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Supporting information for article:

Reflectivity spectra as absorption resonant spectra – is it correct?

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1. *Reflectivity from a low absorption semi-infinite medium in the presence of a small resonance scattering in the total external reflection region*

For semi-infinite mirror with scalar susceptibility χ

$$\chi = \chi^{nr} + \chi^{res}(\omega) \ , \tag{S1}$$

where the resonant part $\chi^{res}(\omega) = -2\delta^{res}(\omega) + 2i\beta^{res}(\omega)$ is much smaller than the nonresonant part $\chi^{nr} = -2\delta^{nr} + 2i\beta^{nr}$, the Fresnel formula for the reflectivity amplitude R^{Fr}

$$R^{Fr} = \frac{\sin\theta - \sqrt{\sin^2\theta + \chi}}{\sin\theta + \sqrt{\sin^2\theta + \chi}} \tag{S2}$$

can be essentially simplified in the total reflection region, where $\mathrm{Re}\,\chi^{nr}$ is large enough compared with $\sin^2\theta$ and negative. Let's insert the designation:

$$\sqrt{\sin^2\theta - 2\delta^{nr}} = i\rho \ , \tag{S3}$$

and if $\beta = \beta^{nr} + \beta^{res} << \rho^2 = 2\delta^{nr} - \sin^2\theta$ and $\delta^{res} << \rho^2$, the approximate expression for the square roots in (S2) can be obtained:

$$\begin{aligned}\sqrt{\sin^2\theta + \chi} &= \sqrt{\sin^2\theta - 2\delta^{nr} + 2i\beta^{nr} - 2\delta^{res} + 2i\beta^{res}} = \\ &= \sqrt{\sin^2\theta - 2\delta^{nr}}\sqrt{1 + \frac{2i\beta - 2\delta^{res}}{\sin^2\theta - 2\delta^{nr}}} = \\ &= i\rho\sqrt{1 + \frac{2i\beta - 2\delta^{res}}{-\rho^2}} \cong i\rho\left(1 + \frac{\delta^{res} - i\beta}{\rho^2}\right) = i\rho + i\delta^{res}/\rho + \beta/\rho\end{aligned} \ . \tag{S4}$$

So (S2) takes a form:

$$R^{Fr} \cong \frac{\sin\theta - (i\rho + i\delta^{res}/\rho + \beta/\rho)}{\sin\theta + (i\rho + i\delta^{res}/\rho + \beta/\rho)} = \frac{\rho\sin\theta - \beta - i(\rho^2 + \delta^{res})}{\rho\sin\theta + \beta + i(\rho^2 + \delta^{res})} \ . \tag{S5}$$

The squared module of (S5) gives the expression for the reflected intensity $\left|R^{Fr}\right|^2$:

$$\left|R^{Fr}\right|^2 \cong \frac{(\rho\sin\theta-\beta)^2+(\rho^2+\delta^{res})^2}{(\rho\sin\theta+\beta)^2+(\rho^2+\delta^{res})^2} \cong \frac{\rho^2(\sin^2\theta+\rho^2)-2\rho\beta\sin\theta+2\rho^2\delta^{res}}{\rho^2(\sin^2\theta+\rho^2)+2\rho\beta\sin\theta+2\rho^2\delta^{res}} = \\ = \frac{(\sin^2\theta+\rho^2)-2\,\beta/\rho\,\sin\theta+2\delta^{res}}{(\sin^2\theta+\rho^2)+2\,\beta/\rho\,\sin\theta+2\delta^{res}}, \tag{S6}$$

where we neglect δ^{res2} and β^2. Taking into account that from (S3)

$$\sin^2\theta+\rho^2=2\delta^{nr}, \tag{S7}$$

(S6) can be transformed to:

$$\left|R^{Fr}(\omega)\right|^2 \cong \frac{\delta^{nr}-\beta/\rho\sin\theta+\delta^{res}}{\delta^{nr}+\beta/\rho\sin\theta+\delta^{res}} \cong \left(1-\frac{\beta\sin\theta}{\rho\delta^{nr}}+\frac{\delta^{res}}{\delta^{nr}}\right)\left(1-\frac{\beta\sin\theta}{\rho\delta^{nr}}-\frac{\delta^{res}}{\delta^{nr}}\right) \cong \\ \cong \left(1-\frac{2\sin\theta}{\rho\delta^{nr}}(\beta^{nr}+\beta^{res}(\omega))\right). \tag{S8}$$

