Comment on “Normalization of quasinormal modes in leaky optical cavities and plasmonic resonators”

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Recently, Kristensen, Ge and Hughes have compared [Phys. Rev. A 92, 053810 (2015)] three different methods for normalization of quasinormal modes in open optical systems, and concluded that they all provide the same result. We show here that this conclusion is incorrect and illustrate that the normalization of [Opt. Lett. 37, 1649 (2012)] is divergent for any optical mode having a finite quality factor, and that the Silver-Müller radiation condition is not fulfilled for quasinormal modes.

In a recent paper [1], Kristensen et al. have considered three different normalizations of quasinormal modes: (i) the normalization given in [2], which is a generalized version of the work by Leung et al. [3] and thus called here Leung-Kristensen (LK); (ii) the normalization introduced in [4], which is analytically exact; and (iii) the normalization suggested in [5], based on perfectly matched layers (PML). Kristensen et al. concluded that all three normalizations provide the same result. We show in this Comment that (i) the LK normalization is divergent, and therefore ill-defined. A regularized variant of the LK normalization, put forward in [1], is not suited for numerically determined resonant states (RSs); (ii) the claimed equivalence of LK and PML normalizations is incorrect since the Silver-Müller radiation condition used in the argumentation is not valid for RSs.

The LK normalization, Eq. (5) of [1], for an optical system surrounded by vacuum is defined by an infinite-volume limit

$$N^\infty_{LK} = \lim_{V \to \infty} N_{LK}$$

of the normalization

$$N_{LK} = \int_V \varepsilon(r) \mathbf{E}^2(r) dV + \frac{i}{2k} \int_{S_V} \mathbf{E}^2(r) dS,$$

where

$$P_l(\xi) = \sum_{m=0}^{l} \frac{(l+m)!}{(l-m)!m!} \xi^m$$

and

$$\xi = \frac{1}{-2iz}.$$  

Now, $$P_l(\xi)$$ is a polynomial of order $$l$$, and all resulting terms of Eq. (3) diverge for complex $$z$$, owing to the exponentially large factor $$e^{2iz}$$. Consequently, Eq. (10) in [1], based on Eq. (9) and stating that $$\partial_R \hat{I}^\dagger_l(R) = 0$$, is incorrect, and should read instead

$$\partial_R \hat{I}^\dagger_l(R) = \frac{\epsilon_{2ikR}}{k^4 R^2} \left( 1 + \frac{i}{kR} \right).$$

The authors of [1] write “In practice, direct application of Eq. (5) leads to an integral that seems to quickly converge towards a finite value, but in fact oscillates about this value with an amplitude that eventually starts to grow (exponentially) with the distance, almost slowly compared to the length scales in typical calculations.” This was noted in Ref. [5], where the oscillations were observed only for the cavity with the lowest quality factor ($$Q \approx 16$$). In the cited reference [2], we find “For very low-$$Q$$ cavities, however, the convergence is nontrivial due to the exponential divergence of the modes that may cause the inner product to oscillate around the proper value as a function of calculation domain size,” and otherwise “quick convergence” is claimed. The residual $$f^{\dagger}_{LK}(R)$$ of the LK normalization, which is given in Eq. (11) of [1] diverges – its precise form is

$$f^{\dagger}_{LK}(R) = \frac{R^2}{2} \left[ h_0^2(z) - h_{l-1}(z) h_{l+1}(z) + \frac{i}{z} h_1^2(z) \right]$$

and

$$= \frac{\epsilon_{2ikR}}{k^5 R^2} Q_{2l-2}(\xi).$$
where $Q_n(\xi)$ is an $n$-th order polynomial of $\xi = (-2ikR)^{-1}$, with the leading term at small $\xi$ (i.e. at large $R$) given by $Q_{2l-2}(0) = -i(-1)^{l+1}(l+1)/2$, see [8] for more details. Therefore, $N_{\text{LK}} \to \infty$ as $R \to \infty$.

The authors of [1] describe this divergence as “Thus, while Eqs. (9) and (10) appear to be formally correct also for complex arguments, the limit $R \to \infty$ in practice leads to a position dependent phase difference between the Hankel function and its limiting form, which makes the limit nontrivial to perform along the real axis.” We note that (i) there is no difference between formalism and practise in mathematical limits; (ii) the limit $V \to \infty$ is defined for real volumes, and thus real $R$; (iii) the limit of $N_{\text{LK}}$ along the real axis of $R$ is not “nontrivial”, it simply does not exist due to the divergence.

