Leveraging beam deformation to improve the detection of resonances

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Decades of work on beam deformation on reflection and especially on lateral shifts have spread the idea that a reflected beam is larger than the incident beam. However, when the right conditions are met, a beam reflected by a multilayered resonant structure can be 10% narrower than the incoming beam. Such an easily measurable change occurs on a very narrow angular range close to a resonance, which can be leveraged to improve the resolution of sensors based on the detection of surface-plasmon resonances by a factor of 3. We provide theoretical tools to deal with this effect and a thorough physical discussion that leads to expect similar phenomena to occur for temporal wave packets and in other domains of physics.

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Detecting an optical resonance classically reduces to send a beam on a structure and use the amount of light that is reflected (or transmitted) to accurately determine for which angle or for which frequency the resonance occurs. The beam is almost always large enough so that the finite size of the beam has no influence on the measurement. On the other hand, it is common knowledge that, when a narrow enough beam is reflected by a bare interface, the reflected beam can be deformed by the reflection to the extent that even the basic laws of the specular reflection do not seem to hold anymore [1,2]. The changes are thus said to be nonspecular and have been continuously explored since Newton [3,4]. Especially, the lateral shift of reflected beams has attracted most of the attention [5–15] after the pioneering experimental work of Goos and Hänchen [16] and some theoretical work in the 1970s [17,18]. Nonspecular lateral shifts can actually be influenced by many physical phenomena [19–21]. Generally, the study of lateral shifts, especially large ones which result from the excitation of leaky modes, leads to the conclusion that, in general, the reflected beam is always larger than the incoming one. This corresponds to the commonly shared idea that, in physics, the deformation of a wave packet by a linear physical phenomenon leads to a widening and to dispersion. For these reasons, very little attention has ever been paid to the change in width undergone by a beam when it is reflected by a multilayered structure.

Here we show that, for any multilayered structure whose resonance leads to a reflection dip, the reflected beam can actually be narrower than the incoming beam because of a destructive interference between the beam reflected on the first interface and the resonance. This phenomenon can be leveraged to push the theoretical resolution limits of surface-plasmon resonance (SPR) detection [22] as it occurs on an angular range that is narrower (typically three times) than the range on which the reflection coefficient varies. We provide analytic formulas to describe the variation in the beam width on reflection and a thorough physical analysis why this change occurs on such a narrow angular range. Conversely for many nonspecular phenomena that have been predicted relying on formulas that are valid only for very large beams [23], hindering their use for any practical application, the phenomenon we want to monitor occurs for finite realistic beams. Finally, we underline that the validity of our analysis extends to temporal wave packets and other domains of physics, such as electronics and quantum mechanics.

We introduce first the very general formulas that describe how a Gaussian beam is shifted and widened or narrowed on reflection on a multilayered structure [24] whatever the width of the incoming beam and not just in the large waist limit that most of the authors, following Artmann [23], consider.

The electric field, in s polarization, of an incoming beam can be described in terms of its plane-wave expansion, each plane wave being characterized by a wave-vector $\alpha = nk_0 \sin\theta$ where θ is the associated incidence angle and n is the optical index of the medium. It can thus be written

$$E_i(x,z,\omega) = \frac{1}{2\pi}\int \tilde{E}_i(\alpha) e^{i(\alpha x - \gamma z - \omega t)} d\alpha, \tag{1}$$

where $\gamma = \sqrt{\varepsilon\mu k_0^2 - \alpha^2}$ and where the angular spectral amplitude is given by

$$\tilde{E}_i(\alpha) = \frac{w}{2\sqrt{\pi}} e^{-(w_i^2/4)(\alpha-\alpha_0)^2}. \tag{2}$$

This corresponds to a Gaussian beam with a waist w_i, angularly centered on θ_0 with $\alpha_0 = nk_0 \sin\theta_0$ where $k_0 = \frac{2\pi}{\lambda}$. Light is reflected by the structure beginning at $z = 0$, producing a beam with an angular spectrum,

$$\tilde{E}_r = r(\alpha)\tilde{E}_i = \rho(\alpha) e^{i\phi(\alpha)} \tilde{E}_i, \tag{3}$$

where r is the reflection coefficient and ρ and ϕ are its modulus and phase, respectively. This formalism of course holds to describe the H_y field in p polarization.