That is the formula (5) in the article. It predicts the linear dependence of reflectivity in the total external reflection region on the imaginary part of the small resonant contribution to the refractive index.

2. *Reflectivity from a semi-infinite medium with a relatively high absorption in the presence of a small resonance scattering in the total external reflection region*

If $\beta^{nr} >> \beta^{res}$ the expression (S6) is calculated by a more complicated way:

$$\left|R^{Fr}\right|^2 \cong \frac{(\rho\sin\theta-\beta)^2+(\rho^2+\delta^{res})^2}{(\rho\sin\theta+\beta)^2+(\rho^2+\delta^{res})^2} = \\ = \frac{(\sin\theta-\beta^{nr}/\rho-\beta^{res}/\rho)^2+(\rho+\delta^{res}/\rho)^2}{(\sin\theta+\beta^{nr}/\rho+\beta^{res}/\rho)^2+(\rho+\delta^{res}/\rho)^2} \cong \\ \cong \frac{(\sin\theta-\beta^{nr}/\rho)^2+\rho^2-2\beta^{res}(\sin\theta-\beta^{nr}/\rho)/\rho+2\delta^{res}}{(\sin\theta+\beta^{nr}/\rho)^2+\rho^2+2\beta^{res}(\sin\theta+\beta^{nr}/\rho)/\rho+2\delta^{res}} \cong \\ \cong \left(\frac{(\sin\theta-\beta^{nr}/\rho)^2+\rho^2}{(\sin\theta+\beta^{nr}/\rho)^2+\rho^2}+\frac{-2\beta^{res}(\sin\theta-\beta^{nr}/\rho)/\rho+2\delta^{res}}{(\sin\theta+\beta^{nr}/\rho)^2+\rho^2}\right)\times \\ \times\left(1-\frac{2\beta^{res}(\sin\theta+\beta^{nr}/\rho)/\rho+2\delta^{res}}{(\sin\theta+\beta^{nr}/\rho)^2+\rho^2}\right). \tag{S9}$$

Neglecting again $(\delta^{res})^2$ and $(\beta^{res})^2$, the nominator of the resonant term is calculated by the following way:

$$\begin{aligned}
&\left[2\delta^{res} - 2\beta^{res}(\sin\theta - \beta^{nr}/\rho)/\rho\right]\left[(\sin\theta + \beta^{nr}/\rho)^2 + \rho^2\right] - \\
&\quad -\left[2\delta^{res} + 2\beta^{res}(\sin\theta + \beta^{nr}/\rho)/\rho\right]\left[(\sin\theta - \beta^{nr}/\rho)^2 + \rho^2\right] = \\
&= 2\delta^{res}\left[(\sin\theta + \beta^{nr}/\rho)^2 + \rho^2 - (\sin\theta - \beta^{nr}/\rho)^2 - \rho^2\right] - \\
&\quad - 2\beta^{res}(\sin\theta - \beta^{nr}/\rho)/\rho\left[\sin^2\theta + 2\sin\theta\beta^{nr}/\rho + (\beta^{nr}/\rho)^2 + \rho^2\right] - \\
&\quad - 2\beta^{res}(\sin\theta + \beta^{nr}/\rho)/\rho\left[\sin^2\theta - 2\sin\theta\beta^{nr}/\rho + (\beta^{nr}/\rho)^2 + \rho^2\right] = \\
&= 8\delta^{res}\sin\theta\,\beta^{nr}/\rho - 4\beta^{res}\sin\theta/\rho\,(\sin^2\theta + \rho^2 + (\beta^{nr}/\rho)^2) + 8\beta^{res}\beta^{nr}/\rho^2\sin\theta\beta^{nr}/\rho = \\
&= 8\delta^{res}\sin\theta\,\beta^{nr}/\rho - 4\beta^{res}\sin\theta/\rho\,2\delta^{nr} - 4\beta^{res}\sin\theta/\rho(\beta^{nr}/\rho)^2 + 8\beta^{res}(\beta^{nr}/\rho)^2\sin\theta/\rho = \\
&= 8\delta^{res}\sin\theta\,\beta^{nr}/\rho - 4\beta^{res}\sin\theta/\rho\,(2\delta^{nr} - (\beta^{nr}/\rho)^2)
\end{aligned} \quad . \text{(S10)}$$

