring optical potentials for atom control, and possibly Bose-Einstein condensates, is analogous to the use of micromagnetic fields for a similar purpose [10, 11, 12, 13, 14, 15, 16, 17]. Atom diffraction from a transmission optical grating provided one of the early examples of light-field atom manipulation [18]. A proposal for [19] and realization of [20] a reflection light-field grating quickly followed. These early developments stimulated many subsequent experimental and theoretical studies, and a pertinent review has recently appeared [20]. Until now reflection gratings for matter waves have been implemented by the formation of one dimensional evanescent standing waves produced by counterpropagating laser beams undergoing total internal reflection through a glass prism.

The approach we present here contrasts markedly with this earlier work on standing waves of sinusoidal form. We study diffractive scattering of cold atoms from an evanescent field, spatially modulated by an array of nanometric objects with high index of refraction and subwavelength periodicity deposited on a glass surface [21, 22]. These evanescent fields and their interaction with atoms will exhibit several novel features. First, rather than a pure sinusoidal evanescent standing wave, nanostructured periodic corrugation generates fields containing higher-order harmonics and an intricate polarization distribution. Second, spatial gradients of field intensity and polarization at length scales well below the diffraction limit interact with the external and internal atomic degrees of freedom in ways that strongly depend on the geometry and material of the nanostructures employed. Third, the intensity and polarization map above the nanostructure array also depends strongly on the intensity and polarization of the exciting light source.

Since the cold-atom de Broglie wavelength is not much
The periodic optical near-field above the nanostructured array is generated by light with incident wave vector $k$ and diffracts into orders $k_{\pm 1}$. The periodic optical near-field above the nanostructured array is generated by light with incident wave vector $k_0$ and diffracts into orders $k_{\pm 1}$. The nanostructures are cubes of high-refractive-index material with subwavelength dimensions and periodicity (see text for model details). Note that the incident plane of the light $P_0$ is along the diagonal of the cubes while the incident plane of the atoms $P_A$ is shifted 45 degrees and parallel to the cube edges. Note also that the diffracted orders $k_{\pm 1}$ are "out-of-plane" with respect to the plane of incidence of the light.

smaller than the characteristic scale length of the optical field, an accurate description of atomic motion calls for a quantum treatment of external as well as internal degrees of freedom. In order to analyze the dynamics of cold atoms scattering off periodic optical potentials we need to marry two well-developed numerical techniques: calculation of the optical near-field and atom wave packet propagation. The situation we consider is shown in Fig. 1. First, we calculate the three-dimensional electric field and polarization distribution in the near field surrounding the nanostructures. At frequency detunings far from resonance, where absorption is negligible, this information is used to construct a conservative potential for a full three-dimensional treatment of the center-of-mass motion of the atom, including ground internal states. Using the field information above the nanostructures, we calculate the three-dimensional atom-field interaction potential $V_2$. Since the field polarization will vary significantly over the length scale of the nanostructures, and since various field polarizations may lead to population transfer among atomic internal states, we include the internal Zeeman states of a $^2S_{1/2}$ atomic ground level in the calculation of the atom-optical field scattering. Second, we apply a time-dependent wave packet method to describe the scattering problem of cold atoms diffracting from an optical grating with subwavelength periodicity. Inclusion of the ground-level internal states leads to a three-dimensional, coupled channel problem that we solve with wave packet propagation techniques already successfully applied to atom or molecule surface scattering and quantum molecular dynamics in several degrees of freedom [21, 22, 23, 24, 25, 26, 27, 28, 29, 30]. After the wave packet representing the atom reflects and diffracts from the optical potential, it is projected onto final scattering states to yield the desired diffraction probabilities [28].

In this paper we emphasize general principles and seek to establish a methodology without restriction to any specific experimental set-up. In fact the numerical solution of Maxwell’s equations in the near field and Schrödinger’s equation for the atomic motion can easily be adapted to explore atom manipulation in sub-wavelength optical light fields of arbitrary geometry. However to illustrate this methodology we present calculations obtained with realistic parameters corresponding to an experiment using a flux of cold $^2S_{1/2}$ atoms incident at about 40 degrees from the normal and scattering off a two-dimensional optical grating with subwavelength period. The results of our calculation yields out-of-plane diffraction into a few orders, with markedly large diffraction angles. The results are encouraging for planned experiments.