The lateral shift on reflection is the difference between the center of the reflected beam and the center of the incoming beam,

$$\delta = \frac{\int x|E_r|^2 dx}{\int |E_r|^2 dx} - \frac{\int x|E_i|^2 dx}{\int |E_i|^2 dx}. \tag{4}$$

It is possible to show (see Appendix A) that this shift is given whatever the beam width and even if the modulus of the reflection coefficient is not 1 by

$$\delta = -\frac{\int \rho^2 \phi' |\tilde{E}_i|^2 d\alpha}{\int \rho^2 |\tilde{E}_i|^2 d\alpha}, \tag{5}$$

where the $'$ denotes a derivation with respect to α.

We are interested here in the change in the width of the beam on reflection [1]. It can be simply defined as a difference between second-order centered moments, just like the shift is a difference between first-order moments,

$$\Delta = \frac{\int (x-\delta)^2 |E_r|^2 dx}{\int |E_r|^2 dx} - \frac{\int x^2 |E_i|^2 dx}{\int |E_i|^2 dx}. \qquad (6)$$

We underline that, with the above definition of a Gaussian beam, we have $\int x^2 |E_i|^2 dx / \int |E_i|^2 dx = \frac{1}{4} w_i^2$, clearly showing how meaningful the second-order moments are. If the reflected beam can be considered Gaussian with a waist w_r, then we have $\Delta = \frac{1}{4}(w_r^2 - w_i^2)$, but usually the reflected beam is not rigorously Gaussian. Using the same kind of demonstration as for the shift, a relatively straightforward calculation (see Appendix B) yields

$$\Delta = \frac{\int \frac{1}{2}(\rho'^2 - \rho\rho'')|\tilde{E}_i|^2 d\alpha}{\int \rho^2 |\tilde{E}_i|^2 d\alpha} + \left[\frac{\int \rho^2 \frac{w^2}{4} \tilde{E}_i'^2 d\alpha}{\int \rho^2 |\tilde{E}_i|^2 d\alpha} - \frac{\int \frac{w^2}{4} \tilde{E}_i'^2 d\alpha}{\int |\tilde{E}_i|^2 d\alpha} \right] + \left[\frac{\int \rho^2 \phi'^2 |\tilde{E}_i|^2 d\alpha}{\int \rho^2 |\tilde{E}_i|^2 d\alpha} - \delta^2 \right]. \qquad (7)$$

When the width of the incoming beam becomes asymptotically large, its angular spectrum becomes a Dirac distribution so that the lateral shift tends to a finite limit $\delta \to -\phi'$. This is Artmann's [23] formula,

$$\lim_{w_i \to \infty} \delta = \delta_\infty = -\phi' = -\frac{1}{n k_0 \cos\theta_0} \frac{d\phi}{d\theta}. \qquad (8)$$

In the asymptotic regime, the second and the third terms of Eq. (7) both vanish. The third term vanishes because $\delta^2 \to (\phi')^2$. The first term is the only one whose limit is not zero but instead,

$$\lim_{w_i \to \infty} \Delta = \Delta_\infty = \frac{\rho'^2 - \rho\rho''}{2\rho^2}. \qquad (9)$$

This very simple formula is the equivalent of Artmann's formula for the width of the beam instead of its position. We underline that only ρ appears in this formula and that the quantity $\rho'^2 - \rho\rho''$ plays a central role even outside of the asymptotic limit as shown in expression (7).

The formula thus predicts that, when $\rho = 1$ whatever the angle, there is simply no change in the reflected beam's width. This may sound correct for total internal reflection but is quite at odds with conventional knowledge [17,18] when the beam is narrow and when a resonance is excited in the structure. For a narrow beam, the excitation of a leaky mode, for instance, is generally expected to lead to a large lateral shift and to a widening of the reflected beam (see Fig. 1). Our simulations show that the asymptotic formula is right: In the asymptotic regime when the beam is very large and when $\rho = 1$, there is absolutely no change in the width of the beam on reflection, confirming our predictions.

Now, when ρ presents a minimum because of a resonance, then the formula predicts that the reflected beam should be as follows: (i) narrower than the incidence beam at resonance because $\rho' = 0$ and $\rho'' > 0$ for a minimum so that $\rho'^2 - \rho\,\rho'' < 0$ and (ii) wider than the incident beam slightly off-resonance when ρ can be considered linear so that ρ' is maximum and ρ'' vanishes which yield $\Delta > 0$ for a wide enough beam. And this occurs of course on an angular range that is much narrower than the dip in the reflection coefficient itself. This leads to think that at resonance precisely, the reflected beam is in general narrower than the incoming beam.