Finally, we get the formula (6) in the article:

$$\left|R^{Fr}(\omega)\right|^2 \cong \frac{(\sin\theta - \beta^{nr}/\rho)^2 + \rho^2}{(\sin\theta + \beta^{nr}/\rho)^2 + \rho^2} - \beta^{res}(\omega)\frac{4\sin\theta(2\delta^{nr} - (\beta^{nr}/\rho)^2)}{\rho\left[(\sin\theta + \beta^{nr}/\rho)^2 + \rho^2\right]^2} + \delta^{res}(\omega)\frac{8\sin\theta\,\beta^{nr}}{\rho\left[(\sin\theta + \beta^{nr}/\rho)^2 + \rho^2\right]^2} \quad \text{(S11)}$$

3. *Reflectivity at the exact critical angle in the presence of a small resonant scattering*

At the exact critical angle when

$$\sin^2\theta - 2\delta^{nr} = 0, \quad \text{(S12)}$$

the Fresnel formula for the reflectivity amplitude is simplified to the expression:

$$R^{cr} = \frac{\sin\theta - \sqrt{\sin^2\theta + \chi}}{\sin\theta + \sqrt{\sin^2\theta + \chi}} = \frac{\sqrt{2\delta^{nr}} - \sqrt{i2\beta^{nr} + \chi^{res}}}{\sqrt{2\delta^{nr}} + \sqrt{i2\beta^{nr} + \chi^{res}}} \quad . \quad \text{(S13)}$$

If $\chi^{res}(\omega) = -2\delta^{res}(\omega) + 2i\beta^{res}(\omega)$ is small enough, taking into account that $\sqrt{2i} = (1+i)$, the square root in (S13) can be approximated by the expression

$$\begin{aligned}\sqrt{i2\beta^{nr} + \chi^{res}} &\cong \sqrt{i2\beta^{nr}}\left(1 + \frac{\chi^{res}}{i4\beta^{nr}}\right) = \sqrt{\beta^{nr}}\,(1+i)\left(1 - i\frac{-2\delta^{res} + i2\beta^{res}}{4\beta^{nr}}\right) = \\ &= \frac{1}{\sqrt{\beta^{nr}}}(1+i)\left(\beta^{nr} + \beta^{res}/2 + i\delta^{res}/2\right) = \\ &= \frac{1}{\sqrt{\beta^{nr}}}\left((\beta^{nr} + \beta^{res}/2 - \delta^{res}/2) + i(\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)\right)\end{aligned} \quad . \qquad \text{(S14)}$$

So, the reflectivity amplitude (S13) takes a form:

$$R^{cr} = \frac{\sqrt{2\delta^{nr}\beta^{nr}} - \left((\beta^{nr} + \beta^{res}/2 - \delta^{res}/2) + i(\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)\right)}{\sqrt{2\delta^{nr}\beta^{nr}} + \left((\beta^{nr} + \beta^{res}/2 - \delta^{res}/2) + i(\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)\right)}. \qquad \text{(S15)}$$