The rest of the paper is organized as follows: Section II gives details of the calculation of the scattering probabilities. The sub-wavelength light field calculations are reported elsewhere [28], so only the essential steps are summarized here. In Section III we present a model configuration and in Section IV we show the numerical results for illustration.

II. THEORY

A. The optical near field

The evanescent wave field created by the totally internally reflected laser beam is strongly modified by the periodic nanostructures on the glass substrate surface. The calculation of this intricate electric vector field above the nanostructures can be carried out using several methods that solve Maxwell’s equations in these nontrivial geometries. These methods are well established in the field of scanning near-field optical microscopy (SNOM) [4, 6]. Among the most widely used are the finite-differences scheme [14], the differential theory of gratings (DTG) [15, 24, 27] and the Green’s function method [11]. This latter approach is well-adapted to study single, finite-size nano-objects, and has been used extensively to study a wide range of nanostructures [15, 11]. However, in the case of periodic surface structures, it becomes inefficient, since it does not explicitly take the periodicity into ac-
count. In such cases, the DTG method is more appropriate, because it solves Maxwell’s equations by means of a Fourier expansion of each field component.

To be more specific, we define \( r = (x, y, z) \) with \( z \) taken as the direction perpendicular to the surface. For convenience, we define a vector \( \mathbf{l} = (x, y) \) in the plane of the substrate surface. We will denote the electric field by \( \mathbf{E} \) in the glass half-space and by \( \mathbf{B} \) in the vacuum half-space, \( n_1 \) being the glass index and \( n_2 \) the vacuum index. The two-dimensional periodicity of the nanostructures defines a unit cell of length \( L_x \) and \( L_y \) along the \( x \) and \( y \) directions, respectively. The direction of the incoming laser is given by \((k_L^x, k_L^y, k_L^z)\), with \( k_L = n_12\pi/\lambda_0 \), \( \lambda_0 \) being the laser wavelength in vacuum.

In the DTG method, an index-modulated zone, labelled 3 and characterized by \( n_3(r) \), the high index material, is introduced at the vacuum/glass substrate interface. We have then to solve in all space Helmholtz’s equation:

\[
\Delta \mathbf{E}^{(l)}(r) + n_3^2k_0^2\mathbf{E}^{(l)}(r) = 0; \quad l = 1, 2, 3
\]

Since the system is periodic along \( x \) and \( y \) we can expand the dielectric constant (i.e. \( n_3^2 \)) in the modulated zone:

\[
n_3^2(r) = \sum_{m,n} \alpha_{mn} \exp(2i\pi \frac{mx}{L_x} + \frac{ny}{L_y}),
\]

where \( \alpha_{mn} \) are the Fourier coefficient of \( n_3^2 \). It is clear that electric and magnetic fields outside the modulated zone will also be periodic and thus conveniently written,

\[
\mathbf{E}^{(l)}(r) = \sum_{m,n=\pm\infty} \mathbf{E}_{mn}^{(l)} e^{i\gamma_{mn}z} e^{i\mathbf{k}_{mn} \cdot \mathbf{r}}; \quad l = 1, 2, 3
\]

\[
\mathbf{B}^{(l)}(r) = \sum_{m,n=-\infty} \mathbf{B}_{mn}^{(l)} e^{i\gamma_{mn}z} e^{i\mathbf{k}_{mn} \cdot \mathbf{r}}; \quad l = 1, 2
\]

In this expression, \( \mathbf{k}_{mn}^{(l)} \) denote the \( x,y \) components of the wave vector \( \gamma_{mn} \) obeys the dispersion equation:

\[
(k_{mn}^y)^2 + (\gamma_{mn})^2 = (k_L^x)^2 + (k_L^y)^2 + (k_L^z)^2
\]

for which we have two solutions, corresponding to “rising” and “descending” waves. The rising zero order in the glass substrate corresponds to the incident laser field. Then, if we know the Fourier components \( \mathbf{E}_{mn} \) and \( \mathbf{B}_{mn} \) of the electric and magnetic field in a plane just above the nano–objects, the field distribution anywhere above the structures are determined by Eqs. (2). From Eq. (3), it may be seen that the coefficient \( \gamma_{mn} \) is either real or purely imaginary. The real values of \( \gamma_{mn} \) correspond to radiative harmonics while imaginary values introduce evanescent components.