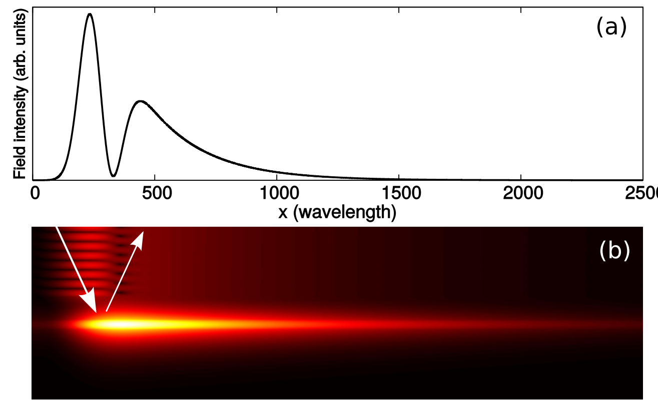

FIG. 1. Excitation of a leaky mode in a waveguide ($\epsilon = 3$, thickness of 0.285λ) surrounded by air using a Gaussian beam (incidence angle of 33.9°, $w = 100\lambda$) propagating in a high index medium (the prism $\epsilon_2 = 5$). The distance between the prism and the waveguide is 0.65λ. (a) A profile of the reflected beam's intensity. (b) A map of the corresponding field intensity [5λ vertically, 2500λ horizontally as for (a)].

In order to better illustrate this phenomenon and to show its potential, we consider the realistic case of a surface-plasmon resonance excited in the Kretschman-Raether configuration at a wavelength of 632.8 nm as illustrated in Fig. 2. We have used MOOSH [25,26] to simulate the excitation of the SPR by a Gaussian beam (p polarized) propagating in a prism (BK7 glass with an index of 1.47) with an incidence angle larger than the critical angle of the glass-air interface. A thin gold film (55 nm) is attached to the prism with a 2-nm-thin chromium layer. These parameters are actually carefully chosen so that the reflection coefficient is not too low at resonance ($\theta_{\rm SPR} = 45.5^\circ$), or the reflected beam would be too weak to allow for any measurement and to maximize the effect we are looking for. Figure 2(b) shows the modulus of the reflection coefficient ρ as a function of the incidence angle as well as the quantity Δ_∞. It is obvious how Δ_∞ is supposed to present swift variations. This too is totally at odds with what one would expect for a narrow incoming beam [17,18] since the resonance is the actual excitation of a leaky mode supposed to widen the reflected beam, the surface plasmon.

We compute Δ as a function in the incoming beam's width. The results are shown in Fig. 3 for two different incidence angles. The first angle corresponds exactly to the resonance ($\theta_{\rm SPR} = 45.5^\circ$), and the other is slightly off-resonance (45.2°). The absolute widening Δ is positive off-resonance and negative at the precise angle of resonance, and the difference between the two behaviors is striking as shown in Fig. 3(a). When the incoming beam is very narrow, no difference can be noticed.

