Total absorption of light by gratings in grazing incidence: a connection in the complex plane with other types of anomaly

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An explanation is given for the effect of total absorption of light in grazing incidence by a sinusoidal grating, recently reported by us. The behavior of the zeros of both the first and the zeroth diffraction orders is studied numerically in the complex α plane. A link between the grating anomaly, non-Littrow perfect blazing, and plasmon excitation in relief metallic gratings is established. A total analysis of the behavior of the zeroth-order zero in grazing incidence is carried out, including groove depth, wavelength, and profile dependences.

I. Introduction

In 1902, Wood[1] was the first to note anomalous diffraction behavior, writing: "I was astonished to find that under certain conditions, the drop from maximum illumination to minimum, a drop certainly from 10 to 1, occurred within a range of wavelengths not greater than the distance between the sodium lines" and he called this phenomenon "singular anomalies." Since then, investigation of this fascinating topic has undergone a spiral development: accumulation of experimental data, an attempt of general explanation, a new collection of anomalies not corresponding to the initial explanation, and so on. It is not easy to follow all the papers devoted to the problem. One can find earlier reviews on Wood's anomalies published by Twersky[2,3] or Millar.[4,5] In recent years the works of Neviere[6] and Maystre[7] have made a significant contribution to the physical understanding of anomalies connected with surface wave excitation.

Here we outline only the most important moments, in our opinion, in the history of grating anomalies, contributions of great meaning to today's concepts—either discovering new types of anomalies or explaining these new facts and putting them in proper connection with other already known phenomena. After the works of Wood, Lord Rayleigh[8,9] was the first to make an attempt to explain theoretically the anomalous (i.e., unpredictable) behavior of gratings: he proposed that it is due to threshold effects—cutoff or appearance of a new spectral order when grating or incident wave parameters vary. As pointed out by Maystre[7] his prediction was all the more remarkable as the author first ignored the groove frequency of the grating used by Wood, and thus could not verify this assumption with experimental data. However, Rayleigh was able to explain the existence of anomalies only for the TM polarization (electric field vector perpendicular to the grooves).

Despite its great successes (mainly in the prediction of the position of anomaly) Rayleigh's theory was unable to describe the exact form of the diffraction efficiency curve. Nevertheless, the so-called Rayleigh hypothesis, the pillar of his method, although not rigorous in a mathematical sense, seems still quite attractive to theoreticians.

By making more careful measurements, done by several authors,[10–12] it became possible to demonstrate the existence of weaker anomalies in TE polarization especially pronounced for deeper groove gratings. In the review paper of Siegman and Fauchet[13] the role of Palmer's work[11] has been discussed in detail. A contribution to the analysis of anomaly interaction (and repelling) was made in the work of Stewart and Gallaway.[12]

Fano[14] was the first to distinguish between two types of anomaly: (i) an edge anomaly, with a sharp behavior connected with the passing off of a higher diffraction order, and (ii) an anomaly, generally consisting of minimum and maximum in efficiency, which appears in a much broader interval.

The second type of anomaly was described by Fano as a resonance one—connected with the excitation of a guided (leaky) wave along the grating surface. Hessel

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and Oliner[15] published a pioneering paper that shows for the first time theoretically (based on a rigorous analysis of electromagnetic scattering from a generic model of a periodic structure yielding a simple closed-form solution) that Wood's anomaly TM resonances are of two types, one due to branch point singularities that correspond physically to the onset of a new propagating spectral order (first indicated by Lord Rayleigh), and the other to pole singularities that correspond to the condition of resonance for leaky surface waves guided by the structure.[16] Although the main problem in the equivalent surface-impedance approach used by Hessel and Oliner[15] remained, to know the surface impedance for a particular structure, they were able to depict in detail the behavior of diffraction efficiency both in the vicinity of Rayleigh and resonance anomalies. Furthermore, they established in the theory of gratings the so-called phenomenological approach—a means for deeper understanding of the physical nature of resonance behavior. As became obvious later on, this approach provided a valid and powerful tool connecting the symmetry of the system with the qualitative properties of anomalies and enabled prediction of new effects.

