

BUFF-EM: A Volume-Integral Solver Suite for Classical Scattering and Fluctuational Electrodynamics

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Abstract

The \mathbb{T} -matrix approach to fluctuational electrodynamics, pioneered by the MIT Casimir theory group led by Professors Kardar and Jaffe, has yielded a bountiful smorgasbord of analytical formulas expressing quantities in fluctuational electrodynamics—including equilibrium and non-equilibrium Casimir forces and thermal heat-transfer rates for compact and extended bodies—in terms of the \mathbb{T} -matrices of the bodies in question [?, ?]. Although the analytical insight afforded by these formulas is immensely valuable, their practical application has typically been restricted to the small catalog of highly symmetric bodies—such as homogeneous spheres—for which \mathbb{T} -matrix element may be computed in closed form.

In its earliest incarnation, BUFF-EM was born as an attempt to extend the \mathbb{T} -matrix approach to a more general class of bodies by computing \mathbb{T} -matrices numerically. However, in the course of implementing these calculations I discovered that the \mathbb{T} -matrix formalism may in fact be understood as simply a disguised version of the well-known volume-integral-equation (VIE) approach to computational electromagnetism, and that in implementing a numerical tool for computing \mathbb{T} -matrices one is in fact implementing a VIE solver.

The BUFF-EM suite¹ consists of a core library (LIBBUFF) implementing this solver—using SWG basis functions [?]¹—together with application modules for classical scattering (BUFF-SCATTER) and non-equilibrium fluctuational electrodynamics (BUFF-NEQ).

¹BUFF-EM stands for **bulk field formulation of electromagnetism**.

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1 VIE formulation of classical EM scattering

In this section I rederive the volume-integral-equation (VIE) approach to classical electromagnetic scattering. This formulation is standard, but I here describe it using terminology and symbols that emphasize the connection to the T-matrix scattering approach used by the Kardar-Jaffe group.

1.1 Continuous VIE formulation

Consider a material body with relative permittivity tensor $\epsilon(\mathbf{x})$ lying in vacuum and irradiated by monochromatic sources which may lie inside or outside the body. Let the electric field due to the sources be \mathbf{E}^{inc} and let $\mathbf{J}^{\text{I}}(\mathbf{x})$ be the induced volume current density throughout the bulk of the body. (We work at frequency ω and assume time dependence of all field and currents $\propto e^{-i\omega t}$.) The total electric field at any point is a sum of “incident” and “scattered” contributions:²

$$\mathbf{E}^{\text{tot}} = \mathbf{E}^{\text{inc}} + \mathbf{E}^{\text{scat}} \quad (1)$$

$$= \mathbf{E}^{\text{inc}} + ikZ_0\mathbb{G} * \mathbf{J}^{\text{I}} \quad (2)$$

where $k = \omega/c$ is the (free-space) wavenumber, $Z_0 = \sqrt{\mu_0/\epsilon_0}$ is the impedance of free space³, $*$ denotes convolution, and \mathbb{G} is the free-space dyadic Green’s function:

$$\mathbb{G}(\mathbf{x}, \mathbf{x}') = \left(\mathbf{1} - \frac{1}{k^2} \nabla \times \nabla \right) \frac{e^{ikr}}{4\pi r} \quad (r \equiv |\mathbf{r}| = |\mathbf{x} - \mathbf{x}'|) \quad (3)$$

$$= \frac{e^{ikr}}{4\pi k^2 r^3} \left[f_1(ikr) \delta_{ij} + f_2(ikr) \frac{r_i r_j}{r^2} \right] \quad (4)$$

$$f_1(x) \equiv -1 + x - x^2, \quad f_2(x) \equiv 3 - 3x + x^2.$$

On the other hand, the induced current is related to the total field according to

$$\begin{aligned} \mathbf{J}^{\text{I}}(\mathbf{x}) &= -i \frac{k}{Z_0} [\epsilon(\mathbf{x}) - \mathbf{1}] \cdot \mathbf{E}^{\text{tot}}(\mathbf{x}) \\ &\equiv -\frac{1}{ikZ_0} \mathbb{V}(\mathbf{x}) \cdot \mathbf{E}^{\text{tot}}(\mathbf{x}) \end{aligned} \quad (5)$$

where $\mathbb{V} \equiv k^2[\mathbf{1} - \epsilon(\mathbf{x})]$ is sometimes [?] known as the “potential.” At points not in free space, i.e. points at which $\epsilon(\mathbf{x}) \neq \mathbf{1}$, we can invert this equation to

²We put the terms “incident” and “scattered” in quotes to remind readers that the “incident”-field sources may in fact lie *inside* the body; in this case it is not quite right to refer to the field they produce as being “incident” on the body, but the terminology is convenient nonetheless.

³Here and throughout we consistently eliminate all reference to the free-space permittivity and permeability constants ϵ_0, μ_0 in favor of $Z_0 = \sqrt{\mu_0/\epsilon_0}$ and $c = 1/\sqrt{\epsilon_0\mu_0}$. For example, we write the combinations $\{\epsilon_0\omega, \mu_0\omega\}$ respectively in the form $\{\frac{k}{Z_0}, kZ_0\}$ where $k = \omega/c$ is the free space wavelength.

read

$$-ikZ_0\Lambda(\mathbf{x}) \cdot \mathbf{J}^I(\mathbf{x}) = \mathbf{E}^{\text{tot}}(\mathbf{x})$$

where $\Lambda \equiv \mathbb{V}^{-1}$. Now insert (2):

$$-ikZ_0\Lambda(\mathbf{x}) \cdot \mathbf{J}^I(\mathbf{x}) = \mathbf{E}^{\text{inc}} + ikZ_0\mathbb{G} \star \mathbf{J}^I \quad (6)$$

Rearranging and writing out the convolution, we obtain a volume-integral equation for \mathbf{J}^I :

$$-ikZ_0 \left[\Lambda(\mathbf{x}) \cdot \mathbf{J}^I(\mathbf{x}) + \int \mathbb{G}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{J}^I(\mathbf{x}') d\mathbf{x}' \right] = \mathbf{E}^{\text{inc}}(\mathbf{x}). \quad (7)$$

In what follows it will be convenient to think of the RHS here as the convolution of just a single operator with \mathbf{J}^I :

$$-ikZ_0 \int \mathbb{L}(\mathbf{x}, \mathbf{x}') \cdot \mathbf{J}^I(\mathbf{x}') d\mathbf{x}' = \mathbf{E}^{\text{inc}}(\mathbf{x}). \quad (8)$$

where

$$\mathbb{L}(\mathbf{x}, \mathbf{x}') = \Lambda(\mathbf{x})\delta(\mathbf{x} - \mathbf{x}') + \mathbb{G}(\mathbf{x}, \mathbf{x}'). \quad (9)$$

(The symbol \mathbb{L} is pronounced “tee-inverse” or “eet”.)

1.2 Discretized VIE formulation

Now let \mathbf{b}_α be some convenient set of N vector-valued basis functions and approximate the induced current in the form

$$\mathbf{J}^I(\mathbf{x}) \approx \sum_{\alpha} j_{\alpha}^I \mathbf{b}_{\alpha}(\mathbf{x}). \quad (10)$$

Insert into (8) and “test” both sides with the elements of the set $\{\mathbf{b}_{\alpha}\}$ to obtain a discretized version of (8) in the form of an $N \times N$ linear system:

$$\mathbf{L} \cdot \mathbf{j}^I = \mathbf{v} \quad (11)$$

where the elements of the vector \mathbf{j}^I are the expansion coefficients in (10) and the elements of \mathbf{L} and \mathbf{v} are

$$L_{\alpha\beta} = \langle \mathbf{b}_{\alpha} | \mathbb{L} | \mathbf{b}_{\beta} \rangle, \quad v_{\alpha} = -\frac{1}{ikZ_0} \langle \mathbf{E}^{\text{inc}} | \mathbf{b}_{\alpha} \rangle. \quad (12)$$

VIE matrix for geometries containing multiple bodies

Equation (11) applies to the case in which we have only a single material body. For a geometry involving N separate bodies, this is generalized to read

$$\underbrace{\begin{pmatrix} \mathbf{L}_1 & \mathbf{G}_{12} & \cdots & \mathbf{G}_{1N} \\ \mathbf{G}_{21} & \mathbf{L}_2 & \cdots & \mathbf{G}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{G}_{N1} & \mathbf{G}_{N2} & \cdots & \mathbf{L}_N \end{pmatrix}}_{\mathbf{M}} \underbrace{\begin{pmatrix} \mathbf{j}_1^i \\ \mathbf{j}_2^i \\ \vdots \\ \mathbf{j}_N^i \end{pmatrix}}_{\mathbf{j}} = \underbrace{\begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_N \end{pmatrix}}_{\mathbf{v}}. \quad (13)$$

where \mathbf{M} is the VIE matrix for the composite system. Here the diagonal blocks involve just the matrix elements of the inverse \mathbb{T} -operator [defined by equation (9) with the \mathbb{A} operator appropriate for the n th body] while the off-diagonal blocks involve only the matrix elements of the \mathbb{G} operator.

The matrices \mathbf{M} and \mathbf{v} in equation (13) are the quantities computed by the `AssembleVIEMatrix()` and `AssembleRHSVector()` methods of the `SWGGeometry` class in BUFF-EM.

