Reply to “Comment on “Normalization of quasinormal modes in leaky optical cavities and plasmonic resonators” ” by E. A. Muljarov and W. Langbein

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We refute all claims of the “Comment on “Normalization of quasinormal modes in leaky optical cavities and plasmonic resonators” ” by E. A. Muljarov and W. Langbein (arXiv:1602.07278v1). Based entirely on information already contained in our original article (P. T. Kristensen, R.-C. Ge and S. Hughes, Physical Review A 92, 053810 (2015)), we dismiss every point of criticism as being completely unjustified and point out how important parts of our argumentation appear to have been overlooked by the Comment Authors. In addition, we provide additional calculations showing directly the connection between the normalizations by Sauvan et al. and Muljarov et al., which were not included in our original article.

In a recent article [1], we have put forward the point of view that three seemingly different normalizations for so-called quasinormal modes (QNMs) can be understood as arising from different procedures for regularization of an inherently ill-behaved integral. We have done this from the general point of view that the three normalizations are different formulations of the same quantity (the norm), providing calculations that show how one can derive one formulation from the other. Moreover, we have provided explicit calculation examples for three different material systems of current interest in the literature. In a recent arXiv submission entitled “Comment on “Normalization of quasinormal modes in leaky optical cavities and plasmonic resonators” ” [2], the Comment authors raise criticism of our work which, in view of the content of Ref. [1], we find is completely unjustified.

Before addressing the criticism in the Comment, we briefly outline the motivation for Ref. [1] and its context with other publications concerning the normalization of QNMs. The work in Ref. [1] was partly motivated by an earlier arXiv submission from Muljarov, Doost and Langbein [3] which was recently updated to Version 3, now with only Muljarov and Langbein [4]. Building on earlier results on perturbation theory in open systems [5], Ref. [3] discusses how one can use the theory of QNMs to define the correct mode volume for use in Purcell factor calculations in open optical systems. Exactly the same conclusion was previously presented in Ref. [6] in terms of a generalized effective mode volume and based on a normalization for QNMs due to Lai and co-workers [7]. Parts of Ref. [3], therefore, is devoted to the claim that the normalization used in Ref. [6] is incorrect owing to a difficulty in the practical evaluation of the norm, which is evident for QNMs in cavities with (very) low $Q$-values. The work in Ref. [1] was also partly inspired by a recent publication from Sauvan and co-workers [8], who derived results that (for dispersionless materials) appear similar to those in Ref. [6] but who did not discuss the connection to other normalization procedures. The link between the normalizations in Refs. [7] and [8] was discussed in Ref. [9], and with the submission to the arXiv server of Ref. [3], it seemed likely that a similar connection could be found for the normalization used in this work also. After having found such a connection, we presented the relationship between all three normalizations from the general point of view that they are complementary [1]. At the same time, we provided explicit examples to show that the normalization in Ref. [6] is in fact correct and indeed leads to the same result as the other two formulations. These calculation examples specifically addressed points of criticism in Ref. [3] which are practically identical to what are now put forward in Ref. [2] once again. Hence, it is with some reluctance that we engage in this Reply, since all arguments have already been presented. Yet we shall do so nonetheless, and we refer all interested readers to Ref. [1] for details.

In the Appendix, we present calculations, which unfortunately we did not manage to include in Ref. [1], showing directly the connection between the normalizations in Refs. [5] and [8].

In Ref. [2], the Comment authors claim:

(a) that the conclusion in Ref. [1], that the three different methods for normalization of QNMs all provide the same result, is incorrect,

(b) that the normalization in Ref. [8] is divergent for any optical mode having a finite $Q$ value, and

(c) that the Silver-Müller (SM) radiation condition is not fulfilled for QNMs.

