1. The open-source numerical tool (QNM_NEBC) of the quasinormal mode expansion theory for mesoscale plasmonic nanoresonators proposed in Ref. [1]

Reference [1] proposes a quasinormal mode (QNM) expansion theory for calculating the optical response of plasmonic nanoresonators with mesoscale (2-20 nm) feature sizes (such as the size of nanogap). The optical response of such mesoscale plasmonic nanoresonators is significantly affected by the nonlocality, surface damping and electron spill-out nonclassical quantum effects, which can be fully described by the nonclassical electromagnetic boundary condition (NEBC) expressed with the surface-response Feibelman $d_\perp$ and $d_\parallel$ parameters. Using the easy-to-solve classical QNMs under classical electromagnetic boundary condition (CEBC) as a complete set of basis functions, the theory can provide rigorous expansion expressions for the source-excited nonclassical electromagnetic field and source-free nonclassical QNMs (both under the NEBC). With an analytical dependence on the non-perturbative NEBC and classical QNMs, the theory can be used as a physically intuitive and computationally efficient tool for designing mesoscale plasmonic nanoresonators.

2. The softwares used in the tool

The open-source numerical tool uses COMSOL Multiphysics software to calculate the classical QNMs, and uses the MATLAB software (via the COMSOL LiveLink for MATLAB) to calculate the expansion expressions for the source-excited nonclassical electromagnetic field and source-free nonclassical QNMs.

3. Codes of the tool for typical examples

The codes for producing all the curves in Figs. 2(a2) and 3(c) as typical examples in Ref. [1] are provided in the folders named “Fig2(a2)” and “Fig3(c)”, respectively, as listed in the following two tables.

Table 1

<table>
<tr><th>Curves in Fig. 2(a2)</th><th>Corresponding codes in folder “Fig2(a2)”</th></tr>
<tr><td>Blue circles
(FEM, NEBC)</td><td>Single_nanowire_NPoM_antenna_h6_PF_fullwave_web.mph</td></tr>
<tr><td>Red circles
(FEM, CEBC)</td><td>Single_nanowire_NPoM_antenna_h6_PF_fullwave_web.mph
(The NEBC reduces to CEBC if $d_\perp = 0$ and $d_\parallel = 0$. Thus, the results under CEBC can be obtained by setting the corresponding parameters as dnormal=0[m] and dparallel=0[m] in the COMSOL model.)</td></tr>
<tr><td>Blue-solid curve
(Model 1, NEBC)</td><td rowspan="4">Single_nanowire_NPoM_antenna_h6_classicalQNM_web.mph
NEBC_QNM_expan_singlenanowire_NPoM_antenna_PF.m
(To carry out the MATLAB program, the COMSOL model should be run first to obtain the results of classical QNM.)</td></tr>
<tr><td>Blue-solid curve
(Model 2A, NEBC)</td></tr>
<tr><td>Blue-dashed curve
(Model 2B, NEBC)</td></tr>
<tr><td>Red-solid curve
(Model 1, CEBC)</td></tr>
</table>

Table 2

<table>
<tr><th>Curves in Fig. 3(c)</th><th>Corresponding codes in folder “Fig3(c)”</th></tr>
<tr><td>Blue circles
(FEM, NEBC)</td><td>Asym_nanowire_dimer_NPoM_antenna_h6_PF_fullwave_web.mph</td></tr>
<tr><td>Red circles
(FEM, CEBC)</td><td>Asym_nanowire_dimer_NPoM_antenna_h6_PF_fullwave_web.mph
(setting dnormal=0[m] and dparallel=0[m])</td></tr>
<tr><td>Blue-solid curve
(Model 1, NEBC)</td><td rowspan="5">Asym_nanowire_dimer_NPoM_antenna_h6_classicalQNM_web.mph
Air_AlOx_Au_PF_Eb_fullwave_web.mph
NEBC_QNM_expan_dimer_antenna_Esca_PF.m
(To carry out the MATLAB program, the COMSOL models should be run first to obtain the results of classical QNMs and the classical electromagnetic field of the background medium.)</td></tr>
<tr><td>Blue-solid curve
(Model 2A, NEBC)</td></tr>
<tr><td>Blue-dashed curve
(Model 2B, NEBC)</td></tr>
<tr><td>Yellow-dashed curves
(Model 2A, 1 QNM, NEBC)</td></tr>
<tr><td>Red-solid curve
(Model 1, CEBC)</td></tr>
<tr><td>Green-solid curve
(Model 1, NEBC, $\kappa_{1,2}=\kappa_{2,1}=0$)</td><td rowspan="2">Asym_nanowire_dimer_NPoM_antenna_h6_classicalQNM_web.mph
Air_AlOx_Au_PF_Eb_fullwave_web.mph
NEBC_QNM_expan_dimer_antenna_Esca_PF_without_crosscoupl.m
(To carry out the MATLAB program, the COMSOL models should be run first to obtain the results of classical QNMs and the classical electromagnetic field of the background medium.)</td></tr>
<tr><td>Green-solid curve
(Model 2A, NEBC, $\kappa_{1,2}=\kappa_{2,1}=0$)</td></tr>
</table>

4. Citing QNM_NEBC

We kindly request that you cite the following Ref. [1] in any published work for which you used our provided codes here.

5. Reference

[1] Can Tao, Ying Zhong, and Haitao Liu, Quasinormal mode expansion theory for mesoscale plasmonic nanoresonators: an analytical treatment of nonclassical electromagnetic boundary condition, Physical Review Letters **129**, 197401 (2022).