Computation of scattered fields

For a geometry irradiated by incident fields $\{\mathbf{E}, \mathbf{H}\}^{\text{inc}}$, the total fields at \mathbf{x} are

$$\mathbf{E}^{\text{tot}}(\mathbf{x}) = \mathbf{E}^{\text{inc}}(\mathbf{x}) + \mathbf{E}^{\text{scat}}(\mathbf{x}) \quad (14)$$

$$\mathbf{H}^{\text{tot}}(\mathbf{x}) = \mathbf{H}^{\text{inc}}(\mathbf{x}) + \mathbf{H}^{\text{scat}}(\mathbf{x}) \quad (15)$$

$$\mathbf{E}^{\text{scat}}(\mathbf{x}) = \sum_{\alpha} j_{\alpha} \mathbf{E}_{\alpha}(\mathbf{x}) \quad (16)$$

$$\mathbf{H}^{\text{scat}}(\mathbf{x}) = \sum_{\alpha} j_{\alpha} \mathbf{H}_{\alpha}(\mathbf{x}) \quad (17)$$

where $\{\mathbf{E}, \mathbf{H}\}_{\alpha}(\mathbf{x})$ are the fields due to basis function \mathbf{b}_{α} populated with unit strength:

$$\mathbf{E}_{\alpha}(\mathbf{x}) \equiv ikZ_0 \int_{\text{sup } \mathbf{b}_{\alpha}} \mathbb{G}(\mathbf{x}, \mathbf{x}') \mathbf{b}_{\alpha}(\mathbf{x}') d\mathbf{x}' \quad (18)$$

$$\mathbf{H}_{\alpha}(\mathbf{x}) \equiv -ik \int_{\text{sup } \mathbf{b}_{\alpha}} \mathbb{C}(\mathbf{x}, \mathbf{x}') \mathbf{b}_{\alpha}(\mathbf{x}') d\mathbf{x}'. \quad (19)$$

Scattered and total fields are computed by the `GetFields()` method of the `SWGGeometry` class in the BUFF-EM core library.

2 Computation of power, force, and torque

As is true for surface-integral solvers like SCUFF-EM, in volume-integral solvers like BUFF-EM there are multiple distinct ways of computing the power, force, and torque (PFT) on a body.

2.1 Displaced surface-integral (DSI) PFT

A first approach is to evaluate surface integrals of the Poynting vector and Maxwell stress tensor over a closed bounding surface \mathcal{S} containing the body but displaced from its surface:

$$\begin{aligned} P^{\text{abs}} &= \frac{1}{2} \oint_{\mathcal{S}} \mathcal{F}^\dagger(\mathbf{x}) \mathcal{N}^{\text{P}}(\hat{\mathbf{n}}(\mathbf{x})) \mathcal{F}(\mathbf{x}) dA \\ \mathbf{F} \cdot \hat{\mathbf{u}} &= \frac{1}{2} \oint_{\mathcal{S}} \mathcal{F}^\dagger(\mathbf{x}) \mathcal{N}^{\text{F}}(\hat{\mathbf{n}}(\mathbf{x}), \hat{\mathbf{u}}) \mathcal{F}(\mathbf{x}) dA \\ \mathcal{T} \cdot \hat{\mathbf{u}} &= \frac{1}{2} \oint_{\mathcal{S}} \mathcal{F}^\dagger(\mathbf{x}) \mathcal{N}^{\text{T}}(\hat{\mathbf{n}}(\mathbf{x}), \hat{\mathbf{u}}) \mathcal{F}(\mathbf{x}) dA \end{aligned}$$

Here $\mathcal{F} = \begin{pmatrix} \mathbf{E} \\ \mathbf{H} \end{pmatrix}$ is the 6-vector of fields computed from (15), and the \mathcal{N} matrices are certain constant 6×6 matrices whose entries depend on the surface normal $\hat{\mathbf{n}}$ to \mathcal{S} at \mathbf{x} .

2.2 JDEPFT

An alternative to the surface-integral method of the previous section is to compute the power, force and torque on a body using a volume-integral approach:

$$P^{\text{abs}} = \frac{1}{2} \text{Re} \int \mathbf{J}^* \cdot \mathbf{E} dV \quad (20a)$$

$$F_i = \frac{1}{2\omega} \text{Im} \int \mathbf{J}^* \cdot \partial_i \mathbf{E} dV \quad (20b)$$

$$\mathcal{T}_i = \frac{1}{2\omega} \text{Im} \int \left[\mathbf{J}^* \times \mathbf{E} + \mathbf{J}^* \cdot \partial_{\theta_i} \mathbf{E} \right] dV \quad (20c)$$

where \mathbf{J} is the induced current and \mathbf{E} is the total field. Equation (20a) is just the usual Joule heating, while Equations (20b,c) follow from Lorenz-force considerations and are derived in Appendix B. I call equations (20) the “J dot E” or JDE approach to power, force, and torque computation. [The second term in (20c) is typically small and will be neglected below]

For implementation purposes, it is convenient to separate the total field \mathbf{E} in equations (20) into incident and scattered portions and to write

$$\{P^{\text{abs}}, F_i, \mathcal{T}_i\} = \{P^{\text{abs}}, F_i, \mathcal{T}_i\}^{\text{JI}} + \{P^{\text{abs}}, F_i, \mathcal{T}_i\}^{\text{JJ}} \quad (21)$$

where the “JI” terms involve the interaction of \mathbf{J} with the incident field \mathbf{E}^{inc} alone, while the “JJ” terms involve the interaction of \mathbf{J} with itself.

The JI contribution to the power is

$$P^{\text{JI}} = \frac{1}{2} \text{Re} \int \mathbf{J}^* \cdot \mathbf{E}^{\text{inc}} dV \quad (22a)$$

$$= \frac{1}{2} \text{Re} \sum_{\alpha} j_{\alpha}^* \langle \mathbf{b}_{\alpha} | \mathbf{E}^{\text{inc}} \rangle \quad (22b)$$

and similarly

$$F_i^{\text{JI}} = \frac{1}{2\omega} \text{Im} \sum_{\alpha} j_{\alpha}^* \langle \mathbf{b}_{\alpha} | \partial_i \mathbf{E}^{\text{inc}} \rangle \quad (22c)$$

$$\mathcal{T}_i^{\text{JI}} = \frac{1}{2\omega} \text{Im} \sum_{\alpha} j_{\alpha}^* \langle \mathbf{b}_{\alpha} \times \mathbf{E}^{\text{inc}} \rangle. \quad (22d)$$

The three-dimensional integrals involved in the matrix elements in (22) are non-singular and evaluated in BUFF-EM by low-order numerical cubature (Appendix D).

On the other hand, the JJ contributions to the power, force, and torque involve *six*-dimensional integrals:

$$P^{\text{JJ}} = \frac{1}{2} \text{Re} \int \mathbf{J}^*(\mathbf{x}) \cdot \mathbf{E}^{\text{scat}}(\mathbf{x}) d\mathbf{x} \quad (23a)$$

Using $\mathbf{E}^{\text{scat}} = ik\mathbb{G} \star \mathbf{J}$, this becomes

$$= \frac{kZ_0}{2} \text{Re} \iint J_i^*(\mathbf{x}) \left(i\mathbb{G}_{ij}(\mathbf{x}, \mathbf{x}') \right) J_j(\mathbf{x}') d\mathbf{x} d\mathbf{x}' \quad (23b)$$

and similarly

$$F_i = \frac{Z_0}{2c} \text{Im} \iint J_j^* \left(i\partial_i \mathbb{G}_{jk} \right) J_k d\mathbf{x} d\mathbf{x}' \quad (23c)$$

$$\mathcal{T}_i = \frac{Z_0}{2c} \text{Im} \varepsilon_{ijk} \iint J_j^* \left(i\mathbb{G}_{k\ell} \right) J_{\ell} d\mathbf{x} d\mathbf{x}' \quad (23d)$$

Although equations (23) appear to be singular integrals, this appearance is misleading, as is demonstrated by the following rewriting, which follows from Onsager reciprocity [$\mathbb{G}_{ij}(\mathbf{x}, \mathbf{y}) = \mathbb{G}_{ji}(\mathbf{y}, \mathbf{x})$]:

$$P^{\text{JJ}} = -\frac{kZ_0}{2} \iint \left[\text{Re} (J_i^* J_j) \text{Im} \mathbb{G}_{ij} \right] dV dV' \quad (24a)$$

$$F_i^{\text{JJ}} = -\frac{Z_0}{2c} \iint \left[\text{Im} (J_j^* J_k) \text{Im} \partial_i \mathbb{G}_{jk} \right] dV dV' \quad (24b)$$

$$\mathcal{T}_i^{\text{JJ}} = \frac{Z_0}{2c} \varepsilon_{ijk} \iint \left[\text{Im} (J_j^* J_{\ell}) \text{Im} \mathbb{G}_{k\ell} \right] dV dV' \quad (24c)$$

These equations involve only the imaginary part of \mathbb{G} , which is *non-singular*; indeed, in the short-distance limit one finds immediately from (4) that

$$\text{Im } \mathbb{G}_{ij}(\mathbf{r}) = \frac{k}{6\pi} \delta_{ij} - \frac{k^3 r^2}{30\pi} \left[\delta_{ij} - \frac{1}{2} \frac{r_i r_j}{r^2} \right] + \frac{k^5 r^4}{560\pi} \left[\delta_{ij} - \frac{2}{3} \frac{r_i r_j}{r^2} \right] + O(r^6) \quad (25)$$

The discretized versions of equations (24) read, upon accounting for simplifying symmetries,

$$P^{\text{JJ}} = -kZ_0 \sum'_{\beta \geq \alpha} \left(\text{Re } j_{\alpha}^* j_{\beta} \right) \left\langle \mathbf{b}_{\alpha} \left| \text{Im } \mathbb{G} \right| \mathbf{b}_{\beta} \right\rangle \quad (26a)$$

$$F_i^{\text{JJ}} = -\frac{Z_0}{c} \sum_{\beta > \alpha} \left(\text{Im } j_{\alpha}^* j_{\beta} \right) \left\langle \mathbf{b}_{\alpha} \left| \text{Im } \partial_i \mathbb{G} \right| \mathbf{b}_{\beta} \right\rangle \quad (26b)$$

$$\mathcal{T}_i^{\text{JJ}} = -\frac{Z_0}{c} \sum_{\beta > \alpha} \left(\text{Im } j_{\alpha}^* j_{\beta} \right) \varepsilon_{ijk} \left\langle b_{\alpha j} \left(\text{Im } \mathbb{G}_{k\ell} \right) b_{\beta \ell} \right\rangle \quad (26c)$$

where the primed sum in (26) indicates that summands with $\alpha = \beta$ are to be weighted by $\frac{1}{2}$. The matrix elements in (26) involve nonsingular 6-dimensional integrals which are evaluated in BUFF-EM by simple numerical cubature.

