

## Atomic diffraction assisted by a stimulated Raman transition

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We show that internal state transitions may induce energy transfer among different directions of motion and lead efficiently to large scattering angles in atomic reflection from evanescent-wave mirrors. The proposed scattering mechanism is reminiscent of the so-called Sisyphus effect of laser cooling. Perturbative calculations are presented and discussed for the diffraction of atomic beams at grazing incidence on evanescent fields with polarization gradients and for the reflection of atoms by a rough mirror. [S1050-2947(97)050507-5]

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In this paper we discuss a simple mechanism for the scattering of multilevel atoms from an atomic mirror formed by an evanescent laser wave. Provided the laser field contains a weak component with a polarization different from the field establishing the mirror, the atoms may change internal state in the vicinity of the turning point of their approach towards the mirror. We show that the resulting exchange between internal energy and kinetic energy of the atomic center-of-mass motion leads to efficient large-angle scattering. A similar idea has been proposed for the construction of a magnetically assisted reflection beam splitter where the internal states are mixed by a homogeneous magnetic field [1]. We show here that this mechanism also applies for purely optical potentials. In particular, we present a perturbative analysis of two cases, atomic diffraction from a partially stationary evanescent wave with a polarization gradient and diffuse reflection at an evanescent wave above a rough dielectric surface.

*Distorted-wave Born theory.* A mirror for atoms ideally reflects all incident atoms, and at first sight a perturbative approach to the scattering process seems less justified. This problem is well known in atom-surface scattering and its solution is not to consider transitions between traveling waves (momentum eigenstates) as in the usual lowest-order perturbation theory, but to consider the coupling among wave functions that already have both an incoming and a specularly reflected component [2]. We present here a brief outline of such a distorted-wave Born theory that we shall use to compute the scattering probabilities for atoms reflected at an evanescent-wave mirror.

Our theory applies to situations where atoms interact with a far-off resonant laser field of the form

$$\mathbf{E}(\mathbf{r}, t) = [\mathbf{E}^0(\mathbf{r}) + \mathbf{E}^1(\mathbf{r})]e^{-i\omega t} + \text{c.c.}, \quad (1)$$

where  $\mathbf{E}^0(\mathbf{r}) = E_0 \mathbf{e}_0 \exp(i\mathbf{K} \cdot \mathbf{R} - \kappa z)$  is a traveling evanescent wave, and we have adopted the notation  $\mathbf{r} = (\mathbf{R}, z)$ . The effect of the weak-field component  $\mathbf{E}^1(\mathbf{r})$  on the atomic motion is treated perturbatively. If the laser detuning with respect to the atomic transition frequency,  $\Delta = \omega - \omega_A$ , is sufficiently

large, the excited states are not populated, and we obtain an effective ground-state potential operator,

$$\hat{\mathbf{V}} = \frac{d^2}{\hbar \Delta} (\mathbf{d}^- \cdot \mathbf{E}^*) (\mathbf{d}^+ \cdot \mathbf{E}), \quad (2)$$

where the operator character within the space of ground-state Zeeman sublevels is given by the raising and lowering parts of the atomic dipole operator  $d d^\pm$ .

Inserting the expression for the electric field in Eq. (2) we obtain a term,  $V^0(\mathbf{r}) \propto |\mathbf{E}^0(\mathbf{r})|^2$ : this is the usual evanescent-wave potential. The atomic eigenstates in this potential are product states of an in-plane momentum eigenstate  $\exp(i\mathbf{P} \cdot \mathbf{R}/\hbar)$  and a wave function  $\phi_{p_z}(z)$  that approaches asymptotically a sine wave corresponding to a superposition of incoming and outgoing plane waves. Another term, quadratic in  $\mathbf{E}^1(\mathbf{r})$ , is neglected due to the weakness of  $\mathbf{E}^1(\mathbf{r})$ , whereas we use first-order perturbation theory to treat the interference term,  $V^1(\mathbf{r})$ .