The six components of the electromagnetic field \( \mathbf{E}^{(l)}(r) \), \( \mathbf{B}^{(l)}(r) \) are then deduced from two independent parameters, usually named the principal components, which in the present case are chosen to be the \( y \)-components \( E^{(l)y}(r) \) and \( B^{(l)y}(r) \). In order to calculate the Fourier components of the electric field just above the nanostructures, we have to solve a system of linear differential equations for \( E^{(l)y}(r) \) and \( B^{(l)y}(r) \) in the region of space where the index is modulated by the nanostructures. This system mixes all the Fourier orders of the electric and the magnetic field through the product \( n_3^2 E_r^{(3)y}(r) \) in Helmholtz’s equation. Then, for numerical applications the Fourier expansion converges at some sufficiently large value \( N \), i.e. the order \( n \) and \( m \) will both vary from \(-N \) to \(+N \). We solve this system using standard bounding conditions for this problem, i.e. we assume there is no field arriving from infinity in the vacuum, and the only Fourier components of the incident field in the glass substrate are those of zero-order. Finally, we can express the Fourier components \( E_{mn}^{(2)y} \) and \( B_{mn}^{(2)y} \) in a horizontal plane just above the nano-objects as a linear combination of the \( y \)-components of the incident fields \( E_i, B_i \), which define the polarization state of the incoming laser:

\[
E_{mn}^{(2)y} = T_{EE} E_i^{(1)y} + T_{EB} B_i^{(1)y}
\]

\[
B_{mn}^{(2)y} = T_{BB} E_i^{(1)y} + T_{BB} B_i^{(1)y}.
\]

These transmission coefficients, \( T_{EE}, T_{EB}, T_{BB} \) depend only on the geometry of the sample, the frequency and the angle of incidence of the illuminating laser. The setup for the field calculation is shown in Fig. 2. A more detailed description of this calculation can be found in Refs. [22, 27]. With the optical field mapping in hand we turn our attention to atom scattering in the presence of these fields.
B. Calculation of atom-surface scattering

In the limit of low saturation and a blue detuning $\delta$ which is large compared to the Doppler shift and natural linewidth, the atom-field interaction can be treated within the framework of coherent atomic motion where spontaneous emission is neglected [22, 29, 30]. We will consider an atom transition dipole, typical of the first alkali $^2S_{1/2} \rightarrow P$ transition, neglecting fine and hyperfine structure in the excited state, but including the two-component angular momentum degeneracy of the ground state. The excited level can be eliminated adiabatically, which results in atomic motion that is described by a two-component, three-dimensional wavepacket that evolves within the framework of coherent atomic motion where the atomic motion can be treated in real space [31, 39, 40]. Briefly, one simulates the collision of the atom with the surface by sampling the density matrix elements among them. In fact it is only recently that modern and very efficient numerical wave packet propagation techniques have permitted the calculation of diffractive scattering by solving Eq. 6 directly on grids in real space [31, 22, 29, 43].

\[
V_{m_jm'_j}(r) = \frac{\hbar^2}{2\hbar} \sum_{q, q', m_e} E_q(r) E_{q'}(r) \langle j_g, m_j; 1, q | j_e, m_e \rangle \langle j_e, m_e | j_g, m'_j; 1, q' \rangle
\]  

(8)

In this expression the terms in parenthesis are Clebsch-Gordan coefficients with $j_g$ and $j_e$ being the total angular momentum of the ground and excited state respectively. The reduced dipole moment is denoted by $d$ and the field enters through its spherical components $E_q(r)$, $q = 0, \pm 1$. This expression forms the basis of numerous studies of atomic diffraction from standing evanescent waves as has been used by many authors [8, 22, 29, 30, 43]. In general the polarization state of the electric field above the nanostructured objects is a very complicated function of space. Hence, according to Eqs. [8, 22] transitions between the different Zeeman sublevels can occur during the interaction of the atom with the light fields. As a consequence, we performed the collision on the coupled ground state levels.