Accordingly for the reflected intensity the following expression takes place:

$$\left|R^{cr}\right|^2 \cong \frac{\left(\sqrt{2\delta^{nr}\beta^{nr}} - (\beta^{nr} + \beta^{res}/2 - \delta^{res}/2)\right)^2 + (\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)^2}{\left(\sqrt{2\delta^{nr}\beta^{nr}} + (\beta^{nr} + \beta^{res}/2 - \delta^{res}/2)\right)^2 + (\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)^2} \; . \qquad \text{(S16)}$$

The calculations of $(\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)^2$ in the first order of smallness of χ^{res} gives

$$\begin{aligned}(\beta^{nr} + \beta^{res}/2 + \delta^{res}/2)^2 &= (\beta^{nr} + \beta^{res}/2)^2 + (\delta^{res}/2)^2 + 2(\beta^{nr} + \beta^{res}/2)\delta^{res}/2 \cong \\ &\cong \beta^{nr2} + \beta^{nr}\beta^{res} + \beta^{nr}\delta^{res}\end{aligned} \qquad \text{(S17)}$$

and correspondingly for $(\beta^{nr} + \beta^{res}/2 - \delta^{res}/2)^2$ we have:

$$(\beta^{nr} + \beta^{res}/2 - \delta^{res}/2)^2 \cong \beta^{nr2} + \beta^{nr}\beta^{res} - \beta^{nr}\delta^{res}. \qquad \text{(S18)}$$

So, their sum is simplified to:

$$(\beta^{nr}+\beta^{res}/2+\delta^{res}/2)^2+(\beta^{nr}+\beta^{res}/2-\delta^{res}/2)^2\cong 2\beta^{nr}(\beta^{nr}+\beta^{res})\,. \tag{S19}$$

With this simplification and neglecting δ^{res2} and β^{res2}, (S16) can be presented in the form:

$$\begin{aligned}\left|R^{cr}\right|^2 &\cong \frac{\delta^{nr}+\beta^{nr}+\beta^{res}-\sqrt{2\delta^{nr}\beta^{nr}}\left(1+\beta^{res}/(2\beta^{nr})-\delta^{res}/(2\beta^{nr})\right)}{\delta^{nr}+\beta^{nr}+\beta^{res}+\sqrt{2\delta^{nr}\beta^{nr}}\left(1+\beta^{res}/(2\beta^{nr})-\delta^{res}/(2\beta^{nr})\right)}\cong\\ &\cong\left(\frac{\delta^{nr}+\beta^{nr}-\sqrt{2\delta^{nr}\beta^{nr}}}{\delta^{nr}+\beta^{nr}+\sqrt{2\delta^{nr}\beta^{nr}}}+\frac{\beta^{res}-\sqrt{2\delta^{nr}\beta^{nr}}\left(\beta^{res}/(2\beta^{nr})-\delta^{res}/(2\beta^{nr})\right)}{\delta^{nr}+\beta^{nr}+\sqrt{2\delta^{nr}\beta^{nr}}}\right)\times\\ &\times\left(1-\frac{\beta^{res}+\sqrt{2\delta^{nr}\beta^{nr}}\left(\beta^{res}/(2\beta^{nr})-\delta^{res}/(2\beta^{nr})\right)}{\delta^{nr}+\beta^{nr}+\sqrt{2\delta^{nr}\beta^{nr}}}\right)\end{aligned} \tag{S20}$$