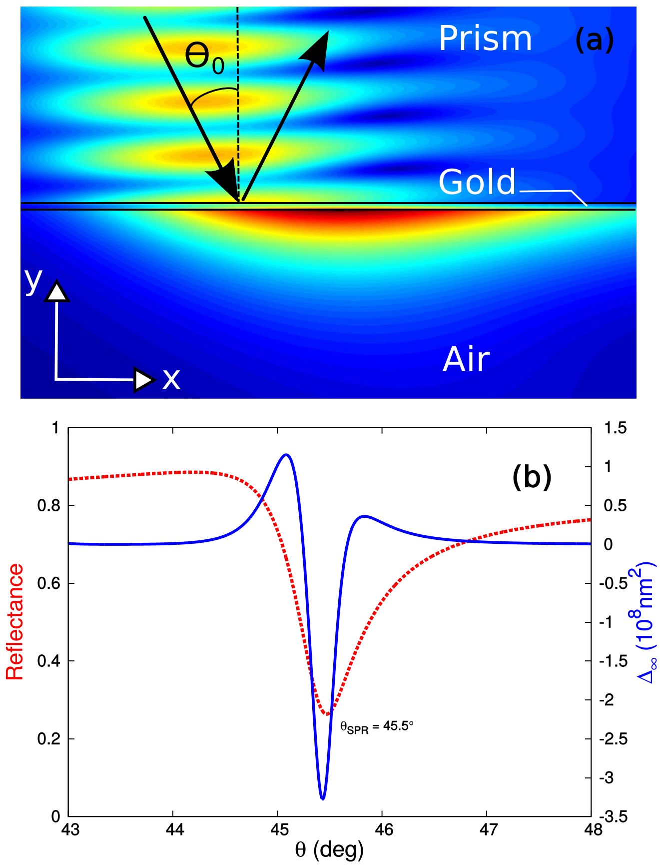

FIG. 2. (a) Modulus of the magnetic field obtained by simulation in the case of a surface-plasmon resonance excitation. A gold layer (55 nm) is deposited on the bottom of a prism. The incoming beam comes from above with an incidence angle of 45.5° and propagates inside the prism. The reflected beam interferes locally with the incoming beam, hence, the fringes. (b) The dotted red line (scale on the left) represents the modulus of the reflection coefficient whereas the asymptotic beam width change is represented by a solid blue line (scale on the right).

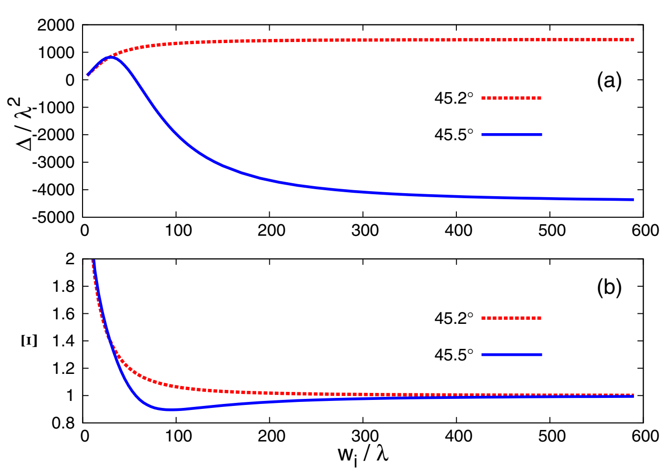

FIG. 3. Absolute (Δ, top) and relative (Ξ, bottom) beam width changes on reflection for two different incidence angles: $\theta_{\rm SPR} = 45.5^\circ$ (solid blue line) and 45.2° (dotted red line) as a function of the incoming beam waist (expressed in wavelength units).

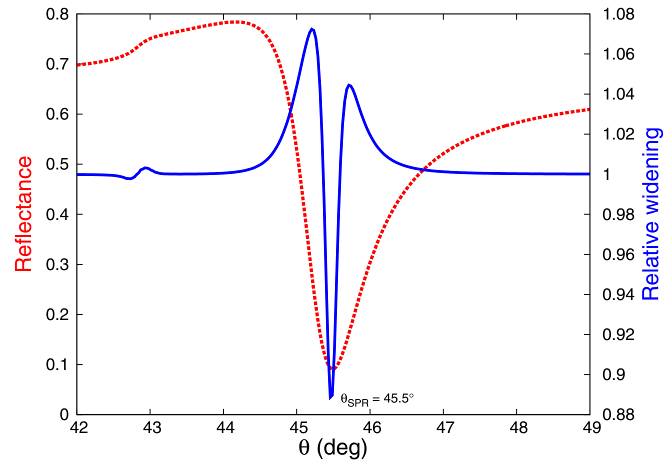

FIG. 4. Reflection coefficient (dotted red line) (scale on the left) and relative reflected beam width change (solid blue line) (scale on the right) as a function of the incidence angle for an incoming beam with a waist of 75λ.

However, the absolute widening is not a perfectly relevant quantity from an experimental point of view. This idea is very important: If a nonspecular phenomenon can only be observed for very large beams, then the relative effect will be so small that detecting it can prove impossible. As the absolute expansion tends to a limit in the asymptotic regime, the relative widening defined as the ratio,

$$\Xi = \sqrt{\left(\frac{\int (x-\delta)^2 |E_r|^2 dx}{\int |E_r|^2 dx}\right) \Big/ \left(\frac{\int x^2 |E_i|^2 dx}{\int |E_i|^2 dx}\right)}, \qquad (10)$$

actually tends to 1 whatever the angle. This ratio in the asymptotic limit is $\frac{w_r^2}{w_i^2}$, but w_r is generally not well defined since the reflected beam is distorted. This means that there is no relative widening in the asymptotic regime, whereas it is the right quantity to consider if ever we want to measure such a phenomenon experimentally. That is the reason why asymptotic formulas, such as Artmann's or (9) should not fully be trusted: Sometimes the asymptotic regime is so difficult to reach that the relative effect (such as the ratio of the lateral shift over the incident beam's waist) is negligible.