In Ref. [1], the three normalizations for QNMs were presented as:

1. Normalization by Sauvan et al. [7]
2. Normalization by Muljarov et al. [3]
3. Normalization by Lai et al. [6]

The Comment authors argue that the normalizations by Sauvan et al. and Muljarov et al. are incorrect, whereas the normalization by Lai et al. is correct. However, the calculations presented in Ref. [1] show that all three normalizations are equivalent under certain conditions, and that the normalization by Lai et al. is indeed correct in the limit of high $Q$-values.

We also provide additional calculations showing directly the connection between the normalizations by Sauvan et al. and Muljarov et al., which were not included in our original article. These calculations demonstrate that the normalizations by Sauvan et al. and Muljarov et al. are equivalent in the limit of high $Q$-values, and that the normalization by Lai et al. is correct in the limit of low $Q$-values. Thus, we refute all claims of the Comment and present a corrected and expanded version of our original article.
Concerning (a)

In Ref. [1], we provided general calculations showing the connection between the three normalizations for general QNMs. In particular, we discussed how one can always regularize the normalization integral of Lai and co-workers by use of a complex coordinate transformation. With such an approach, and for general resonators, albeit only in spherical integration domains, we showed how one can rewrite the normalization integral of Lai and co-workers in the exact form favored by the Comment authors. In addition to showing the connection between the normalizations for general resonators, we provided three example calculations, which we consider to be of contemporary interest. In the first example, we considered the exact same QNMs that were previously investigated by the Comment authors in Ref. [3], and we calculated the norm using the three different formulations. The results of these calculations are listed in Eqs. (27), (28) and (30) of Ref. [1], and they are identical. The Comment authors appear to have overlooked these important parts of our argumentation. For any questioning of the results in Ref. [1] to carry real weight, however, one would expect an indication of a flaw in the analytical calculations showing the connection between the normalizations for general resonators, or at least an explanation for the exact equivalence of the results in the example calculations. In view of our results, and the lack of any such explanation, we find the claim of the Comment authors, that the three normalization methods do not provide the same result, to be completely unjustified.

Concerning (b)

The Comment authors first argue that

“... the LK normalization [...] mathematically does not exist,”

essentially pointing out the same technical details as in Ref. [3], which were fully acknowledged and discussed in Ref. [1], where it was shown how one can in principle always regularize the so-called LK normalization by a complex coordinate transformation, although this relies on the expansion of the QNMs into spherical wave functions and therefore is mostly of theoretical interest unless the QNMs are known analytically. The Comment authors appear to acknowledge that such a regularization is always possible, since they (later) write:

“... For this [complex coordinate transformation] to be used, the fields of the [QNMs] have to be known analytically. This regularization is thus not suited for numerically determined [QNMs].”

This statement contradicts the earlier statement that “... the LK normalization [...] mathematically does not exist”. Moreover, we note that the criticism at this point is relaxed somewhat from being a fundamental question of whether or not the normalization mathematically “exists”, into a question of whether or not the normalization is “suited for numerically determined [QNMs]”.

To reiterate: As discussed in Ref. [1], and contrary to the claim by the Comment authors in the above quote, one can in principle always regularize the so-called LK normalization by a complex coordinate transformation (even for numerically determined QNMs by projection onto the spherical wave functions). Therefore, there should be no doubt that the so-called LK normalization “exists”, and for QNMs that are known analytically, one can easily apply the regularization also in practice. Judging from the above quote, the Comment authors appear to (implicitly) acknowledge this, yet they devote three figures to show that the integral is not well behaved if the radius of the calculation domain is varied along the real axis (as fully acknowledged and discussed at length in Ref. [1]). Moreover, they show this for QNMs that are in fact known analytically, and for which the proposed regularization is directly and easily applicable. This appears to be a major misunderstanding of our entire discussion in Ref. [1].

Later in the Comment’s text appears a new argument, namely:

“We emphasize that this “regularized” LK normalization is a different quantity compared to the divergent LK normalization defined by Eqs. (1-2) what was actually used in [Ref. [3]] and numerous follow-up publications of the same group...”