One way of proceeding is to expand the wavefunction into plane waves parallel to the surface which results in a set of coupled diffraction channels for the direction perpendicular to the surface [22]. Diffraction then occurs as transitions between these diffractive states, the probabilities of which can be calculated by a semi-classical treatment within the Landau-Zener theory [22] or by numerical wave packet propagation [43]. This treatment corresponds to the well-known CCWP (close-coupling wave packet) method used in standard atom or molecule surface scattering [42]. However, with increasing diffraction orders one may need to take a large number of diffractive states into account, together with all the coupling matrix elements among them. In fact it is only recently that modern and very efficient numerical wave packet propagation techniques have permitted the calculation of diffractive scattering by solving Eq. 6 directly on grids in real space [31, 22, 29, 43]. Briefly, one simulates the collisional process by a wave packet propagation from the initial state to the final interaction–free zone, where it is projected onto any desired observable, which in our case is the total population in the different diffraction channels. To achieve a good energy resolution, one needs to construct an initial wave packet that is sufficiently large such that its energy width is negligible. From a numerical point of view, this is very disadvantageous, since it requires a large grid in the direction perpendicular to the surface. Therefore, we used a method proposed by Mowrey and Kouri [22], who started with a spatially narrow wave packet that comprised a wide range of energies, and extracted energetically resolved results by projecting onto asymptotic states of well-defined energy, $E$.

The initial state of the atom is taken to be a specific Zeeman sublevel $m^0$ of the ground state manifold with center of mass motion described by the box-normalized wavefunction

\[
\Psi_{m^0}^i(r) = \left(2\pi \xi^2 L_x^2 L_y^2\right)^{-1/4} \times \\
\exp\left(-(z - z_0)^2/4\xi^2 + i k_z z + i \mathbf{k}_i \cdot \mathbf{r}\right)
\]  

(9)

with the initial transverse momentum $\mathbf{k}_i = (k_x^i, k_y^i)$ and the initial momentum in z-direction described by a Gaussian distribution centered around $\xi^2$. The propagation of this three dimensional wavepacket is performed on the coupled surfaces defined by Eqs. [8, 22] until the final scattered wave function $\Psi_{m}^f(r)$ is entirely in the asymptotic region.

The (unnormalized) modulus square of the transition amplitudes is given by projection of the final wave packet onto diffractive states [22]:

\[
|b_{m_j}^{mn}(E)|^2 = \frac{1}{k_{mn}^2} \left| \int \mathbf{r} \ e^{-i(k_{mn}z + (\mathbf{k}_i + \mathbf{G}_{mn}) \cdot \mathbf{r})} \Psi_{m_j}^f(r) \right|^2
\]  

(10)
FIG. 3: Top panel: schematic view of the 100 nm TiO$_2$ cubes deposited on a silica surface. Bottom panel: Light field intensity distribution 125 nm above the nanostructures (the arrow $\mathbf{k}_0$ indicates the plane of the incident laser of mode TM and $\mathbf{k}_i$ the plane of incidence of the atoms. The contour lines correspond to (in units of $|E|^2$: 0.397, 0.412 (dashed lines) and 0.427, 0.442 (full lines)

where $\mathbf{G}_{mn} = (\frac{2\pi m}{L_x}, \frac{2\pi n}{L_y})$ denotes the reciprocal lattice vector and $k^z_{mn}$ is determined by energy conservation:

$$k^z_{mn} = \sqrt{2M\mathcal{E} - (k_i + \mathbf{G}_{mn})^2}$$ (11)

The probability to diffract into a specific order $(m, n)$ as a function of total collision energy is then given by [10, 12]:

$$P_{mn}(\mathcal{E}) = \left( \sum_{m_j = \pm \frac{1}{2}} |b_{m_n}^{m_n}(\mathcal{E})|^2 \right) / \left( \sum_{m_j = \pm \frac{1}{2}} \sum_{m_n} |b_{m_n}^{m_n}(\mathcal{E})|^2 \right)$$ (12)

