Emerging beam resonances in atom diffraction from a reflection grating

Bum Suk Zhao, Gerard Meijer, and Wieland Schöllkopf
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany
(Dated: May 20, 2010)

PACS numbers: 03.75.Be, 34.35.+a, 37.25.+k, 42.25.Fx, 68.49.Bc

We report on the observation of emerging beam resonances, well known as Rayleigh-Wood anomalies and threshold resonances in photon and electron diffraction, respectively, in an atom-optical diffraction experiment. Diffraction of He atom beams reflected from a blazed ruled grating at grazing incidence has been investigated. The total reflectivity of the grating as well as the intensities of the diffracted beams reveal anomalies at the Rayleigh angles of incidence, i.e., when another diffracted beam emerges parallel to the grating surface. The observed anomalies are discussed in terms of the classical wave-optical model of Rayleigh and Fano.

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incident beam and the angular resolution of detection are required to be on the order of 100 μrad. Another prerequisite for observing the effect is to have a significant flux diffracted into the very beam that, at Rayleigh conditions, emerges above the surface so as to have an appreciable effect on the other outgoing beam intensities. In the experiment described here these requirements have been met by reflecting a highly collimated helium atom beam at grazing incidence from a blazed ruled diffraction grating. The use of helium atoms at grazing incidence ensures sufficient coherent reflection probability \(24\), while the grating blaze angle in combination with a well chosen azimuthal orientation of the grating leads to an effective enhancement of the intensity of the emerging diffracted beam.

The high angular resolution diffraction apparatus has been used in previous experiments \([24, 25]\). The continuous atom beam is formed by supersonic expansion of He gas at stagnation temperature \(T_0 = 8.7\) K and pressure \(P_0 = 0.5\) bar through a 5-μm-diameter orifice into high vacuum. After passing a skimmer of 500 μm diameter, the beam is collimated by two 20 μm wide slits (slit 1 and slit 2) separated by 100 cm as indicated in Fig. 1(a). In combination with the 25 μm wide detector-entrance slit (slit 3), located 78 cm downstream from the second slit, the observed angular width of the atom beam is 120 μrad (full width at half maximum). The third slit and the detector (an electron-impact ionization mass spectrometer) are mounted on a frame which is rotated precisely (including \(\phi < \varphi\)) around the z-axis. In this configuration out-of-plane diffraction is without effect on the measurements because the vertical acceptance angle of slit 3 (≈ 10 mrad) is far larger than the vertical diffraction angles (tens of μrad). As indicated in Fig. 1(c) the grating can be rotated by the azimuth angle \(\phi\) around the z-axis. By varying \(\phi\) the effective periodic length \(d_{\text{eff}}\) and the effective blaze angle \(\alpha_{\text{eff}}\) can be adjusted, as depicted in Figs. 1(c) and (d). The former is given by trigonometry of the triangle in Fig. 1(c), \(d_{\text{eff}} = d/|\sin\phi|\), while the latter is approximated by \(\alpha_{\text{eff}} \approx \alpha \phi\), which is derived from \(\sin \alpha_{\text{eff}} = \sin \alpha \sin \phi\). We define \(\phi\) to be negative (positive) when the blaze arrow is rotated clockwise (counterclockwise) from the y-axis. In this convention Fig. 1(c) shows the case of \(\phi < 0\). Since the effect of blazing is to enhance those diffracted beams which are specularly reflected with respect to the facet normal, negative (positive) diffraction orders get enhanced for \(\phi < 0\) (\(\phi > 0\)).

The fraction of He atoms that are coherently scattered from the grating, measured for three different azimuth angles \(\phi < 0\), is plotted as a function of incidence angle \(\theta\) in Fig. 2. It is determined from the summation of the areas \(A_n\) of the diffraction peaks in intensity vs. detection angle plots (see below). The sum is taken over all diffraction orders \(n\) (including \(n = 0\), the specular peak) and normalized to the incidence beam area \(A_{\text{inc}}\). The latter is measured when the grating is moved out of the beam path. The vertical lines in Fig. 2 each labeled by an integer, indicate the positions of the Rayleigh angles of incidence \(\theta_{R,m}\) with the integer indicating the