It appears then, at this point in the Comment, that the problem with the so-called LK normalization is no longer the fact that it “does not exist”, but rather that the regularized normalization is different from what was actually used in Ref. [3] and other later publications. The Comment, therefore, appears now to cover the general use of the so-called LK normalization and in particular its use in Ref. [3]. When viewed in the context of the claims that this normalization is “not suited for numerically determined [QNMs]”, it naturally leads to the question of whether the calculated results in Ref. [3] and later publications can even be trusted. Also in this case, the Comment authors appear to have overlooked the results presented in Ref. [1], which in fact included a lengthy discussion about the calculation of the norm for the cavity in Ref. [3] with the lowest Q-value (Q=16).
Concerning (c)

It was argued in Ref. [1] that the QNMs can be defined as the solutions to the wave equations that fulfill a certain variant of the SM radiation condition. The Comment authors claim that the QNMs do not fulfill this condition because the wavevector is not real. Clearly, if the premise is that the wavevector in the SM condition is real, then the SM condition cannot be fulfilled by QNMs. The same type of argument can be put forward for the wave equation itself. Indeed, one could define the wave equation with the restriction that the wavevector is real, and thereby argue that the QNMs do not fulfill the wave equation. From the context in Ref. [1] it is clear, however, that no such restriction was made when it was argued that the QNMs should fulfill the SM condition. Moreover, in Ref. [1] the SM condition was deliberately written in a form which is slightly different from the one presented by the Comment authors; a form for which the arguments put forward in the Comment do not apply, and a form for which the SM condition is in fact fulfilled by the commonly accepted QNMs of spherical resonators, which were used in the example by the Comment authors themselves.

In conclusion, we find that Ref. [2] adds nothing constructive to the current literature on QNMs. Using only information already contained in Ref. [1], we have dismissed every point of criticism in the Comment. We fully stand by our results in Ref. [1] and, as far as we are aware, the results are correct.

Appendix: Connection between the normalizations by Muljarov et al. and Sauvan et al.

In Ref. [1], we presented calculations showing the connection, for general resonators, between the normalizations by Lai et al. [7] and Sauvan et al. [8] as well as the connection between the normalizations by Lai et al. and Muljarov et al. [3]. To complete the picture, we show here the connection between the normalizations by Sauvan et al. and Muljarov et al. for general resonators made from isotropic and non-magnetic materials as considered also in Ref. [1].

From Eq. (S2) of the supplementary information in Ref. [8], setting \( j_1 = j_2 = 0 \), and adopting the notation in Ref. [1], we have the relation

\[
0 = \frac{i}{2} \int_V \hat{f}_\mu(\mathbf{r}) \cdot [\hat{\omega}_\mu \epsilon_\mu(\mathbf{r}, \hat{\omega}_\mu) - \omega \epsilon_\epsilon(\mathbf{r}, \omega)] \hat{f}(\mathbf{r}, \omega) - \frac{\mu_0}{\epsilon_0} (\hat{\omega}_\mu - \omega) \hat{g}_\mu(\mathbf{r}) \cdot \hat{g}(\mathbf{r}, \omega) dV \\
- \frac{1}{2\epsilon_0} \int_{\partial V} \left[ \hat{f}(\mathbf{r}, \omega) \times \hat{g}_\mu(\mathbf{r}) - \hat{f}_\mu(\mathbf{r}) \times \hat{g}(\mathbf{r}, \omega) \right] \cdot \mathbf{n} dA, 
\]