Although correctly explaining TM anomalies, the authors of Ref. 15 speculated that TE anomalies, already found experimentally by Palmer,[11] could be explained in similar terms. Such an explanation requires the existence of a proper TE surface wave in the limit of small modulation depth. As was pointed out by Tseng *et al.*,[17] "the idealized surface reactance structure considered therein need not always be a physically realizable one." This paper[17] not only gives the theoretical arguments for a correct explanation of TE-type anomaly and its physical nature, but also establishes the foundations of a modern classification. It shows theoretically that (i) for the first time TE anomalies do exist, and (ii) they are not connected with a surface wave on a flat surface, but with the root of the dispersion relation situated on an improper Riemann sheet (nonphysical sheet where the electromagnetic field does not satisfy the radiation conditions at infinity).

Investigating fin-corrugated perfectly conducting surfaces the authors were able to connect this anomaly (exhibited in a Littrow mount) with the half-wavelength mode resonances in the corrugated region. They showed that, by varying the groove depth in the vicinity of an anomaly, the trajectory of the improper root of the dispersion relation is perpendicular to the real axis of $\sin\theta$, where θ is the angle of incidence.

In 1969, Wirgin and Deleuil[18] were able to find both theoretically and experimentally this Bragg-type anomaly, as it was termed by Tseng *et al.*[17], for the case of lamellar perfectly conducting gratings for both polarizations. Effects of finite conductivity and groove shape for fin, triangular, and sinusoidal gratings on different kinds of anomaly were analyzed numerically by Kalhor and Neureuther in 1973[19] and it was established that usually the TE Bragg-type anomaly was exhibited at larger groove depths compared with the TM one.

Ebbeson[20] made a separate theoretical and experimental analysis of the TM Bragg-type anomaly in fin-corrugated surfaces. Wirgin and Deleuil[18] called this Bragg-type anomaly "perfect blazing in Littrow mount," because the improper root of the dispersion relation leads to a zero in the specular order, i.e., all the incident energy is diffracted in the −1st diffraction order. Hessel *et al.* in 1975[21] published a review of the perfect blazing in rectangular groove gratings. They showed a nomogram of groove depth h to period d ratio necessary for TE Littrow perfect blazing (Bragg-type anomaly) as a function of wavelength λ. The most important feature is that these h/d curves do not approach the abscissa ($h = 0$). Their analysis was followed by the work of Roumiguieres *et al.*,[22] also concerning TM polarization. The main difference between the two polarizations is that h/d values necessary for the existence of TM Littrow perfect blazing approaches zero as $\lambda/d = 2$ (i.e., in grazing incidence). This fact was explained later in the papers of Maystre *et al.*[23,24] and Breidne and Maystre.[25]

In these papers[23–25] it was demonstrated theoretically that another type of anomaly, not known up to that time, could exist in a non-Littrow mount, consisting of a zero of the specular order, i.e., a non-Littrow perfect blazing in −first diffraction order was borne out. It could be found only in TM polarization, and its connection with other existing anomalies was not yet established.

In connection with Bragg-type anomalies (exhibited only in a Littrow mount) we have to mention the works of Andrewartha *et al.*[26,27] which discuss in detail cavity resonances (modes inside the grooves) in lamellar gratings, represented with poles in the complex α plane. The lack of the zeroth groove mode for TE polarization can explain why, for shallow groove depth, the poles are far from the real axis, so that they lead to anomalous diffraction efficiency curves only for deep gratings. Some recent work of Maradudin and Wirgin considers the problem of cavity resonances[28,29]: excitation of the groove modes in very deep ($h/d = 6.5$) lamellar gratings can result in a significant electromagnetic field enhancement inside the grooves without any noticeable effect on the far-field zone, provided that only the specular order propagates. These resonances can manifest themselves through surface enhanced Raman scattering (an extended review can be found in Ref. 29).

The other main classes of anomaly are the true singular ones that are connected with the existence of a proper root of the dispersion relation (pole of the scattering matrix of the system[7]), connected with the possibility of guided wave propagation along the flat surface (for more details see Refs. 6 and 7).

Contrary to the Bragg-type anomaly this root lies on the proper Riemann sheet that corresponds to a physically meaningful solution of Maxwell's equation, boundary and radiation conditions.[17,26] These surface waves on the metal–dielectric boundary are plasmons or polaritons[30] and are connected with the collective oscillations of the electrons in metal near the interface.[31] Further development of rigorous electromagnetic theories and their numerical implementation[32] enables one to predict the existence of one of the most interesting phenomena in gratings[33]: a shallow corrugation that can lead to a total absorption of incident light whereas the corresponding flat surface reflects its almost fully. This effect called Brewster's incidence in gratings was confirmed experimentally by Hutley and Maystre[34] and can now be considered well investigated.