\[\begin{align*}
\text{FIG. 1: (Color online) Scheme of the experimental setup and orientation of the plane ruled grating. In each figure the chosen coordinate system is denoted. The grating azimuth angle } \phi \text{ is the angle between the grating blaze arrow (thick arrow in (b) and (c)) and the y-axis. In (b) } \phi = 0, \text{ whereas (c) and (d) correspond to } \phi < 0. \end{align*}\]
with a Gaussian curve. The incidence angle \( \theta \) undergoes diffuse scattering at the surface. There must be a concurrent decrease of the fraction of He atoms that are coherently scattered. There must be an increase of the fraction of He atoms that are diffusely scattered for the outgoing beams, but also to an increase of the fraction of He atoms that are coherently scattered. (The diffraction order sign convention follows Ref. \[12\].) The emergence of another diffraction order leads to a redistribution of flux among the diffraction orders. This indicates that emergence of another diffraction order not only leads to a redistribution of flux among the outgoing beams, but also to an increase of the fraction of He atoms that are coherently scattered. There must be a concurrent decrease of the fraction of He atoms that undergo diffuse scattering at the surface. The azimuth angle \( \phi \) is obtained by analyzing diffraction patterns at various incidence angles. Fig. 2(a) shows diffraction spectra for \( \phi = -41 \) mrad at five different incidence angles in the vicinity of the Rayleigh incidence angle \( \theta_{\text{R},-1} = 1.164 \) mrad, where the \(-1^{\text{st}}\) order peak emerges. The diffraction angles \( \theta_n \) and areas \( A_n \) of the \( n^{\text{th}} \)-order diffraction peak are found by fitting each peak with a Gaussian curve. The incidence angle \( \theta_{\text{in}} \) is determined from the detection angle of the specular peak, \( \theta_0 \). The diffraction angles \( \theta_n \) as a function of \( \theta_{\text{in}} \) are then fitted by the grating equation, \( \cos \theta_n - \cos \theta_{\text{in}} = n \frac{\lambda}{2 d_{\text{eff}}} \) with \( d_{\text{eff}} \) being the only fit parameter. For the data set in Fig. 2, \( d_{\text{eff}} = 493 \pm 1 \) \( \mu \text{m} \) is found corresponding to an azimuth angle \( \phi = -41 \) mrad. The angular spectra shown in Fig. 2(a) illustrate the progressive emergence of the \(-1^{\text{st}}\)-order peak. The height of the latter increases rapidly from 40 to 1050 counts/s within this range of incidence angles, whereas the height of the specular peak increases from 270 to 360 counts/s when \( \theta_{\text{in}} \) is increased from 1.146 to 1.179 mrad, and stays around 360 counts/s at \( \theta_{\text{in}} = 1.203 \) mrad. This indicates a discontinuity of the slope of the specular intensity variation around \( \theta_{\text{in}} = 1.179 \) mrad, which agrees with the calculated Rayleigh angle. As can be seen in Fig. 3(a) this coincides with the incidence angle at which the \(-1^{\text{st}}\)-order diffraction peak starts to be fully separated from the surface. The high intensity of the diffraction beam at grazing emergence is remarkable and might be a manifestation of the reciprocity theorem, as observed before in x-ray grating diffraction \[27\].
angles of incidence. Figure 3(b) exemplifies general aspects of emerging beam resonances, which have also been found for further azimuth angles not shown here. (I) The resonance behavior at $\theta_{R,m}$ observed in the outgoing beams of order $n$ (with $n \neq m$) is the more distinctive, the more intense the emerging beam is. This can be seen in the figure where the resonance behavior is most pronounced at $\theta_{R,-1}$, less distinct at $\theta_{R,-2}$, and hardly visible when the less intense $-3^{rd}$ and $-4^{th}$-order diffraction peaks emerge. (II) Discontinuities seem to appear in all the other diffraction peaks, although they are most pronounced in neighboring diffraction orders, namely, $A_{m+1}$ and $A_{m+2}$. In Fig. 3(b), for instance, at $\theta_{R,-1}$ pronounced discontinuities are found in the slopes of $A_0$ and $A_1$. (III) At the Rayleigh angle of incidence the slope of $A_n$ usually exhibits a discontinuous decrease with increasing incidence angle, except for a few cases where a discontinuous increase is observed. In the figure, $A_0$ and $A_1$ are found to increase steeply (with the slope being close to diverging) at $\theta_0 \leq \theta_{R,-1}$, whereas they hardly change right after the vertical line. Similarly, at $\theta_{R,-2}$ the slope of $A_{-1}$ shows a sudden decrease, the slope of $A_1$, however, abruptly increases.

Following the approach introduced by Rayleigh and Fano [2, 4] the amplitude of the $n^{th}$-order diffraction $S_n$ is approximated by interference of the amplitudes from the first and the second order scattering, $S_n = S_n^{(1)} + S_n^{(2)}$. The first order scattering is the scattering of the incident beam at a given grating unit (red arrow in Fig. 1(d)), while the second order scattering is the scattering of a beam at that grating unit, which has already undergone scattering at another grating unit (blue arrow in Fig. 1(d)). When the $m^{th}$-diffraction-order fulfills the Rayleigh condition, $S_m^{(2)}$ is proportional to $S_m^{(1)}$ and the interference is constructive. Thus, the sudden increase of the emerging $m^{th}$-order intensity increases the other orders (aspects (II) and (III)). The degree of the influence is proportional to $S_m^{(1)}$, namely, $A_m$ (aspect (I)). Therefore, once the $m^{th}$-order peak gets separated from the grating, as seen in the spectra of Fig. 3(a), the contribution of the second order scattering to the other diffraction beams diminishes and their intensities level off.

Emerging beam resonances, i.e., Rayleigh-Wood anomalies in atom optics, have been predicted to provide detailed information of atom-surface interaction potentials [20, 22]. However, more than a century after the first observation of Wood anomalies [1] and 80 years after the first observation of selective adsorption, i.e., a resonance type Wood anomaly in atom surface scattering [13], they were still not observed in atom diffraction experiments. Here we report the first observation of emerging beam resonances in atom optics using a blazed ruled grating at grazing incidence with the grooves oriented almost parallel to the incident beam direction. The total coherent reflectivity of the grating as well as the intensities of the diffracted beams reveal anomalies at the Rayleigh angles of incidence which are interpreted with the approach developed many decades ago to describe the anomalies observed with photons [2, 4]. Therefore, this observation complements the analogy between photon optics (Rayleigh-Wood anomaly and resonance type Wood anomaly) on the one hand and atom optics (emerging beam resonance and selective adsorption) on the other hand.

B.S.Z. acknowledges support by the Alexander von Humboldt Foundation and by the Korea Research Foundation Grant funded by the Korean Government (KRF-2005-214-C00188). We thank J.R. Manson for insightful discussions and H.C. Schewe for help with the apparatus.

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1. Electronic address: zhao@fhi-berlin.mpg.de
2. Electronic address: wschoell@fhi-berlin.mpg.de

[28] For the conical diffraction geometry a modified grating equation holds, taking into account the out-of-plane (i.e. conical) diffraction [28]. However, for our conditions (i.e. $|n\lambda/d| \ll |\sin \phi|$) the in-plane grating equation employed with $d_{\text{eff}}$ is a very good approximation.