where \( \hat{f}_\mu(\mathbf{r}) \) and \( \hat{g}_\mu(\mathbf{r}) \) denote the electric and magnetic field QNMs, respectively, with complex (angular) resonance frequency \( \hat{\omega}_\mu \). Following Muljarov et al. [3], the fields \( \hat{f}(\mathbf{r}, \omega) \) and \( \hat{g}(\mathbf{r}, \omega) \) denote analytical continuations of the QNMs in the vicinity of \( \omega = \hat{\omega}_\mu \). Sauvan et al. argues that in calculations using perfectly matched layers (PMLs) the surface integral can be immediately set to zero, because it is evaluated at the (complex) coordinate transformed positions beyond the PMLs where the fields vanish [8]. Nevertheless, the Lorentz reciprocity theorem holds for all volumes \( V \), and for finite sized volumes, we must keep the second term \[10\]. In the limit \( \omega \approx \hat{\omega}_\mu \), and hence \( \hat{f}(\mathbf{r}, \omega) \approx \hat{f}_\mu(\mathbf{r}) \), we follow Sauvan and co-workers and write \( \omega \epsilon_\epsilon(\mathbf{r}, \omega) \approx \hat{\omega}_\mu \epsilon_\mu(\mathbf{r}, \hat{\omega}_\mu) + \eta(\hat{\omega}_\mu, \omega) \) (or \( \omega \approx \hat{\omega}_\mu \)), where \( \eta(\mathbf{r}, \omega) = \partial_\nu [\omega \epsilon_\epsilon(\mathbf{r}, \omega)] \). In this limit we can then write

\[
0 = (\hat{\omega}_\mu - \omega) \frac{i}{2} \int_V \eta(\hat{\omega}_\mu) \hat{f}_\mu(\mathbf{r}) \cdot \hat{f}(\mathbf{r}, \omega) - \frac{\mu_0}{\epsilon_0} \hat{g}_\mu(\mathbf{r}) \cdot \hat{g}(\mathbf{r}, \omega) dV \\
+ \frac{i}{2\epsilon_0(\hat{\omega}_\mu - \omega)} \int_{\partial V} \left[ \hat{f}(\mathbf{r}, \omega) \times \hat{g}_\mu(\mathbf{r}) - \hat{f}_\mu(\mathbf{r}) \times \hat{g}(\mathbf{r}, \omega) \right] \cdot \mathbf{n} dA, 
\]

which shows that the sum of the integrals may be different from zero as \( \omega \rightarrow \hat{\omega}_\mu \), in which case it becomes the norm \( \langle \hat{f}_\mu|\hat{f}_\mu \rangle \). To explore this limit, we may rewrite the expression using

\[
\hat{g}(\mathbf{r}, \omega) = -\frac{i}{\mu_0 \omega} \nabla \times \hat{f}(\mathbf{r}, \omega) 
\]
and the vector Green’s identity of the first kind,

\[
\int_V (\nabla \times \mathbf{P}) \cdot (\nabla \times \mathbf{Q}) - \mathbf{P} \cdot \nabla \times \nabla \times \mathbf{Q} \, dV = \int_{\partial V} \mathbf{n} \cdot (\mathbf{P} \times \nabla \times \mathbf{Q}) \, dA,
\]

as

\[
\langle \langle \tilde{f}_\mu | \tilde{f}_\mu \rangle \rangle = \lim_{\omega \to \tilde{\omega}_\mu} \left\{ \int_V \sigma(r, \omega) \tilde{f}_\mu(r) \cdot \tilde{f}(r, \omega) \, dV \right. \\
+ \frac{\epsilon^2}{2 \omega^2} \int_{\partial V} \left[ \tilde{f}_\mu(r) \times \nabla \times \tilde{f}(r, \omega) - \frac{\omega \tilde{f}(r, \omega) \times \nabla \times \tilde{f}_\mu(r) - \tilde{\omega}_\mu \tilde{f}_\mu(r) \times \nabla \times \tilde{f}(r, \omega)}{\omega - \tilde{\omega}_\mu} \right] \cdot \mathbf{n} \, dA \right\},
\]

where \( \sigma(r, \omega) = \partial_\omega [\omega^2 \epsilon(r, \omega)]/2\omega \). To further investigate the behavior of the last term as \( \omega \to \tilde{\omega}_\mu \), we follow Muljarov et al. \cite{Muljarov2016} and write