Now Fig. 3(b) shows the relative widening as a function of the incoming beam's waist for the two previously chosen incidence angles. As can be seen, both tend to one in the asymptotic regime and are very close when the incoming beam is very narrow, but a clear behavior difference can still be seen between the two for an intermediate and surprising low value of w_i, well before the asymptotic regime is reached. The difference is actually maximum for $w_i = 75\lambda$ and represents a 20% relative change in the reflected beam width for a 0.3° incidence angle change only.

This significant change is better illustrated in Fig. 4 where the relative expansion of the reflected beam Ξ is shown as a function of the incidence angle using the beam width that maximizes this variation. It allows to better capture the very narrow angular range on which the beam width variation occurs. When compared to the change in the reflection coefficient on the same angular range, this leads to think that,

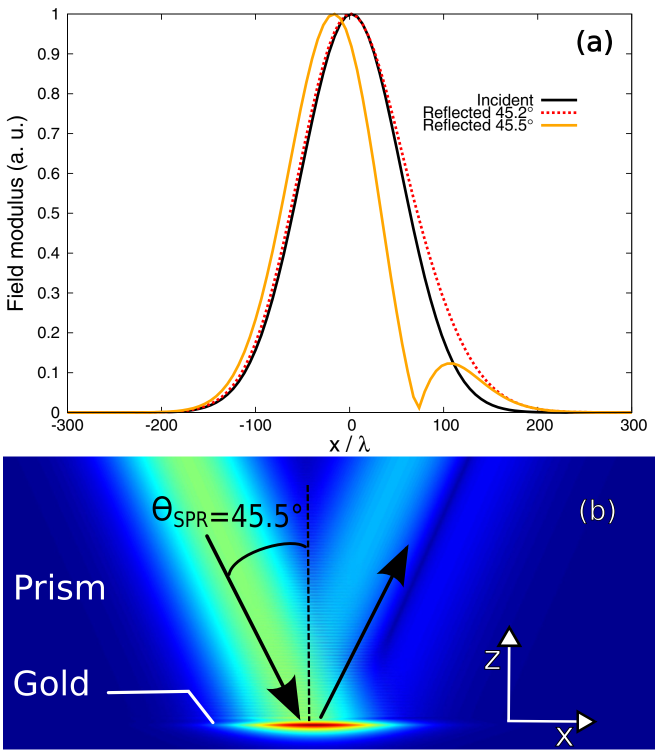

FIG. 5. (a) Profiles of the incoming (solid black line) and of the reflected beam for two incidence angles: $\theta_{SPR} = 45.5^\circ$ (yellow, light gray line) and 45.2° (dotted red line). The profiles are shown with the same maximum for a better comparison. (b) Modulus of the magnetic field exactly at resonance ($\theta_{SPR} = 45.5^\circ$) when the beam reflected by the first interface interferes destructively with the light leaking out of the resonance; size of the map: 160λ vertically and 900λ horizontally.

although the sensitivity of the method would remain the same, monitoring the beam width change would allow to reach a better resolution.

There are two ways this phenomenon can physically be understood. First, the profile of the reflected beam [27] can be interpreted as the result of destructive interference between the beam reflected by the first interface between glass and air and the field leaking out of the surface plasmon itself. At resonance, the interference is destructive enough to strongly reduce the width of the beam. This can be understood better when considering Fig. 1 in which the reflected beam is clearly composed of the beam reflected by the first interface and by the part coming from the leaky mode. The two are easy to distinguish thanks to the destructive interference taking place where they overlap. The profile of the beam when exciting the resonance shown in Fig. 5(a) presents a similar pattern except that here, given the width of the beam and of the resonance, the destructive interference is dominant and reduces the overall width of the reflected beam. Part of the light that leaks out of the surface plasmon can still be seen as a high intensity point. Slightly off-resonance, the interference is no longer destructive so that the leaky mode and the beam reflected by the first interface add up, leading to a widening of the beam. Seen this way, the device can be considered as a new kind of interferometer.