The nominator of the resonant term in the same order of smallness is calculated by the following way:

$$\begin{aligned}&\left[\beta^{res}\left(1-\sqrt{2\delta^{nr}\beta^{nr}}/(2\beta^{nr})\right)+\delta^{res}\sqrt{2\delta^{nr}\beta^{nr}}/(2\beta^{nr})\right]\left[\delta^{nr}+\beta^{nr}+\sqrt{2\delta^{nr}\beta^{nr}}\right]-\\ &-\left[\beta^{res}\left(1+\sqrt{2\delta^{nr}\beta^{nr}}/(2\beta^{nr})\right)+\delta^{res}\sqrt{2\delta^{nr}\beta^{nr}}/(2\beta^{nr})\right]\left[\delta^{nr}+\beta^{nr}-\sqrt{2\delta^{nr}\beta^{nr}}\right]\cong\\ &\cong 2\beta^{res}\left(\sqrt{2\delta^{nr}\beta^{nr}}-\frac{\sqrt{2\delta^{nr}\beta^{nr}}}{2\beta^{nr}}(\delta^{nr}+\beta^{nr})\right)+2\delta^{res}\frac{\sqrt{2\delta^{nr}\beta^{nr}}}{2\beta^{nr}}(\delta^{nr}+\beta^{nr})=\\ &=\sqrt{2\delta^{nr}\beta^{nr}}\left[\beta^{res}\left(1-\frac{\delta^{nr}}{\beta^{nr}}\right)+\delta^{res}\left(1+\frac{\delta^{nr}}{\beta^{nr}}\right)\right]\end{aligned} \tag{S21}$$

Finally, the expression for the reflected intensity at the exact critical angle takes the form (formulas (8) and (9) in the article):

$$\left|R^{cr}(\omega)\right|^2\cong\left|R^{nr}\right|^2+\frac{\sqrt{2\delta^{nr}\beta^{nr}}}{(\delta^{nr}+\beta^{nr}+\sqrt{2\delta^{nr}\beta^{nr}})^2}\left[\delta^{res}(\omega)\left(1+\delta^{nr}/\beta^{nr}\right)+\beta^{res}(\omega)\left(1-\delta^{nr}/\beta^{nr}\right)\right]. \tag{S22}$$

where the first term presents the reflectivity from a nonresonance media:

$$\left|R^{nr}\right|^2 = \frac{\delta^{nr} + \beta^{nr} - \sqrt{2\delta^{nr}\beta^{nr}}}{\delta^{nr} + \beta^{nr} + \sqrt{2\delta^{nr}\beta^{nr}}}. \tag{S23}$$

4. *Reflectivity from an ultrathin resonant layer*

The reflectivity amplitude from an ultrathin resonant layer placed under a reflecting medium can be presented as (M. A. Andreeva and B. Lindgren, JETP Letters **76**(12), 704(2002).):

$$R^{tot}(\omega) \cong R^s + E^2 r^d(\omega) \tag{S24}$$

where R^s is the reflectivity amplitude from an underlying substrate, $r^d(\omega)$ is the reflectivity amplitude of an ultrathin resonant layer, E is the total electric field at the position of the resonant layer. If $r^d(\omega)$ is small enough the expression for the reflected intensity $\left|R^{tot}(\omega)\right|^2$ from an ultrathin resonant layer above a substrate could be presented as:

$$\left|R^{tot}\right|^2 = (R^s + E^2 r^d)(R^{s*} + E^{*2} r^{d*}) \cong \left|R^s\right|^2 + R^s E^{*2} r^{d*} + R^{s*} E^2 r^d \tag{S25}$$

After separation of the real and imaginary parts in R^s, E and r^d, i.e. presenting $R^s = R' + iR''$, $E = E' + iE''$ and $r^d = r' + i r''$, the calculations of the resonant addition to the total reflectivity give the following result:

$$\begin{aligned} &R^s E^{*2} r^{d*} + R^{s*} E^2 r^d = \\ &= (R' + iR'')\, E^{*2} (r' - ir'') + (R' - iR'') E^2 (r' + ir'') = \\ &= (R'r' + R''r'')(E^{*2} + E^2) + i(R''r' - R'r'')(E^{*2} - E^2) = \\ &= 2(R'r' + R''r'')(E'^2 - E''^2) + 4(E'E'')(R''r' - R'r'') = \\ &= \left(2R'(E'^2 - E''^2) + 4R''(E'E'')\right) r' + \left(2R''(E'^2 - E''^2) - 4R'(E'E'')\right) r'' \end{aligned} \tag{S26}$$