Multipole expansion of PFT quantities

Inserting the short-distance expansion (25) into (24a) and keeping only terms of lowest order in k yields

$$P^{\text{JJ}} \approx -\frac{k^2 Z_0}{12\pi} \underbrace{\int J_i^*(\mathbf{x}) d\mathbf{x}}_{i\omega p_i^*} \underbrace{\int J_i(\mathbf{x}') d\mathbf{x}'}_{-i\omega p_i} \quad (27)$$

$$= -\frac{c^2 k^4 Z_0}{12\pi} |\mathbf{p}|^2 \quad (28)$$

where $\mathbf{p} = -\frac{1}{i\omega} \int \mathbf{J} dV$ is the dipole moment of the induced current distribution. Note that (28) is minus the usual expression for the total power radiated by a point dipole radiator.

Proceeding similarly for the force, from (25) one first finds

$$\partial_i G_{jk} = \frac{k^3}{60\pi} \left(r_j \delta_{ik} + r_k \delta_{ij} - 4r_i \delta_{jk} \right) + O(k^5)$$

whereupon (24b) reads

$$\begin{aligned} F_i^{\text{JJ}} &\approx -\frac{k^3 Z_0}{120\pi c} \text{Im} \int \left\{ J_j^*(\mathbf{x})(\mathbf{x} - \mathbf{x}')_j J_i(\mathbf{x}') + J_i^*(\mathbf{x})(\mathbf{x} - \mathbf{x}')_j J_j(\mathbf{x}') \right. \\ &\quad \left. - 4J_j^*(\mathbf{x})(\mathbf{x} - \mathbf{x}')_i J_j(\mathbf{x}') \right\} d\mathbf{x} d\mathbf{x}' \\ &= -\frac{k^3 Z_0}{60\pi c} \text{Im} \left[\mathcal{M}_{jj}^* \mathcal{M}_i + \mathcal{M}_{ij}^* \mathcal{M}_j - 4\mathcal{M}_{ji}^* \mathcal{M}_j \right] \end{aligned} \quad (29)$$

where I defined

$$\mathcal{M}_i \equiv \int J_i(\mathbf{x}) dV, \quad \mathcal{M}_{ij} \equiv \int J_i(\mathbf{x}) x_j dV.$$

The quantity \mathcal{M}_i is related to the electric dipole moment \mathbf{p} by

$$\mathbf{p}_i = -\frac{1}{i\omega} \mathcal{M}_i.$$

On the other hand, \mathcal{M}_{ij} is related to the magnetic dipole and electric quadrupole moments; basically, the magnetic dipole moment \mathbf{m} is the antisymmetric part of \mathcal{M}_{ij} , while the electric quadrupole moment Q_{ij} is the symmetric part. From standard definitions in e.g. Jackson one finds

$$\begin{aligned} m_i &= \frac{1}{2} \varepsilon_{ijk} \int x_j J_k(\mathbf{x}) dV \\ &= \frac{1}{2} \varepsilon_{ijk} \mathcal{M}_{ji} \\ &= -\frac{1}{2} \varepsilon_{ijk} \mathcal{M}_{ij} \\ Q_{ij} &= -\frac{1}{i\omega} \int \left\{ 3J_i x_j + 3x_i J_j - 2J_k x_k \delta_{ij} \right\} dV \\ &= -\frac{1}{i\omega} \left[3\mathcal{M}_{ij} + 3\mathcal{M}_{ji} - 2\delta_{ij} \mathcal{M}_{kk} \right]. \end{aligned}$$

Using these definitions in (30) and performing some algebra, one finds the lowest-order terms in the multipole expansion of the self-force:

$$F_i^{\text{JJ}} \approx \frac{k^4 Z_0}{12\pi} \text{Re}(\mathbf{m}^* \times \mathbf{p})_i + \frac{ck^5 Z_0}{120\pi} \text{Im}(\mathbf{Q}^* \mathbf{p})_i \quad (30)$$

The quantity in the second term involves the matrix-vector product of the 3×3 matrix \mathbf{Q}^* with the 3-vector \mathbf{p} .

Finally, for the torque, inserting (25) into (24b) yields

$$\mathcal{T}_i^{\text{JJ}} \approx -\frac{kZ_0}{12\pi c} \varepsilon_{ijk} \text{Im} \left\{ \left[\int \mathbf{J}_j^* dV \right] \left[\int \mathbf{J}_k dV \right] \right\} \quad (31)$$

$$= -\frac{ck^3 Z_0}{6\pi} \left(\text{Re } \mathbf{p} \times \text{Im } \mathbf{p} \right)_i. \quad (32)$$

2.3 OPFT

From equation (??), the total field \mathbf{E} may be expressed in terms of \mathbf{J} according to

$$\mathbf{E} = -ikZ_0 \mathbb{V}^{-1} \mathbf{J}. \quad (33)$$

Using this in equation (20) yields

$$P = \frac{kZ_0}{2} \text{Im} \int \mathbf{J}^* \cdot \mathbb{V}^{-1} \cdot \mathbf{J} dV \quad (34a)$$

$$F_i = -\frac{Z_0}{2c} \text{Re} \int \mathbf{J}^* \cdot \partial_i [\mathbb{V}^{-1} \cdot \mathbf{J}] dV \quad (34b)$$

$$\mathcal{T}_i = -\frac{Z_0}{2c} \text{Re} \int \mathbf{J}^* \times [\mathbb{V}^{-1} \cdot \mathbf{J}] dV \quad (34c)$$

The discretized versions of these formulas involve only overlap integrals between SWG basis functions, which vanish unless the pairs of basis functions share one or more common tetrahedra. Thus they amount to vector-matrix-vector products with highly sparse matrices and are thus, in principle, the most computationally efficient technique for computing PFTs; However, equation (33) is only approximately satisfied in a numerical solver, so

I refer to (34) as the “overlap PFT” (OPFT) formulas.

3 FVC approach to fluctuation-induced phenomena

In this section I consider a collection of one or more material bodies $\{\mathcal{B}_n\}$, at various temperatures $\{T_n\}$ and embedded in an environment at temperature T_{env} , and derive a sequence of concise matrix-trace formulas expressing thermally and quantum-mechanically averaged heat-transfer rates, forces, and torques on the bodies in terms of the \mathbf{T} and \mathbf{G} matrices discussed in the previous section. Because the resulting energy and momentum transfers may be viewed as arising from fluctuations in volume currents in the bodies, I term this the “fluctuating volume-current” (FVC) approach to fluctuation physics.

The derivation proceeds in two steps.

1. I first consider a fixed, deterministic volume electric current distribution $\mathbf{J}^{\text{F}}(\mathbf{x})$ —confined to the interiors of our material bodies but otherwise arbitrary—and use the VIE formalism of the previous section to derive compact expressions for the rates of energy and momentum absorption by the bodies. These expressions will be quadratic (bilinear) functions of \mathbf{J}^{F} . (The F superscript stands for “free”; it distinguishes the fixed, externally-imposed current \mathbf{J}^{F} from the *induced* current \mathbf{J}^{I} to which it gives rise.)
2. I then average over thermal and quantum-mechanical fluctuations of \mathbf{J}^{F} to derive temperature-dependent mean heat-transfer rates and forces on the bodies.

In what follows I will go back and forth somewhat freely between continuous operator/field notation [involving symbols like \mathbb{G} and $\mathbf{E}(\mathbf{x})$] and discretized matrix/vector notation (involving symbols like \mathbf{G} and \mathbf{e}). For a precise dictionary of the correspondence, see Appendix A.

3.1 Energy and momentum transfer from volume-current bilinears

Consider a collection of material bodies $\{\mathcal{B}_n\}$ and a fixed, deterministic volume current distribution $\mathbf{J}^{\text{F}}(\mathbf{x})$ that is nonzero only inside the bodies. (We work at a fixed frequency ω with all fields and currents varying in time like $e^{-i\omega t}$.) In this section we derive formulas expressing time-average rates of energy and momentum absorption by the bodies as bilinear functions of \mathbf{J}^{F} .

Induced currents from free currents

The free current distribution $\mathbf{J}^{\text{F}}(\mathbf{x})$ excites an induced current distribution $\mathbf{J}^{\text{I}}(\mathbf{x})$ which we can determine using the VIE techniques of the previous section. Indeed, taking \mathbf{J}^{F} as the source of the incident field in a scattering problem, we

have

$$\mathbf{E}^{\text{inc}}(\mathbf{r}) = ikZ_0\mathbb{G} \star \mathbf{J}^{\text{F}} \quad (35)$$

and the RHS vector of the discretized VIE system, equation (13), reads

$$\mathbf{v} = -\mathbf{G}\mathbf{j}^{\text{F}} \quad (36)$$

where, for a geometry consisting of N bodies, the vectors and matrices have an N -fold block structure:

$$\mathbf{v} = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_N \end{pmatrix}, \quad \mathbf{G} = \begin{pmatrix} \mathbf{G}_{11} & \mathbf{G}_{12} & \cdots & \mathbf{G}_{1N} \\ \mathbf{G}_{21} & \mathbf{G}_{22} & \cdots & \mathbf{G}_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{G}_{N1} & \mathbf{G}_{N2} & \cdots & \mathbf{G}_{NN} \end{pmatrix}, \quad \mathbf{j}^{\text{F}} = \begin{pmatrix} \mathbf{j}_1^{\text{F}} \\ \mathbf{j}_2^{\text{F}} \\ \vdots \\ \mathbf{j}_N^{\text{F}} \end{pmatrix}.$$

In particular, the n th subblock of \mathbf{j}^{F} is the projection of the free current distribution⁴ in body \mathcal{B}_n , $\mathbf{J}_n^{\text{F}}(\mathbf{x})$, onto the subset of basis functions whose support lies in body n :

$$j_{n\alpha}^{\text{F}} = \int \mathbf{b}_{n\alpha}(\mathbf{r}) \cdot \mathbf{J}_n^{\text{F}}(\mathbf{r}) d\mathbf{r}. \quad (37)$$

Now taking equation (36) to be the RHS of the VIE scattering problem (13), we obtain an expression for the induced currents in terms of the free currents,

$$\mathbf{M}\mathbf{j}^{\text{I}} = -\mathbf{G}\mathbf{j}^{\text{F}} \quad (38)$$

or

$$\mathbf{j}^{\text{I}} = -\mathbf{W}\mathbf{G}\mathbf{j}^{\text{F}} \quad (39)$$

where $\mathbf{W} = \mathbf{M}^{-1}$ is the inverse of the VIE matrix defined by (13).

