scuff-caspol Implementation Notes

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1 Overview

The Casimir-Polder potential felt by a polarizable particle at a point $\mathbf{x}$ in the vicinity of material bodies is

$$U(\mathbf{x}) = \int_0^\infty \mathcal{U}(\xi, \mathbf{x})\, d\xi \tag{1a}$$

$$\mathcal{U}(\xi, \mathbf{x}) = 2\hbar\xi^2 \mathrm{Tr}\, \boldsymbol{\alpha}(\xi) \cdot \boldsymbol{\mathcal{G}}^{\mathrm{EE}}(\xi; \mathbf{x}, \mathbf{x}) \tag{1b}$$

Here $\boldsymbol{\alpha}(\xi)$ is the 3×3 polarizability tensor of the particle evaluated at imaginary angular frequency $\omega = i\xi$ and $\boldsymbol{\mathcal{G}}^{\mathrm{EE}}(\xi, \mathbf{x}, \mathbf{x})$ is the scattering part of the 3×3 electric-electric dyadic Green's function of the material geometry, defined by

$$\mathcal{G}^{\mathrm{E}}_{ij}(\xi; \mathbf{x}, \mathbf{x}') \equiv -\frac{1}{\kappa Z_0} \left(\begin{array}{l} i\text{-component of scattered } \mathbf{E}\text{-field at } \mathbf{x} \text{ due to a unit-} \\ \text{strength } j\text{-directed point electric dipole radiator at} \\ \mathbf{x}', \text{ all quantities having time dependence} \sim e^{+\xi t} \end{array} \right) \tag{2}$$

where $Z_0 \approx 377\,\Omega$ is the impedance of free space and $\kappa = \frac{\xi}{c}$ is the imaginary wavenumber.

$\mathcal{G}$ is computed numerically by solving a scattering problem in which the incident field arises from a j-directed point dipole at $\mathbf{x}_0$,

$$E_i^{\mathrm{inc}}(\mathbf{x}) = \Gamma^{\mathrm{EE}}_{ij}(\mathbf{x}, \mathbf{x}_0), \qquad H_i^{\mathrm{inc}}(\mathbf{x}) = \Gamma^{\mathrm{ME}}_{ij}(\mathbf{x}, \mathbf{x}_0) \tag{3}$$

where the tensor $\boldsymbol{\Gamma}^{\mathrm{PQ}}$ gives the P field due to a Q source (with {P,Q}∈{electric, magnetic}):

$$\boldsymbol{\Gamma}^{\mathrm{EE}} = -\kappa Z_0 \mathbb{G}, \qquad \boldsymbol{\Gamma}^{\mathrm{EM}} = -\kappa \mathbb{C}, \qquad \boldsymbol{\Gamma}^{\mathrm{ME}} = +\kappa \mathbb{C}, \qquad \boldsymbol{\Gamma}^{\mathrm{MM}} = -\frac{\kappa}{Z_0}\mathbb{G}$$

$$\mathbb{G}_{ij}(\mathbf{r}) = \left(\delta_{ij} - \frac{1}{\kappa^2}\partial_i\partial_j\right) G_0(\mathbf{r}), \qquad \mathbb{C}_{ij}(\mathbf{r}) = -\frac{1}{\kappa}\varepsilon_{ijk}\partial_k G_0(\mathbf{r}), \qquad G_0(\mathbf{r}) = \frac{e^{-\kappa r}}{4\pi r}.$$

Given this incident field, we get one full column of $\mathcal{G}^{\text{EE}}$ by evaluating the components of the scattered field at x_0:

$$\mathcal{G}^{\text{EE}}_{ij}(\xi, \mathbf{x}_0, \mathbf{x}_0) = E^{\text{scat}}_i(\mathbf{x}_0). \tag{4}$$

Implementation in SCUFF-EM

In SCUFF-EM, the scattering problem becomes a linear system of the form

$$\mathbf{Mc} = -\mathbf{f}$$

where $\mathbf{c}$ and $\mathbf{f}$ are respectively the vectors of surface-current coefficients and incident-field projections:

$$\mathbf{c} = \left(\begin{array}{c} \mathbf{k} \\ -\mathbf{n}/Z_0 \end{array}\right), \qquad \mathbf{f} = \left(\begin{array}{c} \mathbf{e}/Z_0 \\ \mathbf{h} \end{array}\right).$$

$$\mathbf{K}(\mathbf{x}) = \sum_\alpha k_\alpha \mathbf{b}_\alpha(\mathbf{x}), \qquad \mathbf{N}(\mathbf{x}) = \sum_\alpha n_\alpha \mathbf{b}_\alpha(\mathbf{x})$$

$$e_\alpha = \big\langle \mathbf{b}_\alpha \cdot \mathbf{E}^{\text{inc}} \big\rangle, \qquad h_\alpha = \big\langle \mathbf{b}_\alpha \cdot \mathbf{H}^{\text{inc}} \big\rangle$$