We are interested in the differential atomic scattering probability  $dw/d\mathbf{Q}$  per in-plane momentum transfer  $\hbar \mathbf{Q} = \mathbf{P}_f - \mathbf{P}_i$ . In the distorted-wave Born approximation, it is related to the matrix element of the perturbing potential  $V^1(\mathbf{r})$  between the wave functions in the zeroth-order potential. The in-plane integral of this matrix element extracts the two-dimensional (2D) Fourier component  $V^1(\mathbf{Q}, z)$  of the perturbing potential at the wave vector  $\mathbf{Q}$ . The scattering probability is now given by

$$\frac{dw}{d\mathbf{Q}} = \frac{4M^2}{\pi^2 \hbar^2 p_{zi} p_{zf} A} |\langle \phi_{p_{zf}} | V^1(\mathbf{Q}, z) | \phi_{p_{zi}} \rangle|^2, \quad (3)$$

where the wave functions  $\phi_{p_{z,i,f}}(z)$  appear. Note that the values of the normal atomic momentum are linked by kinetic-energy conservation  $\mathbf{P}_i^2 + p_{zi}^2 = (\mathbf{P}_i + \hbar \mathbf{Q})^2 + p_{zf}^2$ . In Eq. (3),  $M$  is the atomic mass and  $A$  is the mirror surface area (see Ref. [3]).

For atoms scattered at normal incidence ( $\theta_{in} = 0$ ), the spatial extent  $\sim \kappa^{-1}$  of the perturbing potential in the normal direction limits the in-plane momentum transfers to  $\hbar \mathbf{Q} \lesssim \sqrt{2p_{zi} \hbar \kappa}$ , which is typically less restrictive than the limit set by the in-plane variation of the potential. At oblique incidence, however, the matrix element in Eq. (3) limits the

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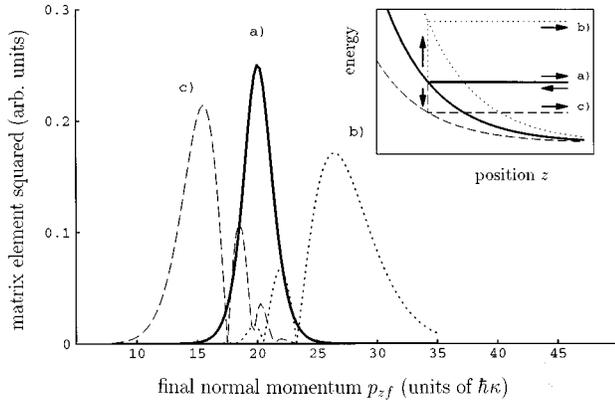


FIG. 1. Squared matrix elements of  $\exp(-2\kappa z)$  between eigenstates  $\phi_p(z)$  in exponential potentials. The initial momentum is fixed with  $p_{zi} = 20 \hbar \kappa$ , and the in-plane momentum transfer  $\hbar \mathbf{Q}$  is varied. Asymptotic kinetic-energy conservation then determines the final normal momentum  $p_{zf}$ . We arbitrarily chose potentials for the final state that differ from the initial-state potential by factors of 1, 2, and  $\frac{1}{2}$ , corresponding to the curves denoted by (a), (b), and (c). The inset illustrates the motion and transitions of the atom for the peak values of the matrix elements.

in-plane scattering to momentum transfers  $\hbar \mathbf{Q} \approx \hbar \kappa / \tan \theta_{in}$  on the order of a single photon momentum: a substantial limitation both for diffraction from a standing-wave pattern and for scattering on a rough mirror [3].

The above analysis is only valid if the atom experiences a *single* position-dependent potential throughout the reflection. For multilevel atoms with different ground-state light shifts this need not be the case, and in Fig. 1 we show the squared matrix element of the  $z$ -dependent quantity  $\exp(-2\kappa z)$  between eigenstates  $\phi_p(z)$  in different exponential potentials. The increased probability for large momentum transfers  $\hbar \mathbf{Q}$ , and hence large changes in  $p_z$ , compared to  $\hbar \kappa$ , is the crucial feature induced by the lifted atomic degeneracy that we wish to emphasize in this paper.

*Stimulated Raman transitions, Franck-Condon enhancement.* When an atom approaches the dielectric its normal kinetic energy is transformed into potential energy. If the atom makes an internal state transition and leaves the surface following a different potential curve, its normal momentum is asymptotically smaller or larger than upon incidence, see inset of Fig. 1. This picture is reminiscent of the spontaneous Sisyphus mechanism of laser cooling [4], suggested also recently for lowering the energy of atoms reflected by an evanescent-wave mirror [5] and for loading a trap formed by two evanescent waves close to a dielectric surface [6]. In Sisyphus cooling, kinetic energy is turned into potential energy during the atomic motion in position-dependent potentials, and transitions among the internal levels release this energy by spontaneous emission of photons having a larger mean energy than the laser photons: energy is exchanged with the photon reservoir. In our problem, the ‘‘Sisyphus effect’’ is stimulated; the transition is driven by a laser field component through the perturbation  $V^1(\mathbf{r})$ , which must both couple the internal atomic states and provide the required in-plane momentum transfer: although total kinetic energy is asymptotically conserved, the atom loses or gains kinetic energy normal to the surface, depending on the initial and final potential curves.