The *total* current is

$$\begin{aligned} \mathbf{j} &= \mathbf{j}^{\text{F}} + \mathbf{j}^{\text{I}} \\ &= [\mathbf{1} - \mathbf{W}\mathbf{G}]\mathbf{j}^{\text{F}}. \end{aligned} \quad (40)$$

Fields from free currents

The \mathbf{E} -field at an arbitrary point in space (either inside or outside a body) is then simply the sum of contributions from fixed and induced currents:

$$\mathbf{E} = ikZ_0\mathbb{G} \star (\mathbf{J}^{\text{F}} + \mathbf{J}^{\text{I}}) \quad (41)$$

⁴Note that $\mathbf{J}_n^{\text{F}}(\mathbf{x})$ is just the restriction of \mathbf{J}^{F} to the interior of \mathcal{B}_n .

or, in discretized form (Appendix A),

$$\begin{aligned}\mathbf{e} &= ikZ_0 \mathbf{G}(\mathbf{j}^F + \mathbf{j}^I) \\ &= ikZ_0 \mathbf{G}(\mathbf{1} - \mathbf{W}\mathbf{G})\mathbf{j}^F\end{aligned}\tag{42}$$

where in going to the last line I used (39).

In what follows I will also need the quantity $\partial_i \mathbf{E}(\mathbf{r})$, i.e. the derivative of \mathbf{E} with respect to the evaluation point. Differentiating both sides of (41), we see that the derivative operates on the first argument of $\mathbb{G}(\mathbf{r}, \mathbf{r}')$ and leaves everything else on the RHS untouched; thus we find simply

$$\partial_i \mathbf{e} = ikZ_0 \left[\partial_i \mathbf{G} \right] (\mathbf{j}^F + \mathbf{j}^I) \tag{43}$$

where the matrix elements of the quantity in square brackets are

$$\left[\partial_i \mathbf{G} \right]_{\alpha\beta} = \int \int \mathbf{b}_\alpha(\mathbf{r}) \left[\frac{\partial}{\partial \mathbf{r}_i} \mathbb{G}(\mathbf{r}, \mathbf{r}') \right] \mathbf{b}_\beta(\mathbf{r}') d\mathbf{r} d\mathbf{r}'.$$

Power absorption

The time-average rate at which body \mathcal{B}_n absorbs power from the source distribution \mathbf{J}^F is obtained by integrating the quantity $\frac{1}{2} \text{Re } \mathbf{J}^* \cdot \mathbf{E}$ over the interior of \mathcal{B}_n ; here \mathbf{J} is the *total* current in \mathcal{B}_n , consisting of both free and induced contributions:

$$\begin{aligned}P_n(\omega) &= \frac{1}{2} \text{Re} \int_{\mathcal{B}_n} \mathbf{J}^*(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r} \\ &= \frac{1}{2} \text{Re } \mathbf{j}_n^\dagger \cdot \mathbf{e}_n\end{aligned}\tag{44}$$

where we used equation (60). The n subscript on vectors picks out the subblock corresponding to body n ; using the projection matrices \mathbf{P}_n defined by (??), we could equivalently write this in the form

$$= \frac{1}{2} \text{Re } \mathbf{j}^\dagger \mathbf{P}_n \mathbf{e}$$

Now insert equations (40) and (42):

$$\begin{aligned}&= \frac{1}{2} \text{Re} \left\{ ikZ_0 \mathbf{j}^{F\dagger} \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right] \mathbf{P}_n \mathbf{G} \left[\mathbf{1} - \mathbf{W}\mathbf{G} \right] \mathbf{j}^F \right\} \\ &= -\frac{kZ_0}{2} \text{Im Tr} \left\{ \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right] \mathbf{P}_n \mathbf{G} \left[\mathbf{1} - \mathbf{W}\mathbf{G} \right] \left[\mathbf{j}^F \mathbf{j}^{F\dagger} \right] \right\}.\end{aligned}\tag{45}$$

As advertised, this expression depends quadratically on \mathbf{J}^F , as witness the appearance of the outer matrix product $\mathbf{j}^F \mathbf{j}^{F\dagger}$.

Momentum absorption

The time-average rate at which body \mathcal{B}_n absorbs i -directed *momentum* from the source distribution \mathbf{J}^F —that is, the i -directed force on the body—may be expressed as a volume-integral expression very similar to that of (44) but with (i) “Re” replaced by “Im,” (ii) \mathbf{E} replaced by $\partial_i \mathbf{E}$, and (iii) an extra factor of ω in the denominator:

$$T_n(\omega) = \frac{1}{2\omega} \text{Im} \int_{\mathcal{B}_n} \mathbf{J}^*(\mathbf{r}) \cdot \partial_i \mathbf{E}(\mathbf{r}) d\mathbf{r}.$$

(This expression is quoted in Ref. ?; I also provide a quick derivation in Appendix B.) Going over to the discrete world, we have

$$= \frac{1}{2\omega} \text{Im} \mathbf{j}^\dagger \mathbf{P}_n(\partial_i \mathbf{e})$$

Insert (40) and (42):

$$\begin{aligned} &= \frac{1}{2\omega} \text{Im} \left\{ ikZ_0 \mathbf{j}^{F\dagger} \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right] \mathbf{P}_n(\partial_i \mathbf{G}) \left[\mathbf{1} - \mathbf{W} \mathbf{G} \right] \mathbf{j}^F \right\} \\ &= \frac{kZ_0}{2\omega} \text{Re} \text{Tr} \left\{ \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right] \mathbf{P}_n(\partial_i \mathbf{G}) \left[\mathbf{1} - \mathbf{W} \mathbf{G} \right] \mathbf{j}^F \mathbf{j}^{F\dagger} \right\} \end{aligned}$$

3.2 Statistical averages of volume-current bilinears

The classical, deterministic expressions derived above for time-average quantities Q (where Q is a power, force, or torque) all take the form

$$Q(\omega) \propto \text{Tr} \left\{ \mathbf{Q}(\omega) \cdot (\mathbf{j}^F \mathbf{j}^{F\dagger}) \right\} \quad (46)$$

where $\mathbf{Q}(\omega)$ is a frequency-dependent matrix. The statistical *average* of such quantities is performed by averaging over all possible free current distributions $\mathbf{J}^F(\mathbf{r})$, which amounts to computing the statistical average of the matrix $\mathbf{j}^F \mathbf{j}^{F\dagger}$:

$$\langle Q(\omega) \rangle \propto \text{Tr} \left\{ \mathbf{Q}(\omega) \cdot \langle \mathbf{j}^F \mathbf{j}^{F\dagger} \rangle_\omega \right\}.$$

This quantity represents just the contribution of frequency- ω fluctuations to the average power, force or torque (PFT); the *total* PFT is given by integrating over all frequencies, $Q = \int_0^\infty \langle Q(\omega) \rangle d\omega$.

The elements of the matrix $\mathbf{j}^F \mathbf{j}^{F\dagger}$ are

$$\left[\mathbf{j}^F \mathbf{j}^{F\dagger} \right]_{\alpha\beta} = \int \int b_{\alpha i}(\mathbf{r}) J_i^F(\mathbf{r}) J_j^{F*}(\mathbf{r}') b_{\beta j}(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \quad (47)$$

Now perform the statistical average. The only quantities on the RHS that experience averaging are the factors of J in the integrand:

$$\langle \mathbf{j}^F \mathbf{j}^{F\dagger} \rangle_{\alpha\beta} = \int \int b_{\alpha i}(\mathbf{r}) \langle J_i^F(\mathbf{r}) J_j^{F*}(\mathbf{r}') \rangle b_{\beta j}(\mathbf{r}') d\mathbf{r} d\mathbf{r}'. \quad (48)$$

We now make use of the fluctuation-dissipation theorem in the form of the Rytov correlation function,⁵

$$\langle J_i^{\mathbf{F}}(\mathbf{r}) J_j^{\mathbf{F}*}(\mathbf{r}') \rangle = \frac{2k}{\pi Z_0} \Theta(T) \delta(\mathbf{r} - \mathbf{r}') \text{Im } \epsilon_{ij}(\mathbf{r}). \quad (49)$$

Inserting this into (48), we find

$$\langle \mathbf{j}^{\mathbf{F}} \mathbf{j}^{\mathbf{F}\dagger} \rangle_{\alpha\beta} = \frac{2k}{\pi Z_0} \int \Theta[T(\mathbf{r})] b_{\alpha i}(\mathbf{r}) [\text{Im } \epsilon_{ij}(\mathbf{r})] b_{\beta j}(\mathbf{r}) d\mathbf{r}.$$

For the situation we consider here—involving N material bodies, throughout the interior of which the temperature is constant—the full matrix takes the form

$$\langle \mathbf{j}^{\mathbf{F}} \mathbf{j}^{\mathbf{F}\dagger} \rangle = \frac{2k}{\pi Z_0} \begin{pmatrix} \Theta(T_1) \boldsymbol{\Sigma}_1 & 0 & \cdots & 0 \\ 0 & \Theta(T_2) \boldsymbol{\Sigma}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \Theta(T_N) \boldsymbol{\Sigma}_N \end{pmatrix} \quad (50)$$

where $\boldsymbol{\Sigma}_n$ is just the matrix of basis-function overlaps with the imaginary part of the relative dielectric function for the n th body, i.e.

$$[\boldsymbol{\Sigma}_n]_{\alpha\beta} = \int b_{\alpha i}(\mathbf{r}) [\text{Im } \epsilon_n(\mathbf{r})]_{ij} b_{\beta j}(\mathbf{r}) d\mathbf{r}. \quad (51)$$

Here ϵ_n is the dielectric tensor for body \mathcal{B}_n . For a basis of localized functions, this matrix is highly sparse (for the SWG basis discussed below it contains just 7 nonzero elements per row). Moreover, numerical evaluation of the matrix elements of $\boldsymbol{\Sigma}$ is essentially costless, particularly compared to the cost of computing matrix elements of \mathbb{G} ; it involves just a single three-dimensional numerical cubature and may be carried out simultaneously with computation of the matrix elements of the \mathbb{A} operator needed to assemble the VIE matrix.