In the case at hand, the elements of the RHS vector are

$$\begin{aligned} e_\alpha/Z_0 &= \frac{1}{Z_0}\Big\langle b_{\alpha;\mu}(\mathbf{x})\Gamma^{\text{EE}}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle \\ &= -\kappa\Big\langle b_{\alpha;\mu}(\mathbf{x})\mathbb{G}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle \\ h_\alpha &= \Big\langle b_{\alpha;i}(\mathbf{x})\Gamma^{\text{ME}}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle \\ &= +\kappa\Big\langle b_{\alpha;\mu}(\mathbf{x})\mathbb{C}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle \end{aligned}$$

which I will write in the form

$$-\mathbf{f} = -\left(\begin{array}{c} \mathbf{e}/Z_0 \\ \mathbf{h} \end{array}\right) = +\kappa \mathbf{v}_j$$

$$\mathbf{v}_j = \left(\begin{array}{c} \mathbf{v}^{\text{E}}_j \\ \mathbf{v}^{\text{M}}_j \end{array}\right)$$

$$\mathbf{v}^{\text{E}}_j = \Big\langle b_{\alpha;\mu}(\mathbf{x})\mathbb{G}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle, \qquad \mathbf{v}^{\text{M}}_j = -\Big\langle b_{\alpha;\mu}(\mathbf{x})\mathbb{C}_{\mu j}(\mathbf{x}, \mathbf{x}_0)\Big\rangle$$

Having computed the surface-current expansion coefficients, the scattered fields at $\mathbf{x}$ are

$$
\begin{aligned}
E_i(\mathbf{x}_0) &= \sum_\alpha \Big\{ k_\alpha \Big\langle \Gamma^{\text{EE}}_{i\mu}(\mathbf{x}_0,\mathbf{x}) b_{\alpha;\mu}(\mathbf{x}) \Big\rangle + n_\alpha \Big\langle \Gamma^{\text{EM}}_{i\mu}(\mathbf{x}_0,\mathbf{x}) b_{\alpha;\mu}(\mathbf{x}) \Big\rangle \Big\} && (5)\\
&= \sum_\alpha \Big\{ -\kappa Z_0 k_\alpha \Big\langle \mathbb{G}_{i\mu}(\mathbf{x}_0,\mathbf{x}) b_{\alpha;\mu}(\mathbf{x}) \Big\rangle - \kappa n_\alpha \Big\langle \mathbb{C}_{i\mu}(\mathbf{x}_0,\mathbf{x}) b_{\alpha;\mu}(\mathbf{x}) \Big\rangle \Big\} && (6)\\
&= -\kappa Z_0 \sum_\alpha \left\{ k_\alpha v^{\text{E}}_{i\alpha} - \frac{n_\alpha}{Z_0} v^{\text{M}}_{i\alpha} \right\} && (7)\\
&= -\kappa Z_0 \mathbf{v}_i^T \mathbf{c} && (8)\\
&= -\kappa^2 Z_0 \mathbf{v}_i^T \mathbf{W} \mathbf{v}_j && (9)
\end{aligned}
$$

where $\mathbf{W} = \mathbf{M}^{-1}$. The dyadic Green's function (2) then reads

$$
\boldsymbol{\mathcal{G}}_{ij} = \kappa \Big[\mathbf{v}_i^T \mathbf{W} \mathbf{v}_j \Big]
$$

and the integrand of the Casimir-Polder potential (1b) reads ($c \equiv 1$)

$$
\begin{aligned}
\mathcal{U}(\xi;\mathbf{x}) &= 2\hbar\xi^3 \sum_{ij} \alpha_{ij} \Big[\mathbf{v}_j^T \mathbf{W} \mathbf{v}_i \Big] \\
&= 2\hbar\xi^3 \Big[\mathbf{v}_j^T \mathbf{W} \Big(\alpha_{ij} \mathbf{v}_i \Big) \Big]
\end{aligned}
$$