Coming back to Fig. 1, the strong peaking of the overlap integrals as a function of the final normal momentum can be understood in terms of the Franck-Condon principle: the  $z$  integral in Eq. (3) obtains its main contributions from a region around the classical turning point of the incoming particle—for smaller  $z$  the wave function is reduced and for larger  $z$  the coupling decreases and the oscillating product of wave functions reduces the contribution to the integral. A maximum of the integral is obtained if the outgoing particle, moving in a different potential, has the same turning point as the incoming one (the situation shown in the inset of Fig. 1).

In Fig. 1 we also observe oscillations in the matrix elements as a function of the final-state momentum. As this quantity is varied, the turning points no longer coincide, and the scattering efficiency is reduced. The matrix element now gets its major contribution from positions around  $z_c$ , defined by

$$V_f^0 e^{-2\kappa z_c} - V_i^0 e^{-2\kappa z_c} = \frac{p_{zf}^2}{2M} - \frac{p_{zi}^2}{2M}, \quad (4)$$

where the potential difference equals the difference between the normal kinetic energies. This is the position where the local de Broglie wavelengths in the two potentials coincide. The oscillations in the matrix elements are due to the variation of the relative phase of the wave functions in the vicinity of this position.

*Diffraction on a mirror with polarization gradient.* The coherent reflection of multilevel atoms from an evanescent light field has recently attracted considerable attention [1,7]. At grazing incidence the diffraction of a two-level atom is negligible due to the difficulty in providing the required momentum transfer in both the normal and the in-plane directions. For multilevel atoms, however, the mechanism described above may come into play. A numerical integration of the time-dependent Schrödinger equation [7] has in fact shown that incorporation of the multilevel atomic structure leads to large diffraction probabilities, in agreement with experiments [8,9]. Higher-order diffraction requires a calculation beyond our distorted-wave Born theory, but it is noteworthy that if diffraction is mediated by the internal level structure rather than by a multiphoton doppleron (velocity tuned resonance) [10], the population of the first-order diffraction peak may be obtained in a perturbation calculation.

We consider a strong evanescent traveling wave  $\mathbf{E}^0(\mathbf{r})$  created by total internal reflection of a TM polarized field (electric-field vector in the plane of incidence, the  $xz$  plane). The weak field  $\mathbf{E}^1(\mathbf{r})$  is taken to be a counterpropagating evanescent wave with TE polarization [ $\mathbf{E}^1(\mathbf{r})$  parallel to the  $y$  axis]. For fields incident far from the critical angle, one then gets, to a quite good approximation, a strong (weak) evanescent wave of  $\sigma^-$  ( $\pi$ ) polarization with respect to the direction of  $\mathbf{E}^1(\mathbf{r})$ . We model the atom by a  $j = 1/2 \rightarrow 3/2$  transition. In the nearly circularly polarized field  $\mathbf{E}^0(\mathbf{r})$ , the ground states then experience different potentials proportional to the Clebsch-Gordan coefficients. The potential matrix  $V^1(\mathbf{r})$  resulting from the interference of this field and the weak field  $\mathbf{E}^1(\mathbf{r})$  describes the Raman transitions that couple the atomic sublevels. The in-plane momentum of the atom then changes by  $\hbar \mathbf{Q} = \pm 2\hbar \mathbf{K}$ , corresponding to the  $n = \pm 1$  diffraction orders. For an incident momentum parallel to  $\mathbf{K}$ ,