Inserting (50) into ...

The total heat transfer to, and the total i -directed force and torque on, a destination body \mathcal{B}_d are given by

$$H_d = \int_0^\infty \mathcal{H}_d(\omega) d\Omega, \quad F_{di} = \int_0^\infty \mathcal{F}_{di}(\omega) d\Omega, \quad T_{di} = \int_0^\infty \mathcal{T}_{di}(\omega) d\Omega$$

where the contribution of each frequency ω may be written as the sum of equilibrium contributions plus non-equilibrium contributions from all other bodies

⁵How do the *units* of this equation work? To answer this question, I think it's easiest to multiply both sides by Z_0 to bring a factor of impedance to the LHS. Since J is the Fourier transform of a volume current density, it has units of $\frac{\text{current}}{\text{length}^2} \cdot \frac{1}{\text{frequency}}$. and the LHS then has units of $\frac{\text{impedance} \cdot \text{current}^2 \cdot \text{time}^2}{\text{length}^4} = \frac{\text{energy} \cdot \text{time}}{\text{length}^4}$ where we used that impedance \cdot current² = power (for example, recall the $\sim I^2 R$ dependence of Joule heating) and power \cdot time = energy. Meanwhile, on the RHS, the dimensionful factors remaining after multiplying by Z_0 are Θ (energy) and $k\delta(\mathbf{r}-\mathbf{r}')$ (length⁻⁴) so everything works out modulo a factor of inverse frequency on the RHS, which I think must be coming from a factor like $\delta(\omega - \omega')$ that is implicit somewhere.

acting as sources, with each contribution expressed as a thermal/statistical factor times a generalized flux:

$$\begin{aligned}\mathcal{H}_d(\omega) &= \sum_s \left[\Theta(\omega, T_s) - \Theta(\omega, T_{\text{env}}) \right] \Phi_{s \rightarrow d}^{\text{energy}}(\omega) \\ \mathcal{F}_{di}(\omega) &= F_{di}^{\text{eq}}(T_{\text{env}}) + \sum_s \left[\Theta(\omega, T_s) - \Theta(\omega, T_{\text{env}}) \right] \Phi_{s \rightarrow d}^{\text{lin mom}}(\omega) \\ \mathcal{T}_{di}(\omega) &= T_{di}^{\text{eq}}(T_{\text{env}}) + \sum_s \left[\Theta(\omega, T_s) - \Theta(\omega, T_{\text{env}}) \right] \Phi_{s \rightarrow d}^{\text{ang mom}}(\omega)\end{aligned}$$

(For the heat transfer there is no equilibrium contribution, as there is no net exchange of energy between equal-temperature bodies. There *is* a net transfer of *momentum*, whereupon the force and torque expressions do contain equilibrium contributions.)

$$\begin{aligned}\Phi_{s \rightarrow d}^{\text{energy}}(\omega) &= -\frac{k^2}{\pi} \text{Im Tr} \left\{ \left[\mathbf{G}(\mathbf{1} - \mathbf{W}\mathbf{G}) \right]_{ds} \boldsymbol{\Sigma}_s \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right]_{sd} \right\} \\ \Phi_{s \rightarrow d}^{\text{lin mom}}(\omega) &= \frac{k^2}{\pi\omega} \text{Re Tr} \left\{ \left[(\partial_i \mathbf{G})(\mathbf{1} - \mathbf{W}\mathbf{G}) \right]_{ds} \boldsymbol{\Sigma}_s \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right]_{sd} \right\} \\ \Phi_{s \rightarrow d}^{\text{ang mom}}(\omega) &= \frac{k^2}{\pi\omega} \text{Re Tr} \left\{ \left[(\partial_\theta \mathbf{G})(\mathbf{1} - \mathbf{W}\mathbf{G}) \right]_{ds} \boldsymbol{\Sigma}_s \left[\mathbf{1} - \mathbf{G}^\dagger \mathbf{W}^\dagger \right]_{sd} \right\}\end{aligned}$$

The trace we compute in these expressions has the form

$$\begin{aligned}\text{Tr} \left[(\mathbf{X}\mathbf{A})_{ds} \boldsymbol{\Sigma}_s (\mathbf{A}^\dagger)_{sd} \right] &= \sum_{ijk} (\mathbf{X}\mathbf{A})_{ds,ij} \Sigma_{s,jk} \left[\mathbf{A}_{sd}^\dagger \right]_{ki} \\ &= \sum_{ijk} (\mathbf{X}\mathbf{A})_{di;s j} \Sigma_{s,jk} A_{di;sk}^*\end{aligned}$$

where

$$\mathbf{A} = (\mathbf{1} - \mathbf{W}\mathbf{G})$$

and

$$\mathbf{X} = \{\mathbf{G}, \partial_i \mathbf{G}, \partial_\theta \mathbf{G}\}.$$

4 SWG Basis Functions

SWG basis functions are the three-dimensional analog of RWG basis functions. They are defined on pairs of adjacent tetrahedra:

$$\mathbf{b}_\alpha(\mathbf{x}) = \begin{cases} +\frac{A_\alpha}{3V_\alpha^+}(\mathbf{x} - \mathbf{Q}_\alpha^+), & \mathbf{x} \in \mathcal{P}_\alpha^+ \\ -\frac{A_\alpha}{3V_\alpha^-}(\mathbf{x} - \mathbf{Q}_\alpha^-), & \mathbf{x} \in \mathcal{P}_\alpha^- \end{cases}$$

where \mathcal{P}_α^\pm are the two tetrahedra associated with basis function α , V_α^\pm are their volumes, \mathbf{Q}_α^\pm are the source/sink vertices, and A_α is the area of the triangular face shared by \mathcal{P}_α^\pm . (I denote tetrahedra by \mathcal{P} , which stands for “pyramid,” to avoid confusion with the symbol \mathcal{T} , which stands for “triangle” in my memos on RWG basis functions.)

The divergence of the SWG basis function is

$$\nabla \cdot \mathbf{b}_\alpha(\mathbf{x}) = \pm \frac{A_\alpha}{V_\alpha^\pm}, \quad \mathbf{x} \in \mathcal{P}_\alpha^\pm.$$

5 SWG Matrix Elements of the \mathbb{G} operator

5.1 Distant case: Volume-integral method

The \mathbb{G} -matrix element between two SWG basis functions is

$$\langle \mathbf{b}_\alpha | \mathbb{G} | \mathbf{b}_\beta \rangle = \int_{\sup \mathbf{b}_\alpha} d\mathbf{x}_\alpha \int_{\sup \mathbf{b}_\beta} d\mathbf{x}_\beta b_{\alpha i}(\mathbf{x}_\alpha) \mathbb{G}_{ij}(\mathbf{R}_0 + \bar{\mathbf{x}}_\alpha - \bar{\mathbf{x}}_\beta) b_{\beta j}(\mathbf{x}_\beta) \quad (52)$$

where

$$\bar{\mathbf{x}}_\alpha \equiv \mathbf{x}_\alpha - \mathbf{x}_{\alpha 0}, \quad \bar{\mathbf{x}}_\beta \equiv \mathbf{x}_\beta - \mathbf{x}_{\beta 0}, \quad \mathbf{R}_0 = \mathbf{x}_{\alpha 0} - \mathbf{x}_{\beta 0}$$

and $\mathbf{x}_{\alpha 0}, \mathbf{x}_{\beta 0}$ are the centroids of the basis functions.

When the two basis functions are well separated (i.e. $|\mathbf{R}_0| \gg |\bar{\mathbf{x}}_\alpha|, |\bar{\mathbf{x}}_\beta|$), we may compute (53) to sufficient accuracy using a volume-integral method:

$$\langle \mathbf{b}_\alpha | \mathbb{G} | \mathbf{b}_\beta \rangle = \sum \pm \int_{\mathcal{P}_\alpha^\pm} d\mathbf{x}_\alpha \int_{\mathcal{P}_\beta^\pm} d\mathbf{x}_\beta \left[\mathbf{b}_\alpha \cdot \mathbf{b}_\beta - \frac{9}{k^2} \right] \Phi(|\mathbf{R}_0 + \bar{\mathbf{x}}_\alpha - \bar{\mathbf{x}}_\beta|) \quad (53)$$

where $\Phi(r) = \frac{e^{ik|r|}}{4\pi|r|}$. in which the 6-dimensional integration over each of the four pairs of tetrahedra is carried out by simple low-order numerical cubature, as discussed in Appendix D.

5.2 Nearby case: Desingularization

When the two basis functions have one or more common vertices, the integral (53) is singular. In this case, BUFF-EM follows the standard desingularization strategy: the first few singular terms in the small- r expansion of $\Phi(r)$ are subtracted off, leaving **(a)** a desingularized version of (53) which is evaluated by low-order cubature, and **(b)** a collection of singular but frequency-independent integrals.