Supposing the amplitude of the incident wave equals 1, and replacing E in (S26) by $E = 1 + R^s = 1 + R' + iR''$ we get

$$\begin{aligned} &R^s E^{*2} r^{d*} + R^{s*} E^2 r^d = \\ &= \left(2R'((1+R')^2 - R''^2) + 4R''^2(1+R')\right) r' + \left(2R''((1+R')^2 - R''^2) - 4R'R''(1+R')\right) r'' \\ &= 2\left(R'(1+R')^2 + R''^2(2+R')\right) r' - 2\left(R''(1 - R'^2 - R''^2)\right) r'' \end{aligned} \tag{S27}$$

Finally, the total reflectivity $\left|R^{tot}(\omega)\right|^2$ from an ultrathin resonant layer placed under a substrate takes a form (formula (15) in the article):

$$\left|R^{tot}(\omega)\right|^2 \cong \left|R^S\right|^2 + 2\left(R' + (2+R')\left|R^S\right|^2\right)r' + 2R''\left(1-\left|R^S\right|^2\right)r'' = \left|R^S\right|^2 + Q_1 r'(\omega) + Q_2 r''(\omega) \quad \text{(S28)}$$

If R^S in (S26), (S27), is the Fresnel reflectivity amplitude from substrate, for separation of its real and imaginary parts the square root in (S2) should be presented in the form:

$$\sqrt{\sin^2\theta + \chi^S} = \sin\theta\sqrt{1 - 2\delta^S/\sin^2\theta + 2i\beta^S/\sin^2\theta} = \\ = \sin\theta\left(\sqrt{\frac{\sqrt{u^2+v^2}+u}{2}} + i\sqrt{\frac{\sqrt{u^2+v^2}-u}{2}}\right) = \frac{\sin\theta}{\sqrt{2}}\left(\sqrt{q+u} + i\sqrt{q-u}\right), \quad \text{(S29)}$$

where δ^S and β^S characterize the susceptibility of the substrate $\chi^S = -2\delta^S + 2i\beta^S$. In (S29) the following notations are used:

$$u = 1 - 2\delta^S/\sin^2\theta, \quad v = 2\beta^S/\sin^2\theta, \quad q = \sqrt{u^2+v^2}. \quad \text{(S30)}$$

With these notations the reflectivity amplitude from a substrate (S2) can be rewritten in the form:

$$R^S = \frac{\sin\theta - \sqrt{\sin^2\theta+\chi^S}}{\sin\theta + \sqrt{\sin^2\theta+\chi^S}} = \frac{\sqrt{2} - \left(\sqrt{q+u} + i\sqrt{q-u}\right)}{\sqrt{2} + \left(\sqrt{q+u} + i\sqrt{q-u}\right)} = \\ = \frac{\left(\sqrt{2} - \sqrt{q+u} - i\sqrt{q-u}\right)\left(\sqrt{2} + \sqrt{q+u} - i\sqrt{q-u}\right)}{\left(\sqrt{2}+\sqrt{q+u}\right)^2 + (q-u)} \\ = \frac{2 - q - u - q + u - i\sqrt{q-u}\left[\left(\sqrt{2}-\sqrt{q+u}\right) + \left(\sqrt{2}+\sqrt{q+u}\right)\right]}{\left(\sqrt{2}+\sqrt{q+u}\right)^2 + (q-u)} = \\ = \frac{2(1 - q - i\sqrt{2}\sqrt{q-u})}{2\left(1 + q + \sqrt{2}\sqrt{q+u}\right)} == \frac{1}{W}\left((1-q) - i\sqrt{2}\sqrt{q-u}\right), \quad \text{(S31)}$$