Finally, the whole phenomenon can be understood from a spectral point of view. The angular spectrum of the reflected beam is the angular spectrum of the incident beam times the reflection coefficient. This allows to understand why the variation in the width of the reflected beam is the largest when the spectral width of the beam is roughly one-third of the spectral width of the resonance. In that case, three domains can clearly be defined, depending on the incidence angle θ_0. For an incidence angle slightly smaller that the resonance angle, ρ is linear and decreasing sharply. The angular spectrum of the reflected beam is thus narrower than the spectrum of the incoming beam, and the reflected beam is then spatially larger. The narrowing of the reflected beam occurs when the incoming angular spectrum is centered on the resonance because the central part of the reflected spectrum is thus diminished, leading to a spectral widening and a spatial narrowing. On the other side of the resonance, the reflected beam is of course spatially widened too.

We have thus provided very general tools to deal with the beam width's change in reflection on a multilayered structure and showed that it is a relevant parameter that can be used to better detect a SPR resonance, eventually opening a new route to improve the resolution of SPR biosensors. In that way nonspecular phenomena, which have been widely studied since Newton [3], could for once find an application. Furthermore, our paper suggests that monitoring nonspecular changes outside of the asymptotic regime is a relevant idea. Asymptotic results are interesting, but as very wide beams are very often required to reach this regime, the effects may be extremely difficult to measure. It is high time, now that we have the numerical tools to deal with realistic finite beams and complex changes in the reflected and transmitted beams, to explore thoroughly what could finally appear as a whole new domain, well beyond the classical nonspecular phenomena as the Goos-Hänchen or the Imbert-Fedorov [28] lateral shifts.

We underline that the spectral explanation given above is very general and this resonant narrowing can thus be expected to occur in other domains of physics, such as for instance in the case of resonant tunneling in quantum mechanics when a wave packet is sent on a potential well buried in a barrier [29,30]. In that case, the part of the wave function that is reflected would be, if the conditions are correctly chosen, spatially narrower than the incoming wave function, despite the time that is spent in the potential well. A physical interpretation is that the beam reflected by the first barrier is interfering destructively with the wave function leaking out of the weakly bound state inside the barrier. In electronics, when a stop-band filter is excited with a temporal wave packet, the resulting signal can be expected to be temporally shorter than the incoming signal in the proper conditions. In all these cases, provided the wave-vector α is replaced with the pulsation ω, the formulas that have been given above will correctly describe the resonant narrowing of the temporal wave packet.

APPENDIX A

In this first appendix, we propose a demonstration of Artmann's formula in the asymptotic regime, showing that the formula is valid even if the modulus of the reflection coefficient changes with the angle of incidence. Even if the formula has been quite successfully used in that context, we underline that all the previous demonstrations of Artmann's formula have been performed assuming a reflection coefficient with a unity modulus. The analytic formulas that are necessary to get to the end of the proof will be extremely useful in the following.

The incident and reflected beam fields E_i and E_r can be expressed whatever the polarization by

$$E_i(x,z,\omega) = \frac{1}{2\pi}\int \tilde{E}_i(\alpha)e^{i(\alpha x-\gamma z-\omega t)}d\alpha, \tag{A1}$$

and

$$E_r(x,z,\omega) = \frac{1}{2\pi}\int \tilde{E}_r(\alpha)e^{i(\alpha x+\gamma z-\omega t)}d\alpha, \tag{A2}$$

where $\tilde{E}_i$ and $\tilde{E}_r$ are the spectral amplitudes, $\gamma = \sqrt{\varepsilon\mu k_0^2-\alpha^2}$, k_0 being the wave number in vacuum, and ε (respectively, μ) being the permittivity (respectively, permeability) of the upper medium.

The reflection coefficient is defined by

$$r = \rho e^{i\phi} = \frac{\tilde{E}_r}{\tilde{E}_i}, \tag{A3}$$

where $\rho = \rho(\alpha)$ is the magnitude and $\phi = \phi(\alpha)$ is the phase of r.