This quantity will be calculated for a selected set of parameters and discussed in the next section. For the three-dimensional, two-component wave packet propagation we used the FFT-Split-Operator scheme, which in the field of quantum molecular dynamics or molecule-surface collisions has proven to be a fast, stable and efficient method to perform this task [48]. Briefly, in this method the total quantum mechanical short-time propagator is approximated by

$$\exp\left[ -\frac{i}{\hbar} \Delta t \left( \begin{array}{cc} T_r + V_{\frac{1}{2}, \frac{1}{2}}(r) & V_{\frac{1}{2}, -\frac{1}{2}}(r) \\ V_{-\frac{1}{2}, \frac{1}{2}}(r) & T_r + V_{-\frac{1}{2}, -\frac{1}{2}}(r) \end{array} \right) \right] \approx \exp\left[ -\frac{i}{\hbar} \Delta t \left( \begin{array}{cc} T_r & 0 \\ 0 & T_r \end{array} \right) \right] \exp\left[ -\frac{i}{2\hbar} \Delta t \left( \begin{array}{cc} V_{\frac{1}{2}, \frac{1}{2}}(r) & V_{\frac{1}{2}, -\frac{1}{2}}(r) \\ V_{-\frac{1}{2}, \frac{1}{2}}(r) & V_{-\frac{1}{2}, -\frac{1}{2}}(r) \end{array} \right) \right] \exp\left[ -\frac{i}{2\hbar} \Delta t \left( \begin{array}{cc} T_r & 0 \\ 0 & T_r \end{array} \right) \right]$$ (13)

This form of symmetric splitting is correct through second order; it is unitary by construction and thus ensures numerical stability [48, 49]. The operator acts on the two-component wavefunction to perform a short-time propagation from time $t$ to $t + \Delta t$. The action of the kinetic operator is calculated in Fourier space, where it is a simple multiplication with a phase factor, and so every time step the two components of the wavefunctions need to be Fourier transformed which can be done very efficiently with three-dimensional FFT algorithms. With this technique, the initial wavepacket Eq. (9) is propagated until it is entirely in the asymptotic region. From which distance the wavepacket can be considered to be effectively free has to be checked carefully since it depends on many parameters. This is especially important in the field of cold collisions where low energies are considered.
Even though not applied in the current approach, we note that the numerical effort can still be reduced by an adiabatic correction of the initial state \[ |00\rangle, \] analyzing the flux out of the scattering region instead of projecting onto final diffractive states \[ |11\rangle \] or using a filter-diagonalization scheme \[ |2\rangle. \]

III. NUMERICAL IMPLEMENTATION

A. Model Configuration

We model a typical experimental setup with a regular square lattice of TiO\(_2\) cubes (100 nm on a side, index of refraction \( n = 2.1 \)) deposited onto a flat silica surface (index of refraction \( n = 1.5 \)) at a center-to-center distance of 250 nm (Figs. 3b). These structures are illuminated by an evanescent light field created by an incoming laser with a vacuum wavelength of 850 nm, intensity of 80 W/cm\(^2\), and subject to total internal reflection. The plane of incidence of the laser beam (denoted \( k_0 \) in Figs. 3a) is chosen to be diagonal with respect to the rectangular nanostructured pattern, and its polarization is taken to be within the plane of incidence (TM polarization). The angle of incidence with respect to the surface normal was chosen to be 60 degrees. Under these conditions, the flat surface without the nanostructures would give rise to an evanescent wave with a decay length \( \gamma_0 \) of about 170 nm, and the atoms would not approach closer than about 200 nm to the surface. Hence the influence of the attractive van der Waals atom-surface potential can be neglected. For different parameters however, it might become important \[ \xi \] and can easily be included in Eqs. 18. The Fourier decomposition Eq. 4 required \( N = 10 \) terms for convergence.

B. Diffractive scattering

We have chosen a model atom with ground state \( S_{1/2} \), the mass of atomic Cs, and transition dipole moment corresponding to the \( 6^2S_{1/2} \rightarrow 6^2P_{3/2} \) atomic Cs transition. The initial internal state was taken to be \( m_j = -1/2 \) and the initial Gaussian distribution of the perpendicular motion was centered around \( k_x = 0.87 \) nm\(^{-1}\) with a width parameter \( \xi = 5.00 \) nm. The initial transverse momentum is taken to be \( k_{x} = 0.73 \) nm\(^{-1}\), \( k_y = 0.0 \). This corresponds approximately to cold Cs atoms produced in a MOT after a free fall of about 1.5 cm before colliding with the nanostructured surface inclined at an angle of about 40 degrees between the vertical axis and the surface normal. Under these conditions, the incoming and specular direction are in the \( y = 0 \) plane, as indicated in Fig. 3b. We found converged results for a cut-off distance of about 600 nm. The asymptotic wavefunction is then analyzed to yield the diffraction probabilities \( P_{mn}(|\mathcal{E}|) \) as outlined in the previous section. In all calculations, grids of 16 points in the \( x \) and 64 in the \( y \) direction were used and 1024 points in the \( z \)-direction.