All singular integrals computed by BUFF-EM for an object described by a given tetrahedral mesh are automatically stored in a binary data file named `Mesh.cache`, (where `Mesh.vmesh` is the name of the file from which the mesh was read). The BUFF-EM core library will automatically look for this file when it needs singular integrals; if the file is not found, the singular integrals are computed on the fly and automatically stored in the file `Mesh.cache`. (Thus, the caching of singular integrals is more transparent to the user than is the case in SCUFF-EM.)

5.3 Evaluation of singular integrals: Taylor-Duffy Method

Singular 6-dimensional integrals in BUFF-EM are evaluated by a complicated technique obtained by generalizing the Taylor-Duffy method for triangles to the case of tetrahedra.

A Dictionary of the operator–matrix correspondence

Infinite-dimensional position-space basis $\iff N_B$ -dimensional basis of discrete expansion functions $\{\mathbf{b}_\alpha(\mathbf{x})\}$.

Notation

- We use blackboard-bold symbols for position-space operators: \mathbb{G}, \mathbb{T} .
- We use upper-case bold letters for discrete-basis matrices: $\mathbf{T}, \mathbf{G}, \mathbf{W}$. The elements of these matrices are, e.g.

$$G_{\alpha\beta} \equiv \int \int \mathbf{b}_\alpha(\mathbf{r}) \mathbb{G}(\mathbf{r}, \mathbf{r}') \mathbf{b}_\beta(\mathbf{r}') d\mathbf{r} d\mathbf{r}'$$

- (At the risk of confusion with the previous item) We use upper-case bold letters for position-space vectors: $\mathbf{J}(\mathbf{x}), \mathbf{E}(\mathbf{x})$.
- We use lower-case bold letters for discrete-basis vectors: \mathbf{j}, \mathbf{e} . The elements of these vectors are e.g.

$$e_\alpha \equiv \int \mathbf{b}_\alpha(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r}.$$

Continuous	Discrete
$\mathbb{G}(\mathbf{r}, \mathbf{r}')$	\mathbf{G} matrix, with elements $U_{\alpha\beta} = \int \int \mathbf{b}_\alpha(\mathbf{r}) \mathbb{G}(\mathbf{r}, \mathbf{r}') \mathbf{b}_\beta(\mathbf{r}') d\mathbf{r} d\mathbf{r}'$
$\mathbf{E}(\mathbf{r})$	\mathbf{e} vector, with elements $e_\alpha = \int \mathbf{b}_\alpha(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r}$

Approximate completeness relation

One way to conceptualize the transition from the continuous to the discrete is to suppose that the basis functions $\{\mathbf{b}_\alpha(\mathbf{x})\}$ satisfy an approximate completeness relation of the form

$$\sum_{\alpha} b_{\alpha i}(\mathbf{r}) b_{\alpha j}(\mathbf{r}') \approx \delta_{ij} \delta(\mathbf{r} - \mathbf{r}') \quad (54a)$$

or

$$\sum_{\alpha} \int b_{\alpha i}(\mathbf{r}) b_{\alpha j}(\mathbf{r}') d\mathbf{r}' = \delta_{ij} \quad (54b)$$

Convolutions becomes matrix-vector products

For example, consider the continuous version of the equation relating the total current to the total field:

$$\mathbf{E} = ikZ_0 \mathbb{G} \star \mathbf{J} \quad (55)$$

or

$$E_i(\mathbf{r}) = ikZ_0 \int \mathbb{G}_{ij}(\mathbf{r}, \mathbf{r}') J_j(\mathbf{r}') d\mathbf{r}'. \quad (56)$$

Insert (54a) [in the form $\sum b_{\beta j}(\mathbf{r}') b_{\beta k}(\mathbf{r}'') = \delta_{jk} \delta(\mathbf{r}' - \mathbf{r}'')$] between \mathbb{G} and \mathbf{J} on the RHS:

$$E_i(\mathbf{r}) = ikZ_0 \sum_{\beta} \left[\int \mathbb{G}_{ij}(\mathbf{r}, \mathbf{r}') b_{\beta j}(\mathbf{r}') d\mathbf{r}' \right] \underbrace{\left[\int b_{\beta k}(\mathbf{r}'') J_k(\mathbf{r}'') d\mathbf{r}'' \right]}_{\mathbf{j}_{\beta}} \quad (57)$$

As it stands this equation exists in a sort of hybrid continuous-discrete form. Now multiply both sides by $\mathbf{b}_{\alpha}(\mathbf{r})$ and integrate over \mathbf{r} to find

$$e_{\alpha} = ikZ_0 G_{\alpha\beta} j_{\beta} \quad (58)$$

or

$$\mathbf{e} = ikZ_0 \mathbf{G} \mathbf{j}. \quad (59)$$

Volume integrals become dot products

Consider, for example, the integral

$$\langle \mathbf{J} \cdot \mathbf{E} \rangle_{\mathcal{B}_n} \equiv \int_{\mathcal{B}_n} \mathbf{J}^*(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}) d\mathbf{r}$$

Rewrite this in the seemingly pedantic form

$$= \int_{\mathcal{B}_n} \int_{\mathcal{B}_n} J_i^*(\mathbf{r}) \delta_{ij} \delta(\mathbf{r} - \mathbf{r}') E_j(\mathbf{r}') d\mathbf{r} d\mathbf{r}'$$

Now insert (54a):

$$\begin{aligned} &= \int_{\mathcal{B}_n} \int_{\mathcal{B}_n} J_i^*(\mathbf{r}) \left[\sum_{\alpha} b_{\alpha i}(\mathbf{r}) b_{\alpha j}(\mathbf{r}') \right] E_j(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \\ &= \sum_{\alpha} \underbrace{\left[\int_{\mathcal{B}_n} b_{\alpha i}(\mathbf{r}) J_i^*(\mathbf{r}) d\mathbf{r} \right]}_{j_{n\alpha}^*} \underbrace{\left[\int_{\mathcal{B}_n} b_{\alpha j}(\mathbf{r}') E_j(\mathbf{r}') d\mathbf{r}' \right]}_{e_{n\alpha}} = \mathbf{j}_n^{\dagger} \mathbf{e}_n. \quad (60) \end{aligned}$$

B Derivation of volume integrals for the force and torque

Consider a body in which exists both a (deterministic) total volume current distribution $\mathbf{J}(\mathbf{x})$ and electric and magnetic fields $\{\mathbf{E}, \mathbf{H}\}(\mathbf{x})$. The time-average force experienced by the currents in an infinitesimal volume dV is

$$d\mathbf{F} = \frac{1}{2} \text{Re} \left[\rho^* \mathbf{E} + \mu_0 \mathbf{J}^* \times \mathbf{H} \right] dV$$

Use $\rho = \frac{1}{i\omega} (\nabla \cdot \mathbf{J})$ and $\mathbf{H} = \frac{1}{i\omega\mu_0} \nabla \times \mathbf{E}$:

$$= \frac{1}{2} \text{Re} \left\{ \frac{1}{i\omega} \left[-(\nabla \cdot \mathbf{J}^*) \mathbf{E} + \mathbf{J}^* \times (\nabla \times \mathbf{E}) \right] \right\} dV$$

or

$$\begin{aligned} dF_i &= -\frac{1}{2\omega} \text{Im} \left[(\partial_j J_j^*) E_i - \underbrace{\varepsilon_{ijk} \varepsilon_{klm}}_{\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}} J_j^* \partial_l E_m \right] dV \\ &= -\frac{1}{2\omega} \text{Im} \left[(\partial_j J_j^*) E_i - J_j^* \partial_i E_j + J_j^* \partial_j E_i \right] dV. \end{aligned} \quad (61)$$

The total force is given by integrating over the volume:

$$F_i = -\frac{1}{2\omega} \text{Im} \int_{\mathcal{B}_n} \left[(\partial_j J_j^*) E_i - J_j^* \partial_i E_j + J_j^* \partial_j E_i \right] dV \quad (62)$$

The first and third terms here together read

$$\int \partial_j (J_j^* E_i) dV = \int \nabla \cdot (E_i \mathbf{J}^*) dV = \oint E_i \mathbf{J}^* \cdot d\mathbf{A} = 0 \quad (63)$$

because $\mathbf{J} \cdot \hat{\mathbf{n}} = 0$ at the surface of the object (no current flows from the body into space). Thus only the middle term in (62) is nonvanishing, and we find simply

$$F_i = \frac{1}{2\omega} \text{Im} \int_{\mathcal{B}_n} J_j^* \partial_i E_j dV = \frac{1}{2\omega} \text{Im} \int_{\mathcal{B}_n} \mathbf{J}^* \cdot \partial_i \mathbf{E} dV. \quad (64)$$

Torque

The contribution of currents in dV to the *torque* about an origin \mathbf{r}_0 is given by

$$d\mathcal{T} = (\mathbf{r} - \mathbf{r}_0) \times d\mathbf{F}$$

or, in components,

$$d\mathcal{T}_i = \varepsilon_{ijk} (\mathbf{r} - \mathbf{r}_0)_j dF_k.$$

Insert (61):

$$= -\frac{1}{2\omega} \text{Im} \left\{ \varepsilon_{ijk} (\mathbf{r} - \mathbf{r}_0)_j \left[(\partial_\ell J_\ell^*) E_k - J_\ell^* \partial_k E_\ell + J_\ell^* \partial_\ell E_k \right] \right\} dV \quad (65)$$

The volume integral of the second term reads

$$\mathcal{T}_i^{(2)} = +\frac{1}{2\omega} \text{Im} \int \mathbf{J}^* \cdot \partial_{\theta_i} \mathbf{E} dV.$$

where the symbol $\partial_{\theta_i} \mathbf{E}$ denotes the derivative of $\mathbf{E}(\mathbf{r})$ with respect to an infinitesimal rotation of the point \mathbf{r} about the i th coordinate axis with origin \mathbf{r}_0 .