The lateral displacement of the reflected beam is the distance between the centers of the incident and the reflected beams. It can be expressed as

$$\delta = \frac{\int x|E_r|^2dx}{\int |E_r|^2dx} - \frac{\int x|E_i|^2dx}{\int |E_i|^2dx}. \tag{A4}$$

Applying the Parseval-Plancherel lemma, we can write

$$\int x|E_r|^2dx = \frac{i}{2\pi}\int \frac{\partial \tilde{E}_r}{\partial\alpha}\tilde{E}_r{}^*d\alpha, \tag{A5}$$

and by inserting expression (A3), we obtain

$$\begin{aligned}\int x|E_r|^2dx &= \frac{i}{2\pi}\int \frac{\partial}{\partial\alpha}(\rho e^{i\phi}\tilde{E}_i)\rho e^{-i\phi}\tilde{E}_i{}^*d\alpha\\ &= \frac{i}{2\pi}\int(\rho\rho' + i\rho^2\phi')|\tilde{E}_i|^2d\alpha\\ &\quad + \frac{i}{2\pi}\int \rho^2\frac{\partial\tilde{E}_i}{\partial\alpha}\tilde{E}_i{}^*d\alpha. \end{aligned}\tag{A6}$$

For an incident Gaussian beam the spectral amplitude is

$$\tilde{E}_i(\alpha) = \frac{w}{2\sqrt{\pi}}e^{-(w^2/4)(\alpha-\alpha_0)^2}e^{-i\alpha x_0}, \tag{A7}$$

where x_0 is the position of the beam's center, given by $\frac{\int x|E_i|^2dx}{\int |E_i|^2dx}$ and $\alpha_0 = \sqrt{\epsilon\mu}k_0\sin\theta_0$, θ_0 being the angle of incidence of the beam.

In this particular case, we can notice that

$$\frac{\partial\tilde{E}_i}{\partial\alpha}\tilde{E}_i{}^* = -ix_0|\tilde{E}_i|^2 - \frac{1}{2}\frac{\partial|\tilde{E}_i|^2}{\partial\alpha}, \tag{A8}$$

so that using an integration by parts, Eq. (A6) yields

$$\int x|E_r|^2dx = -\frac{1}{2\pi}\int\rho^2\phi'|\tilde{E}_i|^2d\alpha + \frac{x_0}{2\pi}\int\rho^2|\tilde{E}_i|^2. \tag{A9}$$

Finally, the lateral displacement is given by the rigorous formula,

$$\delta = -\frac{\int\rho^2\phi'|\tilde{E}_i|^2d\alpha}{\int\rho^2|\tilde{E}_i|^2d\alpha}. \tag{A10}$$

The asymptotic regime is reached when the incident beam is large enough. The spectral amplitude is then so narrow that ρ^2 and $\rho^2\phi'$ can be considered constant. Another point of view is to say that the Gaussian function tends towards the Dirac when $w \to +\infty$ in the sense of distributions so that the asymptotic lateral shift is the same whatever the profile of the beam,

$$\lim_{w\to\infty}\delta = -\phi'. \tag{A11}$$

This result is referred to as Artmann's formula.

APPENDIX B

Here we will find an expression for the variation of the reflected beam width. Let us consider a centered incident beam for which $\int x|E_i|^2dx = 0$. The position of the reflected beam's center, denoted as δ, is given by Eq. (4). The width of a beam is given by the square root of its second centered momentum so that the widening of the reflected beam can be expressed as

$$\Delta = \frac{\int(x-\delta)^2|E_r|^2dx}{\int|E_r|^2dx} - \frac{\int x^2|E_i|^2dx}{\int|E_i|^2dx}, \tag{B1}$$

which can be developed as follows:

$$\Delta = \frac{\int x^2|E_r|^2dx}{\int|E_r|^2dx} - \frac{\int\delta^2|E_r|^2dx}{\int|E_r|^2dx} - \frac{\int x^2|E_i|^2dx}{\int|E_i|^2dx}. \tag{B2}$$

Applying the Parseval-Plancherel lemma, we get

$$\int x^2|E_r|^2dx = -\frac{1}{2\pi}\int\frac{\partial^2\tilde{E}_r}{\partial\alpha^2}\tilde{E}_r^*d\alpha, \tag{B3}$$

and by inserting expression (A3), we obtain

$$\begin{aligned}&2\pi\int x^2|E_r|^2dx\\ &= -\int(\rho\rho'' + 2i\rho\rho'\phi' + i\rho^2\phi'' - \rho^2\phi'^2)|\tilde{E}_i|^2d\alpha\\ &\quad - \int(\rho\rho' + i\rho^2\phi')\frac{\partial|\tilde{E}_i|^2}{\partial\alpha}d\alpha - \int\rho^2\tilde{E}_i{}^*\frac{\partial^2\tilde{E}_i}{\partial\alpha^2}d\alpha.\end{aligned}\tag{B4}$$