IV. RESULTS

A. Sub-wavelength optical near-field

In Fig. 4, we show the geometry of the TiO\(_2\) cubes (a) together with the intensity distribution (b) at a distance of 125 nm above the surface. The arrow indicating the plane of incidence of the laser beam is denoted by \( k_0 \) and plane of incidence of the atoms by \( k_x \). One can clearly see that the light fields bear the periodicity of the nanostructures. We found that illuminating the nanostructures with the plane of laser incidence aligned along the cube diagonals rather than along the sides yields periodic potentials with steeper gradients (more pronounced localization) even at distances far above the surface. At the illustrated distance of 125 nm above the surface, we still find pronounced periodic field intensity modulation. This strong localization of light intensity above high-refractive-index structures is a well-known characteristic of the TM illumination mode. It has been theoretically modelled and experimentally verified by the SNOM technique for a number of nanostructured objects \[ 4. \] In Fig. 4, we show a cross section of the field intensity distribution in the \( y, z \) plane above the nanostructures up to 400 nm. One clearly sees how the intensity contrast above the nanostructures decays with in-
the electric field orously establish the optical potential that governs the wavelength to the optical grating period. In order to rig-
at large distances from the surface, the diffraction angle mains the same; and that even if the atoms are diffracted the contrast diminishes with distance, the periodicity re-
modulation (contrast) at the plane of the mean classi-
surface, therefore experiencing a different amplitude falling atoms will penetrate to different heights above
creasing distance. Depending on the kinetic energy, the falling atoms will penetrate to different heights above the surface, therefore experiencing a different amplitude modulation (contrast) at the plane of the mean classical turning point. It is important to note that even if the contrast diminishes with distance, the periodicity remains the same; and that even if the atoms are diffracted at large distances from the surface, the diffraction angle will still be controlled by the ratio of the atom de Broglie wavelength to the optical grating period. In order to rigorously establish the optical potential that governs the atomic motion, we need the full information of the field above the surface, i.e. the three spherical components of the electric field $E_+, E_-$ and $E_0$, as can be seen from Eq. 8. The quantization axis was chosen to be perpendicular to the plane of laser incidence. From Fig. 5 one can see that the different components of the light fields are a complicated function of space that will interact with the multi-level internal structure of the colliding atom. Note that the $E_0$ component is one order of magnitude smaller than $E_+$ or $E_-$. 

B. Diffraction probabilities including ground state degeneracy

In this section, we show the results for diffractive scattering, using the light field parameters as detailed in the previous section. We stress that these probabilities are calculated using the Cs $6^2S_{1/2} \rightarrow 6^2P_{3/2}$ transition dipole and atomic mass, but that no other specific atomic parameters were used. This particle is still a model atom, however, since we have ignored hyperfine structure in the ground and excited states. The center-of-mass motion is treated entirely quantum mechanically, and the polarization state of the electric field with its spatial variation rigorously included in the calculations. Since we are considering a 2-D potential surface, the diffraction takes place in two spatial directions labelled $G_{mn}$, which are the reciprocal lattice vectors corresponding to the $x−$ and $y−$ directions, respectively. The probability $P(m,n)$ to diffract into a given order $(m,n)$ as a function of energy is given by Eq. 12. Figure 6 plots these diffraction prob-
abilities $P(m,0)$ (top panel) and $P(0,n)$ (bottom panel) as a function of total energy. The symmetrical results for negative values of $m, n$ are not shown for clarity. With the definitions employed $(m,0)$ corresponds to diffraction within the plane of incidence of the atoms while $(0,n)$ corresponds to diffraction perpendicular to this plane. These two cases will be called 'in- plane' and 'out-of-plane' diffraction, respectively. Comparing the top and bottom panels of Fig. 6, we see that probabilities for in-
plane and out-of-plane diffraction differ dramatically.