The volume integral of the first+third terms in (65) is

$$\begin{aligned} \mathcal{T}_i^{(1+3)} &= -\frac{1}{2\omega} \text{Im} \int \varepsilon_{ijk} (\mathbf{r} - \mathbf{r}_0)_j \partial_\ell (J_\ell^* E_k) dV \\ &= -\frac{1}{2\omega} \text{Im} \underbrace{\oint \varepsilon_{ijk} (\mathbf{r} - \mathbf{r}_0)_j E_k \mathbf{J} \cdot d\mathbf{A}}_{=0} + \frac{1}{2\omega} \text{Im} \int \varepsilon_{ijk} \delta_{\ell j} J_\ell^* E_k dV \\ &= +\frac{1}{2\omega} \text{Im} \int (\mathbf{J}^* \times \mathbf{E})_i dV \end{aligned}$$

where the surface integral in the second line vanishes by the argument of (63).

Adding the two contributions, I find

$$\mathcal{T}_i = \frac{1}{2\omega} \text{Im} \int_{B_n} \left[\mathbf{J}^* \cdot \partial_{\theta_i} \mathbf{E} + (\mathbf{J}^* \times \mathbf{E})_i \right] dV. \quad (66)$$

C From Rytov to Johnson-Nyquist

For those of us who learned about noise in resistors before learning about Casimir forces and radiative heat transfer in nanoparticles, it's useful to relate the abstract and possibly mysterious notion of the Rytov correlation function to the concrete and familiar concept of Johnson-Nyquist noise. (Even for those who need no help with fluctuation-dissipation ideas, this exercise is useful for pinning down factors of 2π and other normalization effluvia.)

Johnson-Nyquist Noise

In elementary circuit theory we are taught that, at temperature T , a resistor exhibits a mean-square power of

$$\langle P \rangle = 4kT\Delta f$$

(where Δf is the effective measurement bandwidth in Hertz, usually determined by low-pass and high-pass filters in the circuit). If the resistance of the resistor is R , then the mean-square voltage across its terminals and the mean-square current flowing through it are

$$\begin{aligned}\langle V^2 \rangle &= \langle P \rangle R = 4kTR\Delta f, \\ \langle I^2 \rangle &= \frac{1}{R} \langle P \rangle = \frac{4kT}{R} \Delta f\end{aligned}\tag{67}$$

We would now like to understand equation (67) on the basis of the Rytov correlation function.

Macroscopic current noise from microscopic current-density fluctuations

To this end, consider a resistor consisting of a homogeneous cylinder of length L and cross-sectional area A with relative dielectric function

$$\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega) = \epsilon'(\omega) + i\frac{\sigma}{\epsilon_0\omega}\tag{68}$$

where σ is the microscopic conductivity in units of mho-meters [one mho = 1 inverse ohm ($1\ \Omega^{-1}$) = 1 siemen].⁶ The microscopic resistivity, with units of ohms/meter, is $\rho = 1/\sigma$. The total resistance of the resistor is

$$R = \frac{L}{A}\rho = \frac{L}{A\sigma}.$$

⁶The *absolute* permittivity of the object is $\epsilon_0\epsilon' + i\frac{\sigma}{\omega}$. To check that the imaginary part of (68) is indeed dimensionless, note that $\epsilon_0 = \frac{1}{Z_0 c}$ where $Z_0 \approx 377\ \Omega$ is the impedance of free space and c is the speed of light; thus the units of the imaginary part of (68) are

$$\left[\frac{\sigma}{\epsilon_0\omega} \right] = \frac{[\text{mhos}\cdot\text{meters}]}{[\text{mhos}\cdot\text{seconds}\cdot\text{meters}][\text{seconds}^{-1}]} = \text{dimensionless}.$$

We align the cylinder axis with the z -axis and break up coordinates into transverse and longitudinal components according to $\mathbf{x} = (\boldsymbol{\rho}, z)$.

The instantaneous current density at a point in the cylinder may be expressed as a Fourier synthesis:

$$\mathbf{J}(\mathbf{x}, t) = \int \mathbf{J}(\mathbf{x}, \omega) e^{-i\omega t} d\omega \quad (69)$$

where $\mathbf{J}(\mathbf{x}, \omega)$ is the Fourier transform of the instantaneous current density $\mathbf{J}(\mathbf{x}, t)$:

$$\mathbf{J}(\mathbf{x}, \omega) = \frac{1}{2\pi} \int \mathbf{J}(\mathbf{x}, t) e^{+i\omega t} dt. \quad (70)$$

The instantaneous *current* passing through a cross-sectional plane at height z is

$$I(z, t) = \int I(z, \omega) e^{-i\omega t} d\omega$$

where $I(z, \omega)$ is given by integrating \mathbf{J} over the cross-sectional plane:

$$I(z, \omega) = \int_A \mathbf{J}(\boldsymbol{\rho}, z, \omega) \cdot \hat{\mathbf{n}} d\boldsymbol{\rho}$$

or, in our specific geometry in which the cross section is everywhere normal to the z direction,

$$I(z, \omega) = \int_A J_z(\boldsymbol{\rho}, z, \omega) d\boldsymbol{\rho}.$$

Over a time interval of length τ , the average of the product of $I(t, z)$ and $I(t, z')$ is

$$\begin{aligned} \langle I(z)I(z') \rangle &= \frac{1}{\tau} \int_0^\tau I(z, t) I(z', t) dt \\ &= \frac{1}{\tau} \int_0^\tau dt \int d\omega \int d\omega' I(z, \omega) I(z, \omega') e^{-i(\omega+\omega')t} \\ &= \frac{1}{\tau} \int_0^\tau dt \int d\omega \int d\omega' \int_A d\boldsymbol{\rho} \int_A d\boldsymbol{\rho}' J_z(\boldsymbol{\rho}, z, \omega) J_z(\boldsymbol{\rho}', z', \omega') e^{-i(\omega+\omega')t}. \end{aligned} \quad (71)$$

To proceed we need to address a question about which we haven't said anything thus far—namely, where the current *comes from*. In a deterministic circuit problem we would have some fixed, known, externally applied voltage V across the resistor, which would induce a current equal to $I = V/R$. Here, on the other hand, there is no external voltage, and instead the current arises from thermal and quantum-mechanical *fluctuations* in the microscopic current density. Although we can't track the instantaneous progress of these fluctuations

in time—and thus, for example, we can't write down an expression for the instantaneous current density $\mathbf{J}(\mathbf{x}, t)$ —we can make precise statements about certain statistical *averages* over these fluctuating quantities. One particularly obvious statement is that the time-average value of any Cartesian component of \mathbf{J} vanishes,

$$\langle J_i(\mathbf{x}, t) \rangle = 0 \quad \text{for any } i.$$

A less obvious but even more important statement is that the fluctuation-dissipation theorem allows us to make a very definite prediction about the time-average value of the *product* of two cartesian components of \mathbf{J} . This equation—sometimes known as the *Rytov correlation function*—is easiest to write in the frequency domain, where it takes the form

$$\langle J_i(\mathbf{x}, \omega) J_j(\mathbf{x}', \omega') \rangle = \delta(\omega + \omega') \langle J_i(\mathbf{x}), J_j(\mathbf{x}') \rangle_\omega \quad (72)$$

$$\langle J_i(\mathbf{x}) J_j(\mathbf{x}') \rangle_\omega = \frac{2\omega\epsilon_0}{\pi} \Theta(\omega, T) \delta(\mathbf{r} - \mathbf{r}') \text{Im } \epsilon_{ij}(\mathbf{r}, \omega) \quad (73)$$

Equation (72) here is essentially the same⁷ as equation (122.4) in Landau and Lifshitz (LL), *Statistical Physics Volume 1*. In equation (73), $\Theta(\omega, T)$ is the Bose-Einstein statistical factor at the local temperature near \mathbf{r} (about which we will have more to say shortly) and $\epsilon_{ij}(\mathbf{r}, \omega)$ is the (i, j) component of the relative permittivity tensor of the material at point \mathbf{r} and frequency ω . Inserting (72) into (71) and using the δ functions to perform the $\boldsymbol{\rho}'$ and ω' integrations, we have

$$\begin{aligned} & \langle I(z) I(z') \rangle \\ &= \frac{1}{\tau} \int_0^\tau dt \int d\omega \int d\omega' \int_A d\boldsymbol{\rho} \int_A d\boldsymbol{\rho}' \langle J_z(\boldsymbol{\rho}, z, \omega) J_z(\boldsymbol{\rho}', z', \omega') \rangle e^{-i(\omega + \omega')t} \\ &= \frac{2\epsilon_0}{\pi\tau} \delta(z - z') \int_0^\tau dt \int d\omega \omega \Theta(\omega, T) \int_A d\boldsymbol{\rho} \text{Im } \epsilon_{zz}(\boldsymbol{\rho}, z, \omega) \end{aligned}$$

In the present case [cf. equation (68)] we have $\text{Im } \epsilon_{ij}(\mathbf{r}, \omega) = \delta_{ij} \frac{\sigma}{\epsilon_0 \omega}$ (independent of \mathbf{r}), whereupon we find

$$= \frac{2\sigma}{\pi} \cdot \delta(z - z') \cdot \underbrace{\frac{1}{\tau} \int_0^\tau dt \int d\omega \Theta(\omega, T)}_{kT\Delta\omega} \underbrace{\int_A d\boldsymbol{\rho}}_A$$

Here I used the high-temperature limit $\Theta(\omega, T) \approx kT$ (see below). Finally,

⁷My formula differs from that of Landau and Lifshitz (LL) by a factor of 2π , which arises because of our different conventions for the Fourier analysis and synthesis of time-domain functions: I like to put a factor of $\frac{1}{2\pi}$ in Fourier-analysis equations like (70), and to omit this factor in Fourier-synthesis equations like (69), while LL make the opposite choice.

averaging over the length of the resistor yields

$$\begin{aligned}\langle I^2(z) \rangle &= \frac{1}{L} \int_0^L \langle I(z)I(z') \rangle dz' \\ &= \frac{2kT\Delta\omega}{\pi} \cdot \underbrace{\frac{A\sigma}{L}}_{1/R} \\ &= \frac{4kT}{R} \Delta f\end{aligned}$$

where I used $\Delta\omega = 2\pi\Delta f$. This is equation (67).