Very recently we demonstrated both theoretically and experimentally a heretofore unknown total absorption of light by a diffraction grating in grazing incidence[35] occurring in a specific combination of conditions, namely, the angle of incidence, wavelength, groove shape, groove frequency, depth modulation, and polarization. It must be pointed out that the main difference between the Brewster effect in gratings and this new grazing anomaly is that the latter is exhibited when two diffraction orders are propagating; thus a simultaneous vanishing of both the specular and −1st diffraction orders is observed.

Here we propose an explanation of this grazing anomaly based on numerical tracing of both the zeroth and the first-order zeros in the complex plane of angles of incidence. Moreover a connection with other phenomena in gratings, plasmon excitation and non-Littrow perfect blazing, is obtained. The calculations have been carried out using a numerical method[36] based on the rigorous formalism of Chandezon *et al.*[37] The computer code has been generalized to work for complex values of $\alpha = \sin\theta$, which needs a normalization of the eigenvectors to a modulus of unity. Poles and zeros have been found using an iterative method of Newton for complex variables, which seems to be quite efficient, provided the initial approximation is properly chosen. Some remarks concerning the complex α plane are worth noting. When speaking about resonance anomalies it is more convenient to use the sinus of angle of incidence, rather than the angle itself. The physical meaning of the quantity $\alpha = \sin\theta$ is that it is equal to the component $k\|$ of light wavevector **k** parallel to the grating plane divided by the wavenumber $|k| = 2\pi/\lambda$. It is useful because surface waves are characterized most often by their propagation constants α_g proportional to the component of the wavevector in the interfacing plane. On the other hand, with air being the upper media it is always true that $\alpha_g > 1$, thus θ cannot be used instead of α. From that point of view, a generalization to complex values of α appears most natural, as α_g is always complex, since real media are always lossy. In that case the imaginary part of α_g corresponds to the losses (it is equal to half of the leakage constant in the direction of surface wave propagation). It is $\mathrm{Re}(\alpha_g)$ that is directly connected through the grating equation

$$\sin\theta_m \equiv \alpha_m = \alpha + m\lambda/d, \qquad m = 0,\pm1,\pm2,\ldots, \tag{1}$$

with the proper conditions of surface wave excitation (i.e., resonance anomaly): $\alpha_m = \mathrm{Re}(\alpha_g)$. That is why the phenomenological formula[6,7,15] is usually written in terms of α rather than of θ.