After some integrations by parts, we can write that

$$\begin{aligned}2\pi\int x^2|E_r|^2dx &= \int(\rho^2\phi'^2 - \rho\rho'')|\tilde{E}_i|^2d\alpha\\ &\quad + \int\rho^2\left(\frac{\partial\tilde{E}_i}{\partial\alpha}\right)^2d\alpha.\end{aligned}\tag{B5}$$

On the other hand, the equality,

$$2\pi\int x^2|E_i|^2dx = -\int\frac{\partial^2\tilde{E}_i}{\partial\alpha^2}\tilde{E}_i{}^*d\alpha \tag{B6}$$

can be written

$$2\pi \int x^2|E_i|^2 dx = -\int \left[\frac{1}{2}\frac{\partial^2(|\tilde{E}_i|^2)}{\partial\alpha^2} - \left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2\right] d\alpha, \tag{B7}$$

so that we get

$$\Delta = \frac{\int(\rho^2\phi'^2 - \rho\rho'')|\tilde{E}_i|^2 d\alpha}{\int \rho^2|\tilde{E}_i|^2 d\alpha} + \frac{\int \rho^2\left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 d\alpha}{\int \rho^2|\tilde{E}_i|^2 d\alpha} + \frac{\int \frac{\partial^2(|\tilde{E}_i|^2)}{\partial\alpha^2}}{\int |\tilde{E}_i|^2 d\alpha} - \frac{\int \left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 d\alpha}{\int |\tilde{E}_i|^2 d\alpha} - \frac{\int \delta^2|E_r|^2 dx}{\int |E_r|^2 dx}. \tag{B8}$$

For a centered Gaussian beam, Eq. (2) gives

$$\left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 = \frac{w^4}{4}(\alpha-\alpha_0)^2 {\tilde{E}_i}^2, \tag{B9}$$

and

$$\frac{\partial({\tilde{E}_i}^2)}{\partial\alpha} = -w(\alpha-\alpha_0){\tilde{E}_i}^2. \tag{B10}$$

so that

$$\int \rho^2\left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 d\alpha = -\int \rho^2\frac{w^2}{4}(\alpha-\alpha_0)\frac{\partial({\tilde{E}_i}^2)}{\partial\alpha} d\alpha. \tag{B11}$$

Using integrations by parts, we obtain

$$\int \rho^2\left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 d\alpha = \int \rho^2\frac{w^2}{4}{\tilde{E}_i}^2 d\alpha + \frac{1}{2}\int(\rho\rho'' + \rho'^2){\tilde{E}_i}^2 d\alpha. \tag{B12}$$

Following a very similar way, we get

$$\int \left(\frac{\partial \tilde{E}_i}{\partial\alpha}\right)^2 d\alpha = \int \frac{w^2}{4}{\tilde{E}_i}^2 d\alpha. \tag{B13}$$

Since $\int \frac{1}{2}\partial_\alpha^2({\tilde{E}_i}^2) d\alpha = 0$ for any Gaussian (or finite) beam, Eq. (B8) becomes

$$\Delta = \frac{\int\left[\rho^2\phi'^2 + \frac{1}{2}(\rho'^2 - \rho\rho'')\right]|\tilde{E}_i|^2 d\alpha}{\int \rho^2|\tilde{E}_i|^2 d\alpha} + \frac{\int \rho^2\frac{w^2}{4}{\tilde{E}_i}^2 d\alpha}{\int \rho^2|\tilde{E}_i|^2 d\alpha} - \frac{\int \frac{w^2}{4}{\tilde{E}_i}^2 d\alpha}{\int |\tilde{E}_i|^2 d\alpha} - \frac{\int \delta^2|E_r|^2 dx}{\int |E_r|^2 dx}. \tag{B14}$$

That is the result used in the present paper to estimate the beam width's variation.

In the asymptotic regime δ tends towards $-\phi'$, and the second and third terms of Eq. (B14) cancel each other so that

$$\lim_{w\to\infty} \Delta = \frac{1}{2}\left(\frac{\rho'^2}{\rho^2} - \frac{\rho''}{\rho}\right). \tag{B15}$$

Since in the asymptotic limit the reflected beam can be considered as Gaussian, it is relevant to try to link Δ to a change in the waist of the reflected beam. A straightforward calculation shows that the above formula can, in that case, be written

$$w_r^2 = w_i^2 + 2\left(\frac{\rho''}{\rho} - \frac{\rho'^2}{\rho^2}\right). \tag{B16}$$

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