where we designate

$$W = 1 + q + \sqrt{2}\sqrt{q+u}. \quad \text{(S32)}$$

So, the real and imaginary parts of R^S are determined by the expressions:

$$R' = \frac{(1-q)}{W}, \quad R'' = -\frac{\sqrt{2}\sqrt{q-u}}{W} \tag{S33}$$

Calculations of Q_1 with R^S from (S31) give:

$$\begin{aligned} Q_1 &= 2\left[R'(1+R')^2 + R''^2(2+R')\right] = \\ &= \frac{2}{W^3}\left((1-q)\left(W+(1-q)\right)^2 + \left(\sqrt{2}\sqrt{q-u}\right)^2\left(2W+(1-q)\right)\right) = \\ &= \frac{2}{W^3}\left((1-q)\left(W+(1-q)\right)^2 + \left(\sqrt{2}\sqrt{q-u}\right)^2\left(2W+(1-q)\right)\right) = \\ &= \frac{2}{W^3}(1-q)\left[\left(W+1-q\right)^2 + 2\left(q-u\right)\right] + \frac{8}{W^2}\left(q-u\right) \end{aligned} \tag{S34}$$

After simplifying the expression in the parentheses:

$$\begin{aligned} &\left[\left(W+1-q\right)^2 + 2\left(q-u\right)\right] = \\ &\left[\left(1+q+\sqrt{2}\sqrt{q+u}+1-q\right)^2 + 2\left(q-u\right)\right] = \left(4+4\sqrt{2}\sqrt{q+u}+2(q+u)\right) + 2\left(q-u\right) = , \\ &= \left(4+4\sqrt{2}\sqrt{q+u}+4q\right) = 4W \end{aligned} \tag{S35}$$

the expression for Q_1 (S34) is reduced to

$$Q_1 = \frac{8}{W^2}[(1-q)+(q-u)] = \frac{8(1-u)}{W^2} = \frac{16\delta^S}{W^2\sin^2\theta}. \tag{S36}$$

Similarly, we calculate Q_2 coefficient with R^S from (S31):

$$\begin{aligned} Q_2 &= 2R''(1-R''^2-R'^2) = -\frac{2\sqrt{2}}{W}\sqrt{q-u}\left(1-\left(\frac{\sqrt{2}\sqrt{q-u}}{W}\right)^2-\left(\frac{(1-q)}{W}\right)^2\right) = \\ &= -\frac{2\sqrt{2}}{W^3}\sqrt{q-u}\left(W^2-2(q-u)-(1-q)^2\right) \end{aligned} \tag{S37}$$

The expression in the parentheses can be essentially simplified:

$$\begin{aligned} &\left(W^2-2(q-u)-(1-q)^2\right) = (1+q+\sqrt{2}\sqrt{q+u})^2 + 2u - 1 - q^2 = \\ &= 2(q+u) + 2q + 2\sqrt{2}\sqrt{q+u} + 2q\sqrt{2}\sqrt{q+u} + 2u = \\ &= 4q + 4u + 2\sqrt{2}\sqrt{q+u}(1+q) = 2\sqrt{2}\sqrt{q+u}(\sqrt{2}\sqrt{q+u}+1+q) = 2W\sqrt{2}\sqrt{q+u} \end{aligned} \tag{S38}$$

Taking into account that

$$\sqrt{q-u}\sqrt{q+u}=\sqrt{q^2-u^2}=v\,, \tag{S39}$$

the expression for Q_2 (S37) gets the form:

$$Q_2=-\frac{2\sqrt{2}}{W^3}\sqrt{q-u}\left(2W\sqrt{2}\sqrt{q+u}\right)=-\frac{8v}{W^2}=-\frac{16\beta^s}{W^2\sin^2(\theta)} \tag{S40}$$

The expressions (S36), (S40) present the formulas (18), (19) in the article.