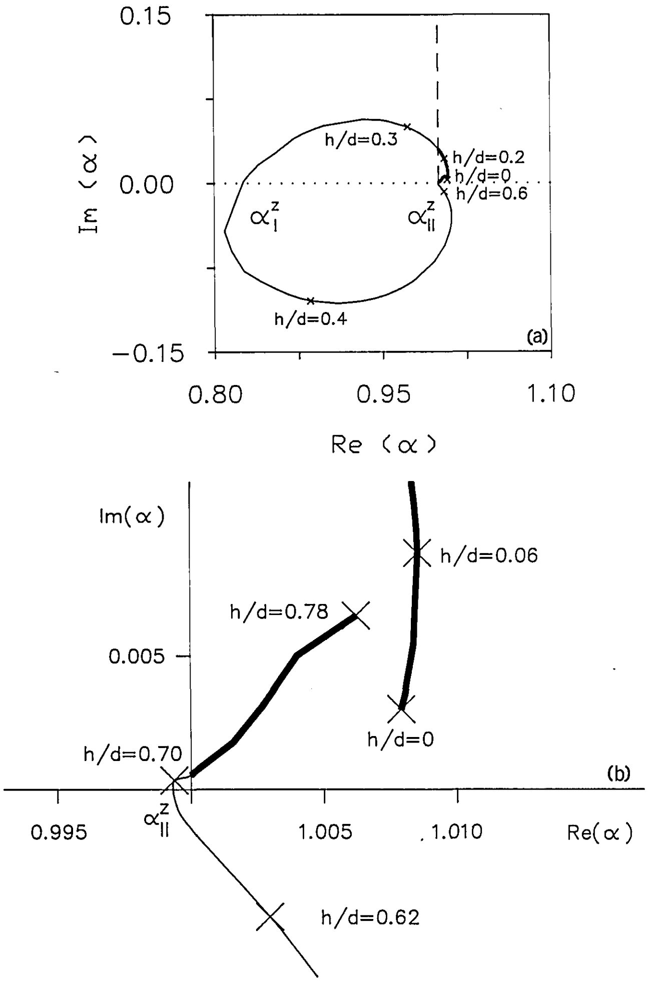

Fig. 1. (a) Trajectory of the pole (heavy solid line) and the zero (solid line) of the zeroth diffraction order in the complex α plane for S polarization (the electric field vector is perpendicular to the grooves) and different values of h/d; $\lambda = 0.6328\ \mu$m, $n = 1.378 + i7.616$, $d = 0.5\ \mu$m. (b) Detailed picture of the vicinity of the point (1,0).

II. Zeroth-Order Zero

The results of the numerical tracing of the zero and the pole of the zeroth diffraction order in the complex α plane are shown in Fig. 1 for a sinusoidal aluminum grating with a period $d = 0.5\ \mu$m. Depth modulation is varied from $h/d = 0$ to 0.8. A vertical dashed line at $\mathrm{Re}(\alpha) = 1$ corresponds to the cut in the complex α plane[7] of the component $k\sigma$ of the reflected zeroth-order wavevector perpendicular to the grating surface:

$$\sigma = (1 - \alpha^2)^{1/2}. \tag{2}$$

The cut is introduced to choose properly the sign of the complex square root in Eq. (2), defined as $\mathrm{Re}(\sigma) + \mathrm{Im}(\sigma) \geq 0$.[7] For small h/d ratios the pole α^p in the complex α plane is connected with surface plasmon excitation. As h/d increases the imaginary part of α^p also goes up, corresponding to the increase of diffraction losses in the −1st propagation order. Crossing the cut, the pole is transferred to a zero. This abrupt change is similar to the transition between the pole and

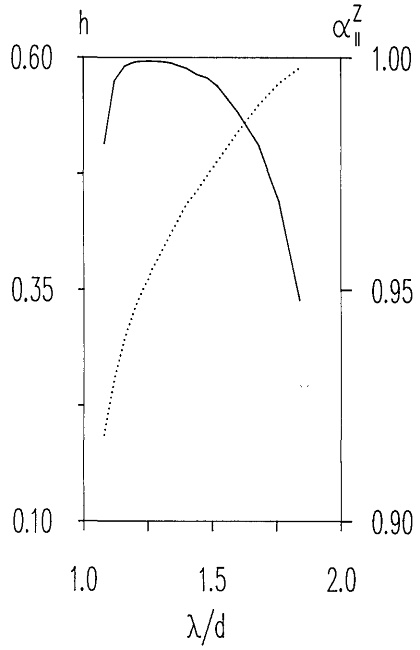

Fig. 2. Spectral dependence of (i) position of the real zeroth-order zero (solid line) and (ii) corresponding to the real zero values of groove depth (dotted line).

the zero in the reflectivity of a plane surface, when the imaginary part of the refractive index decreases.[6] Diminishing n_{Im} to dielectric values, the pole due to plasmon propagation is transferred to a zero, corresponding to Brewster's phenomenon. In our case, the same effect is obtained by increasing the depth modulation rather than by changing n_{Im}.

It is important to note that, if the sign of σ is not properly chosen, one obtains a pole instead of a zero, because in this case one stays on the improper sheet of the Riemann surface (see, for example, Ref. 16).