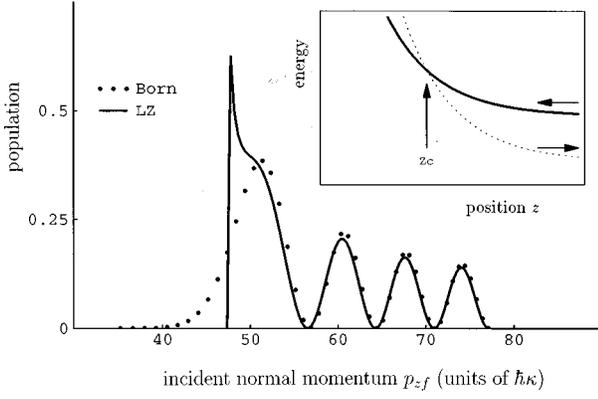


FIG. 2. Population of the  $-1$  diffraction order for an evanescent-wave grating with a weak polarization gradient. The atoms are incident in the state  $|m = +1/2\rangle$  with a lower light shift. The incident in-plane momentum is fixed to  $\mathbf{P}_i = 500\hbar\mathbf{K}$ , and  $|\mathbf{K}| = \sqrt{2}\kappa$ . The transition probability is shown as a function of the normal momentum  $p_{zi}$ , both as a result of the Born theory (dots) and of a semiclassical Landau-Zener treatment (solid curve). The latter is not valid if the classical velocity vanishes in the crossing. The inset illustrates the potential curves crossing at the atom-surface distance  $z_c$ .

the  $n = -1$  order corresponds to a reduced in-plane kinetic energy and a final normal momentum  $p_{zf} > p_{zi}$ . As shown by curve (b) in Fig. 1, this diffraction order may be substantially populated if the atom makes a transition to a state with a larger light shift in the zeroth-order field.

The results of our perturbative calculation (3), indicated by points in Fig. 2, show that if the intensity of the TE field component amounts to a mere 6% of the TM intensity, up to 30% of the atoms are diffracted in the lowest diffraction order. They also show that oscillations appear in the diffraction probability as a function of the incident momentum  $p_{zi}$ .

As the normal kinetic energy changes by a fixed amount, we may follow an idea proposed in Ref. [10] and shift the final potential curve correspondingly. The point  $z_c$  of Eq. (4), which gives the dominant contribution to the overlap integral, now appears as a curve crossing; see inset of Fig. 2. A Landau-Zener treatment of the crossing, and a WKB treatment of the phase accumulated by the wave-function components during propagation on individual potential curves permits us to derive a simple approximation for the diffraction probability, shown as a solid line in Fig. 2 [11]. The oscillations of the diffraction probability have also a simple interpretation in this picture: if the turning points in both the initial- and final-state potentials are closer to the surface than  $z_c$ , a superposition of atomic states is formed upon the first passage of  $z_c$  and the atom will propagate with components in both potentials. During the second passage of  $z_c$  after reflection, the components are recombined into the amplitudes for the reflected atomic states. The two components accumulate different phases, and the oscillations are equivalent to the so-called Stückelberg oscillations, well known in the theory of slow atomic collisions.

*Scattering by mirror roughness.* We now consider an example where the scattering potential contains a continuous distribution of  $\mathbf{Q}$  vectors, and hence the atoms are diffusely

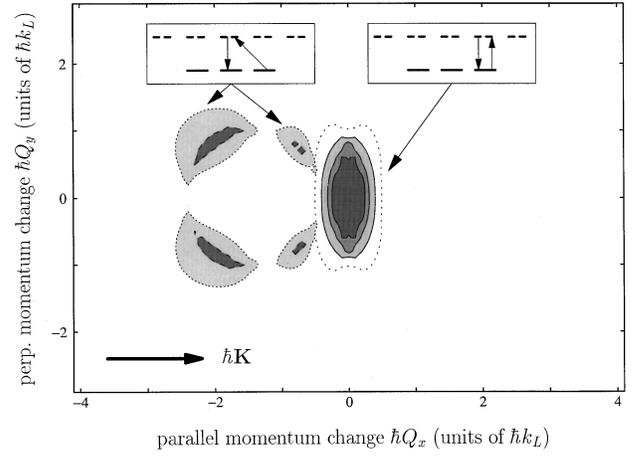


FIG. 3. Distribution functions for the in-plane momentum change  $\hbar\mathbf{Q}$  for atoms incident at an angle of  $70^\circ$  on a rough evanescent mirror [normal momentum  $p_{zi} = 50\hbar k_L$ ; turning point distance  $(\ln 2)/(2\kappa)$ ]. The contour plot indicates the atomic “response function,” which should be multiplied by the surface roughness power spectrum  $|S(\mathbf{Q})|^2$  to yield the true scattering distribution. The components scattered with unchanged internal state and with a change from  $m = 1$  to  $m = 0$  are shown. The arrow at the lower left indicates the photon momentum of the zeroth-order evanescent wave (with  $|\mathbf{K}| = \sqrt{2}k_L$  and  $\kappa = k_L$ ).