The top panel of Fig.6 shows the in-plane diffraction probability as a function of energy for fixed initial transverse momentum of $k_T = 0.73$ nm$^{-1}$. For low energies, we find negligible diffraction. Most of the final population is in the $(0,0)$ channel which represents specular reflection. As the energy $E$ increases, $P(0,0)$ decreases and falls off to almost zero for energies greater than 2.5 mK ($\Delta E = k_B T$). The higher orders of in-plane diffraction $P(m,0)$, $m = \pm 1, \pm 2, \pm 3, \ldots$ are not significantly populated either. The bottom panel of Fig. 6 shows where the scattering flux has gone. Almost the entire population is found in the out-of-plane diffraction orders $(0,n)$, $n = \pm 1, \pm 2, \pm 3$. The fact that we calculate a rapidly decreasing in-plane diffraction corresponds to the well-known averaging of the transverse scattering amplitude of the atomic motion parallel the diffracting structures. With our parameters, we find an interaction time of about 3 ìsec, which together with the initial transverse momentum of $k_T = 0.73$ nm$^{-1}$ implies that the atoms "sample" the modulated potential over a transverse distance of about 800 nm, greater than the peri-
odicity of the potential by more than a factor of three. For the out-of-plane scattering there is no such averaging and the situation is analogous to in-plane diffraction at normal incidence. It is worthwhile noting that this out-of-plane diffraction at grazing incidence (in a quite different experimental arrangement than the one envisaged here) has been observed experimentally.
Using the results shown in Fig. 6, one can now simply read off the probability for specific collision energies. At an energy of 2.35 mK, which corresponds to an angle of incidence of about 40 degrees (indicated by the left arrows in the top and bottom panels of Fig. 6), we have almost the entire population equally distributed in the three diffraction orders \((0,0)\) and \((\pm 1,0)\). Figure 7 shows the complete set of diffraction probabilities \(P(m,n)\) for this case. One sees clearly that the only significant diffraction is out-of-plane, and the three dominating diffraction channels have almost equal probability of 30 percent each. The diffraction angle, given roughly by the ratio of deBroglie wavelength to grating periodicity, is quite large—about 2.6 degrees.

C. Diffraction probabilities neglecting ground state degeneracy

In the previous section, we have calculated the diffraction probability including the ground state degeneracy. As can be seen from Eq. 8, the intricate spatial distributions of polarization in general do not allow treatment of the problem as a one-surface scattering event, but require the solution of multiple internal states coupled to the optical potential. However, as one sees from Fig. 3, the electric field is dominated by the \(E_+\) and \(E_-\) components, with the \(E_0\) one order of magnitude smaller (the axis for the polarization state is chosen to be orthogonal to the plane of incidence of the laser beam). One sees from Eq. 8 that the coupling between the ground state sublevels in the present case of an \(S_{1/2} \to P_{3/2}\) transition is due to the \(E_0\) component. Hence if the component
$E_0$ is sufficiently small, the system of Eqs. 6, 8 decouples and we have the situation of an effective single-surface collision. Consistent with this observation, we find that, starting from a well-defined initial $m_j$ level, less than 0.1 percent of the population is transferred to the other one. As a consequence, one can assume that a treatment on one surface only, which greatly simplifies the computational burden, can yield satisfactory results. Thus in this particular case a one-surface calculation gives very good agreement with the full results, even for the weakly populated diffraction orders. In general, however, with atoms having higher ground-state multiplicity and with different optical materials and excitation geometries, a full coupled-surface calculation will be necessary.

V. CONCLUSIONS

In this paper we have investigated the diffraction of cold atoms by highly structured subwavelength optical potentials generated from evanescent fields. Our approach includes a three dimensional quantum treatment of the atomic center of mass motion. We take into account the spatial distribution of rapidly varying polarization states of the nanostructured optical fields and include the effect of these polarization changes on the atom ground internal state populations.

As an illustration, we have chosen a model system that corresponds to cold cesium atoms (without nuclear spin) diffracting from a nanostructured surface illuminated under conditions of total internal reflection. The interaction of cold atoms with these light fields is calculated in the limit of large detuning and negligible absorption. For experimentally realistic initial conditions, we find diffraction angles on the order of 2 degrees with about two thirds of the initial atomic flux concentrated in the first two diffraction orders. These structures may therefore prove useful in wide-angle atomic interferometers.

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