The next interesting point is found when the curve crosses the real α axis. This first zero, denoted by $\alpha_\perp^z$, does not correspond to a Littrow zero, appearing for $h = 0.194$ μm when $\lambda = 0.6328$ μm. If n_{Im} tends to infinity, $\alpha_\perp^z$ coincides with the non-Littrow zero of the zeroth order for perfectly conducting gratings, as discussed by Maystre *et al.*[23,25] Furthermore, its spectral dependence is quite close to that given in Ref. 25, so we may conclude the identity of the two phenomena. The second cross-point $\alpha_\parallel^z$ is responsible for the reported anomaly in grazing incidence and occurs for $h = 0.345$ μm and $\alpha = 0.99931$. Its spectral dependence is displayed in Fig. 2, up to $\lambda/d = 1.8$. Groove depth values corresponding to real values of $\alpha_\parallel^z$ are also given. Decreasing λ, $\alpha_\perp^z$ tends rapidly toward $\alpha_\parallel^z$ and at $\lambda = 0.54$ μm they merge into each other. Below this critical wavelength real zero does not exist for any groove depth value, because the trajectory of the zero in the complex α plane no longer crosses the real α axis, which fact is illustrated in Fig. 3 for $\lambda = 0.52$ μm. Increasing further the modulation depth (Fig. 1) the trajectory of α^z crosses the cut and is transferred again into a pole. Thus a forbidden gap for the excitation of surface

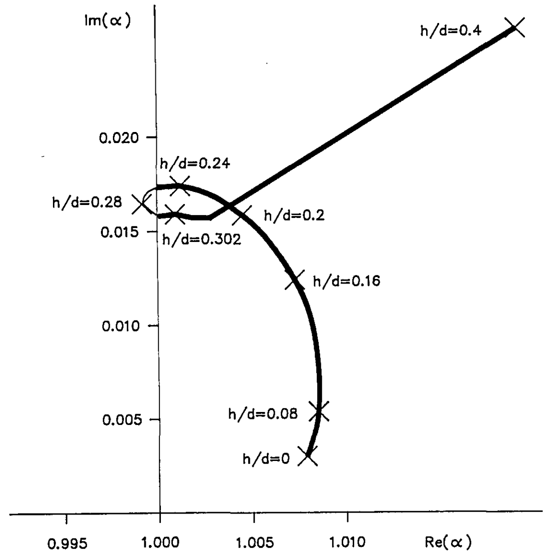

Fig. 3. Same as Fig. 1 except $\lambda = 0.52$ μm.

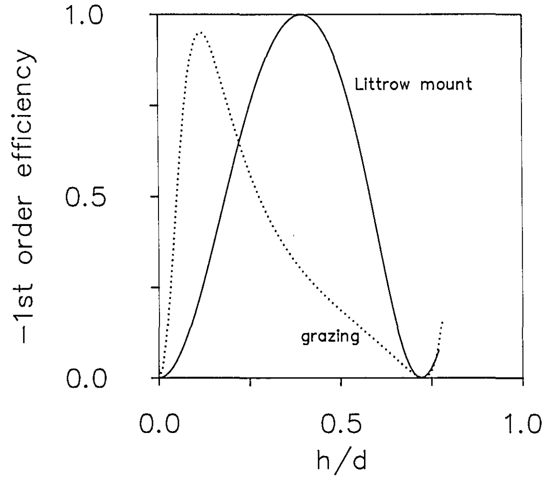

Fig. 4. First-order efficiency as a function of the groove depth for a perfectly conducting grating with $d = 0.5$ μm, $\lambda = 0.6328$ μm; solid line, Littrow mount; dotted line, grazing incidence ($\alpha = 0.99931$).

plasmons in h exists, which gap is smaller for shorter wavelengths and vanishes below 0.52 μm.

III. First-Order Zero and Effect of Total Absorption of Light

Figure 4 shows the groove depth dependence of −1st order efficiency η_{-1} for a perfect metal grating. It was surprising to discover numerically that for $h = 0.3606$ μm (the value of the second zero in Fig. 4) the efficiency does not exceed 10^{-3} over the entire range of angles of incidence, and in particular grazing incidence. Reducing n_{Im} to the imaginary part of the aluminum refractive index, η_{-1} no longer remains pure zero, but always has a minimum, whose position depends on n_{Im}. This dependence, together with the minimum value of η_{-1} is plotted in Fig. 5.