scattered according to Eq. (3). This situation occurs, for example, if an evanescent wave is created outside the rough surface of a dielectric of refractive index  $n$ . Within the Rayleigh approximation, the lowest-order perturbation of the light field with respect to the field outside a planar surface is linearly related to the surface height profile through its Fourier transform  $S(\mathbf{Q})$  and to the electric-field vector  $E_0\mathbf{e}_0$  of the zeroth-order evanescent wave [12],

$$\mathbf{E}^1(\mathbf{K}') = S(\mathbf{K}' - \mathbf{K})(\kappa'_1 - \kappa'_n) \left( \mathbf{e}_0 - \frac{(\mathbf{k}'_1 \cdot \mathbf{e}_0)}{(\mathbf{k}'_1 \cdot \mathbf{k}'_n)} \mathbf{k}'_n \right) E_0, \quad (5)$$

where  $\kappa'_\nu = \sqrt{\mathbf{K}'^2 - \nu^2 k_L^2}$  (real and positive or imaginary with  $\text{Im } \kappa'_\nu < 0$ ,  $\nu = 1$  or  $n$ ), and  $\mathbf{k}'_\nu = (\mathbf{K}', i\kappa'_\nu)$ , see Ref. [3]. The field is monochromatic with  $\omega = ck_L$  and a given  $\mathbf{K}'$  component in  $\mathbf{E}^1(\mathbf{r})$  is either evanescent or propagating with a known normal  $k$ -vector component  $i\kappa'_1$ .

We consider a zeroth-order field with linear (TE) polarization and take the atomic quantization axis along the electric-field vector  $E_0\mathbf{e}_0$ . The atoms are incident in the  $|j = 1, m = 1\rangle$  ground state (the excited state has  $j_e = 2$ ), at an angle of  $70^\circ$  with respect to the normal and with an in-plane momentum  $\mathbf{P}_i$  parallel to the wave vector  $\mathbf{K}$  of the zeroth-order evanescent wave. Figure 3 shows the momentum distribution of the scattered atoms that are detected in the  $m = 1$  and  $m = 0$  states. Note the sizable momentum change associated with the mechanism discussed in the present paper. The absence of scattered atoms along the direction of propagation of the zeroth-order evanescent field is due to the vanishing of the scattered field component with the required polarization,  $(\mathbf{k}'_1 \cdot \mathbf{e}_0) = 0$ . The emergence of distinct peaks on either side of the symmetry line  $Q_y = 0$  reflects the Stückelberg oscillations observed in Fig. 1 [curve (b)].

In conclusion, we have identified a Sisyphus-like mechanism in the scattering of multilevel atoms by evanescent-wave laser fields. In a stimulated Raman transition, the atoms may experience a change of internal energy, which, in turn, is transferred among different directional components of the kinetic energy. The process involves only one absorption and stimulated emission event (on the background of atomic motion in a zeroth-order light-induced potential), and it can therefore be characterized by a simple perturbation approach. In addition, the physical mechanisms responsible for the scattering can be analyzed semiclassically and this facilitates an interpretation of the qualitative behavior of the quantum results.

First we investigated the case of atomic diffraction assisted by a weak-field polarization gradient. The fact that the diffraction in a standing wave with only a single polarization is negligible suggests that our theory applies also in the case of a standing evanescent wave with only one polarization and a small traveling or standing evanescent field component of different polarization. We hence believe that our theory captures the essentials of the recent numerical work on diffraction at grazing incidence [7], and that it represents a good basis for the understanding of recent experiments [8,9].

As a second application, we studied the implications of dielectric surface roughness for evanescent-wave mirrors. We note that, conversely, the state-sensitive detection of scattered atoms may be used to probe the polarization properties of the light field near the dielectric surface as a supple-

ment to existing scanning near-field optical microscopy techniques [13].

We anticipate that the “stimulated Sisyphus effect,” enhanced when the turning points of the atomic motion coincide, may provide a useful picture also in other domains of atom optics (beam splitters, output couplers from trapping geometries, etc.). Also other means to realize the coupling of internal states with different potentials may be considered and have, in fact, already been suggested (see Ref. [1], for example).

Finally, we wish to point out that the potential curve crossing in the inset of Fig. 2 acts as a beam splitter and the two turning points as mirrors for the atomic wave, and thus the system constitutes an atomic equivalent of a Michelson interferometer. Such an interferometer is sensitive to details of the atom-surface interaction, e.g., the van der Waals interaction, and through variation of the parameters, it can probe such details within an adjustable range of atom-surface distances, cf. the location of the enclosed area in the inset of Fig. 2.

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