We show in Figures 1(a-d) the $R$-dependence of $N_{\text{LK}}$ for RSs of a dielectric sphere of radius $a$ with high and low $Q$-factors, and for the fundamental plasmonic RS of a gold sphere. All RS fields used have been normalized using the exact normalization, having analytical expressions [7, 8]. We commence using a RS with a $Q$-factor of about 35 (similar to the RS illustrated in Fig. 3 of [1]), the $l = 7$ transverse electric (TE) whispering gallery mode (WGM) of a dielectric sphere with refractive index $n_r = 2$ in vacuum. Fig. 1 is formatted similarly to Fig. 3 of [1], with $Q = 34.8$. Blue (red) color shows the region of error decreasing (increasing) with $R$. The exact normalization is shown by a black line (a) and a black cross (c-d).

![FIG. 1: LK normalization $N_{\text{LK}}$ (a-c-d) and its absolute error $|N_{\text{LK}} - 1|$ (b) as a function of the radius $R$ of the spherical volume, for a TE $l = 7$ WGM of a dielectric sphere of refractive index $n_r = 2$ and radius $a$, in vacuum. The wave vector of the WGM is $ka = 6.888 - 0.099 i$, corresponding to $Q = 34.8$. Blue (red) color shows the region of error decreasing (increasing) with $R$. The exact normalization is shown by a black line (a) and a black cross (c-d).](image1)

One could argue that for high-$Q$ modes, the LK normalization can be sufficiently accurate, as the error reaches $10^{-3}$ at $R \approx 10a$ in the present example. One could even refine this result by evaluating the center of the spiral, as suggested in [1]. However, one has to keep in mind that simulating the required extended spatial domain in numerical calculations is computationally costly. On the other hand, evaluating the LK normalization close to the system, leads to significant errors due to the slow $1/R^2$ dependence of the residual term Eq. (7), as is clearly shown by the blue line in Figs. 1(b) and (d). The LK normalization used for high-$Q$ RSs is thus at least incon-
are given in the supplement of [8].

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Finally we show that the claim in [1], that the LK normalization the corresponding part is

\[
\frac{i}{2k} \int_{\Delta S} E^2 (\mathbf{k} \cdot \mathbf{n}) dS ,
\]

where \( \mathbf{n} \) is the surface normal, while for the LK normalization the corresponding part is

\[
\frac{i}{2k} \int_{\Delta S} E^2 dS .
\]

This shows that the LK surface term assumes that the propagation direction of the field is always normal to the surface, while the exact normalization takes the actual propagation direction into account. The two terms are equal only if \( \mathbf{n} \parallel \mathbf{k} \) over the whole surface, which is not possible in electrodynamics due to the vectorial nature of the electro-magnetic field.

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of \[5\], is incorrect. This should be clear considering that \( N_{\text{LK}} \) diverges, while the PML normalization is finite, as demonstrated in the supplement of \[5\] for the RS shown in Fig. 3. The PML normalization uses a PML to convert the radiation losses into absorptive losses within the PML, such that the remaining radiation losses at the external border of the PML can be neglected.

The equivalence of the LK and PML normalization is shown in \[1\] analytically, using the Silver-Müller radiation condition. This condition states that the vector field

\[
F = \frac{r}{r} \times \nabla \times E + ikE , \tag{10}
\]

vanishes at large distances from the optical system, i.e. \( F \to 0 \) as \( r \to \infty \). Here \( E \) is the electric field of a wave emitted from the system centered at the origin, with a wave vector \( k \) which is real and positive. However, for a RS, \( k \) is typically complex, so that the Silver-Müller condition does not hold, and a divergence \( F \to \infty \) as \( r \to \infty \) is found instead. To exemplify this, we take TE vector spherical harmonics, which can be used, along with their TM counterparts, for expansion of any mode of a finite system in the outside area. Their field can be written as

\[
E = -r \times \nabla f , \quad \text{where} \quad f(r) = h_l(kr)Y_{lm}(\theta, \varphi) , \tag{11}
\]

so that

\[
F = \frac{r}{r} \times [2 - ikr + (r \cdot \nabla)] \nabla f
= \frac{h_l(kr)}{2ikr^2} \frac{P_l'(\xi)}{P_l(\xi)} \left( e_\varphi \partial_\theta - e_\theta \frac{\partial_\varphi}{\sin \theta} \right) Y_{lm}(\theta, \varphi) , \tag{12}
\]

in which \( e_\varphi \) and \( e_\theta \) are the unit vectors of the spherical coordinate system, and \( \xi = (-2ikr)^{-1} \). We see that \( F \) diverges for \( r \to \infty \) due to the exponentially growing factor in \( h_l(kr) \) and the non-vanishing factor \( P_l'(\xi)/P_l(\xi) \to l(l+1) \). Using \( F \to 0 \) for \( r \to \infty \) in Eq. (17) of \[1\], the authors obtain the LK normalization from the PML normalization. This shows actually that the two normalizations differ by a term proportional to \( F \) which is diverging for \( r \to \infty \), consistent with the fact that the LK normalization is diverging while the PML normalization is not.

Acknowledgments

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