The cross-point of the zeros of the first and zeroth orders (Fig. 5) occurs approximately at $n = n_{Al}$ for $\lambda =$

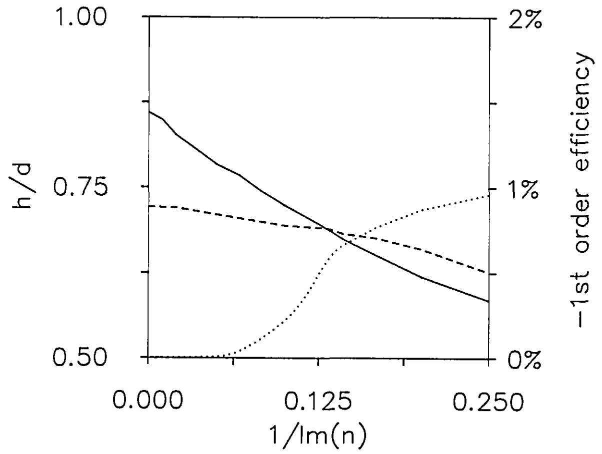

Fig. 5. Values of groove depth h for which (i) the zeroth-order zero α^z is real (solid line), and (ii) the first-order efficiency exhibits a minimum in grazing incidence (dashed line) with the corresponding values of those minima (dotted line), given as a function of the imaginary part of the refractive index of the substrate.

0.6328 μm, thus a total absorption of light is observed. Changing λ, the intersection of the two curves occurs at $n \neq n_{Al}$, but then $\eta_{-1} \neq 0$ for $\alpha = \alpha_{\|}^{z}$. Such peculiar behavior is characteristic only for sinusoidal gratings. As is usual in the anomaly domain the diffraction characteristics are strongly influenced by a small variation in the grating parameters (therefore rigorous electromagnetic theories have to be used in such studies). For example, the influence of the groove profile is illustrated in Fig. 1(b) of Ref. 6: for a symmetrical triangular profile with groove depth $h = 0.345$ μm, computation shows that α^z is not real and the minimum of the zero-order efficiency is therefore not zero. Profile change leads to splitting of the first and zero minima. A real value of $\alpha^z = 0.9966$ is obtained for $h = 0.336$ μm, but then $\eta_{-1} = 76\%$.

IV. Discussion

We have demonstrated theoretically that a close connection exists between the grazing incidence anomaly, perfect blazing in a non-Littrow mounting, and plasmon excitation. Both anomalies are characterized by a zero in the zeroth-order efficiency of the metallic grating, but the grazing one ($\alpha_{\|}^{z}$) is accompanied by an almost zero efficiency in the other (−first) propagating order, too, thus total absorption of incident light occurs. The two anomalies (non-Littrow perfect blazing and grazing total absorption) lie on one and the same trajectory as a function of the groove depth in the complex α plane. This trajectory represents a continuation of the trajectory of the plasmon propagation constant in the region where the resonance (pole—a solution of the surface wave dispersion relation) is transferred into a zero of the zeroth-order efficiency. Thus a proper connection is revealed between the two recently discovered grating anomalies and the well-known plasmon excitation.

This connection provides a direct explanation of the problem described by Breidne and Maystre[25]; they have not been able to find any non-Littrow perfect blazing for TE polarization. Now we can say that this could have been expected: as far as non-Littrow perfect blazing is connected in a peculiar way with surface wave excitation on a flat metal–air interface and for TE polarization no such guided wave exists, TE non-Littrow perfect blazing of the kind discovered in Refs. 23 and 25 is impossible. It is of course worth noting that any other type anomaly in TE polarization is not forbidden.

Although grazing incidence anomaly behaves quite similar to the Brewster effect in shallow gratings,[33,34] they differ much in their nature. Both are characterized by total light absorption by a metallic grating, but the grazing anomaly is a nonresonance phenomenon, contrary to the Brewster effect in shallow gratings. The last is accompanied by a pole, thus a significant increase in evanescent diffraction orders and in total field energy is observed, while the grazing anomaly represents, as far as we know, the first effect of total absorption of light by metallic gratings nonresonant in nature and not accompanied by any noticeable field enhancement.

Three facts are very interesting and need further investigation:

(i) the existence of a forbidden gap in the groove depth dependence of plasmon propagation constant: as a consequence of the results presented in Fig. 1 it directly follows that a solution of the surface wave dispersion relation does not exist in the interval $0.22 < h/d < 0.72$;

(ii) total depression of the first order in the whole angular interval provided in the Littrow mount is equal to zero;

(iii) a possibility to obtain 76% absolute efficiency of the first order for symmetrical triangular gratings at an angle of incidence $\theta = 85.27°$.

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