Limiting behavior of $\Theta(\omega, T)$

The Bose-Einstein statistical factor $\Theta(\omega, T)$, which describes the average energy contained in an electromagnetic⁸ mode of frequency ω , is

$$\Theta(\omega, t) = \hbar\omega \left[\frac{1}{e^{\frac{\hbar\omega}{kT}} - 1} + \frac{1}{2} \right] = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right) \quad (74)$$

In the high- and low-temperature limits (equivalently, the low- and high-frequency) limits, the statistical factor of equation (74) becomes

$$\Theta(\omega, t) \xrightarrow{\frac{\hbar\omega}{kT} \rightarrow 0} kT, \quad \Theta(\omega, t) \xrightarrow{\frac{\hbar\omega}{kT} \rightarrow \infty} \frac{\hbar\omega}{2}. \quad (75)$$

The first case here corresponds to classical equipartition of energy: we have roughly kT worth of energy in each mode, independent of frequency. The second case corresponds to quantum-mechanical zero-point energy; we have some energy in each mode even at zero temperature.

To estimate the crossover between the high- and low-temperature regimes, recall that room temperature ($T=300$ K) corresponds to an energy of $kT \approx 26$ meV (milli-electron-volts), while \hbar has the numerical value

$$\hbar \approx 7 \cdot 10^{-16} \text{ eV} \cdot \text{s} = 7 \cdot 10^{-16} \frac{\text{eV}}{\text{rad/s}}.$$

Thus, for a circuit at frequency $f = 1$ GHz at a temperature of $T=300$ K, we have

$$kT = 0.026 \text{ eV} \quad \ll \quad \hbar\omega = \left(7 \cdot 10^{-16} \frac{\text{eV}}{\text{rad/s}}\right) (2\pi \cdot 10^9 \text{ rad/s}) = 4 \cdot 10^{-6} \text{ eV}$$

and thus, for ordinary circuits at ordinary temperatures, we are well in the high-temperature (low-frequency) regime in which $\Theta(\omega, T) \approx kT$.

⁸Or otherwise bosonic.

D Volume integrals involving SWG basis functions

Integrals over the support of SWG basis functions take the form

$$\int_{\sup \mathbf{b}_\alpha} \mathcal{I}(\mathbf{x}, \mathbf{b}_\alpha) d\mathbf{x} = \int_{\mathcal{P}_\alpha^+} \mathcal{I}(\mathbf{x}, \mathbf{b}_\alpha) d\mathbf{x} + \int_{\mathcal{P}_\alpha^-} \mathcal{I}(\mathbf{x}, \mathbf{b}_\alpha) d\mathbf{x} \quad (76)$$

Consider a tetrahedron with vertices $\{\mathbf{Q}, \mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3\}$. A general integral over this region takes the form

$$\int_{\mathcal{P}} \mathcal{I}(\mathbf{x}, \mathbf{b}) d\mathbf{x} = \mathcal{J} \int_0^1 du \int_0^{1-u} dv \int_0^{1-u-v} dw \mathcal{I}(\mathbf{x}(u, v, w), \mathbf{b}(u, v, w))$$

$$\begin{aligned} \mathbf{x}(u, v, w) &= \mathbf{Q} + u\mathbf{L}_1 + v\mathbf{L}_2 + w\mathbf{L}_3 \\ \mathbf{b}(u, v, w) &= \pm \frac{A}{3V} \left\{ u\mathbf{L}_1 + v\mathbf{L}_2 + w\mathbf{L}_3 \right\} \end{aligned}$$

where

$$\mathbf{L}_i \equiv \mathbf{V}_i - \mathbf{Q}_i$$

and the Jacobian of the transformation is

$$\mathcal{J} = \frac{d(x, y, z)}{d(u, v, w)} = \det \begin{vmatrix} \mathbf{L}_1 & \mathbf{L}_2 & \mathbf{L}_3 \end{vmatrix} = 6V$$

Overlap Matrix Elements

$$\langle \mathbf{b}_\alpha | \mathbf{b}_\beta \rangle = \sum \pm \frac{A_\alpha A_\beta}{9V^2} \int_{\mathcal{V}} (\mathbf{x} - \mathbf{Q}_\alpha) \cdot (\mathbf{x} - \mathbf{Q}_\beta) d\mathbf{x}$$

(where the sum is over the 0, 1, or 2 tetrahedra in the common support of $\{\mathbf{b}_\alpha, \mathbf{b}_\beta\}$)

$$\begin{aligned} &= \sum \pm \frac{2A_\alpha A_\beta}{3V} \int_0^1 du \int_0^{1-u} dv \int_0^{1-u-v} dw \left\{ \left[u\mathbf{L}_{1\alpha} + v\mathbf{L}_{2\alpha} + w\mathbf{L}_{3\alpha} \right] \right. \\ &\quad \left. \cdot \left[u\mathbf{L}_{1\alpha} + v\mathbf{L}_{2\alpha} + w\mathbf{L}_{3\alpha} + \mathbf{Q}_\alpha - \mathbf{Q}_\beta \right] \right\} \\ &= \sum \pm \frac{2A_\alpha A_\beta}{3V} \left\{ \frac{1}{120} \left| \mathbf{L}_{1\alpha} + \mathbf{L}_{2\alpha} + \mathbf{L}_{3\alpha} \right|^2 + \frac{1}{120} \left(|\mathbf{L}_{1\alpha}|^2 + |\mathbf{L}_{2\alpha}|^2 + |\mathbf{L}_{3\alpha}|^2 \right) \right. \\ &\quad \left. + \frac{1}{24} \left(\mathbf{L}_{1\alpha} + \mathbf{L}_{2\alpha} + \mathbf{L}_{3\alpha} \right) \cdot (\mathbf{Q}_\alpha - \mathbf{Q}_\beta) \right\} \end{aligned}$$

This can be simplified by noting that $\mathbf{L}_{1\alpha} + \mathbf{L}_{2\alpha} + \mathbf{L}_{3\alpha} = 3(\mathbf{X}_{0\alpha} - \mathbf{Q}_\alpha)$ where $\mathbf{X}_{0\alpha}$ is the centroid of basis function \mathbf{b}_α :

$$= \sum \pm \frac{2A_\alpha A_\beta}{3V} \left[\frac{3}{40} (\mathbf{X}_{0\alpha} - \mathbf{Q}_\alpha)^2 + \frac{1}{120} (|\mathbf{L}_{1\alpha}|^2 + |\mathbf{L}_{2\alpha}|^2 + |\mathbf{L}_{3\alpha}|^2) + \frac{1}{8} (\mathbf{X}_{0\alpha} - \mathbf{Q}_\alpha) \cdot (\mathbf{Q}_\alpha - \mathbf{Q}_\beta) \right].$$

Dipole and Quadrupole Moments

The dipole moment of the current distribution described by a single unit-strength SWG basis function is

$$\mathbf{p}_\alpha \equiv \frac{i}{\omega} \underbrace{\int_{\sup \mathbf{b}_\alpha} \mathbf{b}_\alpha(\mathbf{x}) d\mathbf{x}}_{\mathcal{J}_\alpha(\mathbf{x})} \quad (77)$$

The Cartesian components of $\mathcal{J}_\alpha(\mathbf{x})$ may be worked out in closed form:

$$\begin{aligned} \mathcal{J}_{\alpha i}(\mathbf{x}) &= 2A \int_0^1 du \int_0^{1-u} dv \int_0^{1-u-v} dw (u + v + w) (\mathbf{Q}^- - \mathbf{Q}^+)_i \\ &= \frac{A}{4} (\mathbf{Q}^- - \mathbf{Q}^+)_i. \end{aligned} \quad (78)$$

Similarly, the quadrupole moments are related to the quantity

$$\mathcal{Q}_{\alpha ij}(\mathbf{x}) = \int_{\sup \mathbf{b}_\alpha} b_{\alpha i}(\mathbf{x} - \mathbf{x}_0)_j d\mathbf{x}$$

where $\mathbf{x}_0 = \frac{1}{3}(\mathbf{V}_1 + \mathbf{V}_2 + \mathbf{V}_3)$ is the centroid of the basis function (which we take to be the centroid of the triangle that constitutes the common face).

$$\begin{aligned} &= 2A \int_0^1 du \int_0^{1-u} dv \int_0^{1-u-v} dw \left\{ \begin{aligned} &\left[u\mathbf{L}_1^+ + v\mathbf{L}_2^+ + w\mathbf{L}_3^+ \right]_i \left[\left(u - \frac{1}{3} \right) \mathbf{L}_1^+ + \left(v - \frac{1}{3} \right) \mathbf{L}_2^+ + \left(w - \frac{1}{3} \right) \mathbf{L}_3^+ \right]_j \\ &- \left[u\mathbf{L}_1^- + v\mathbf{L}_2^- + w\mathbf{L}_3^- \right]_i \left[\left(u - \frac{1}{3} \right) \mathbf{L}_1^- + \left(v - \frac{1}{3} \right) \mathbf{L}_2^- + \left(w - \frac{1}{3} \right) \mathbf{L}_3^- \right]_j \end{aligned} \right\} \\ &= \frac{A}{20} \left\{ Q_i^- \left[\mathbf{Q}^- - \mathbf{x}_0 \right]_j - Q_i^+ \left[\mathbf{Q}^+ - \mathbf{x}_0 \right]_j + x_{0i} \left[\mathbf{Q}^+ - \mathbf{x}_0 \right]_j \right\} \end{aligned}$$