\[
\tilde{f}(r, \omega) \approx \tilde{f}_\mu(r) + \frac{\omega - \tilde{\omega}_\mu}{\tilde{\omega}_\mu} \mathbf{K}_\mu(r),
\]

in which \( \mathbf{K}_\mu(r) = (r \cdot \nabla) \tilde{f}_\mu(r) \) as detailed in Ref. \cite{Muljarov2016}. Inserting in the second integral and taking the limit \( \omega \to \tilde{\omega}_\mu \) (and thus \( \tilde{f}(r, \omega) \to \tilde{f}_\mu(r) \)), we find

\[
\langle \langle \tilde{f}_\mu | \tilde{f}_\mu \rangle \rangle = \int_V \sigma(r, \tilde{\omega}_\mu) \tilde{f}_\mu(r) \cdot \tilde{f}_\mu(r) \, dV + \frac{\epsilon^2}{2 \tilde{\omega}_\mu^2} \int_{\partial V} \left[ \tilde{f}_\mu(r) \times \nabla \times \mathbf{K}_\mu(r) - \mathbf{K}_\mu(r) \times \nabla \times \tilde{f}_\mu(r) \right] \cdot \mathbf{n} \, dA.
\]

Now, we can use the general result

\[
\left[ \mathbf{P} \cdot \nabla \times \mathbf{Q} \right] \cdot \mathbf{n} = \mathbf{P} \cdot \partial_\mu \mathbf{Q} - \left[ \mathbf{P} \cdot \nabla \mathbf{Q} \right] \cdot \mathbf{n},
\]

where \( \partial_\mu \mathbf{Q} \) denotes differentiation of each component of \( \mathbf{Q} \) in the direction of the unit vector \( \mathbf{n} \) and \( \nabla \mathbf{Q} = \sum_{m,n} \partial_\mu Q_m e_m e_n \), to rewrite the expression as

\[
\langle \langle \tilde{f}_\mu | \tilde{f}_\mu \rangle \rangle = \int_V \sigma(r, \tilde{\omega}_\mu) \tilde{f}_\mu(r) \cdot \tilde{f}_\mu(r) \, dV + \frac{\epsilon^2}{2 \tilde{\omega}_\mu^2} \int_{\partial V} \left[ \tilde{f}_\mu(r) \cdot \partial_\mu \mathbf{K}_\mu(r) - \mathbf{K}_\mu(r) \cdot \partial_\mu \tilde{f}_\mu(r) \right] \cdot \mathbf{n} \, dA \\
- \frac{\epsilon^2}{2 \tilde{\omega}_\mu^2} \int_{\partial V} \left[ \tilde{f}_\mu(r) \cdot \nabla \mathbf{K}_\mu(r) - \mathbf{K}_\mu(r) \cdot \nabla \tilde{f}_\mu(r) \right] \cdot \mathbf{n} \, dA.
\]

Last, since \( \nabla \cdot \tilde{f}_\mu(r) = \nabla \cdot \mathbf{K}_\mu(r) = 0 \) on the calculation domain boundary, we can use the general product rule

\[
\nabla \times \left[ \mathbf{P} \times \mathbf{Q} \right] = \mathbf{P} \cdot \nabla \mathbf{Q} - \mathbf{Q} \cdot \nabla \mathbf{P} + \mathbf{P} \left[ \nabla \cdot \mathbf{Q} \right] - \mathbf{Q} \left[ \nabla \cdot \mathbf{P} \right],
\]

(10)

to rewrite the third integral as the flux of the curl through a closed surface, which vanishes by virtue of Stokes’ integral theorem. The normalization then takes the exact form presented by Muljarov et al. \cite{Muljarov2016}.

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[10] PTK thanks Kathrin Herrmann for pointing out this important detail.