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APPENDIX A: EXPECTATION VALUE OF ENERGY TERMS

1. Overview of Calculations

Here, the expectation value of the energy terms in Eqs. (49)-(53) will be evaluated. Finding the first three terms is not very difficult, while obtaining the last two terms is much more involved. Nevertheless, the details are written out fairly completely for all of the steps used in the calculations.

One important approximation should be mentioned at the outset that was used in evaluating $U_{EM,\mathcal{S}-\mathcal{S}}$ and $U_{EM,\mathcal{S}-in}$ and that is related to the size of the volume $\mathcal{V}$ enclosing the particles. This approximation will now be described and argued to be a reasonable one, provided the surface $\mathcal{S}$ is far removed from all particles. Because the following explanation draws on the explicit calculations of Secs. 5 and 6 in this appendix, the reader may wish to proceed with reading the following sections, namely, Secs. 2 through 6, and then subsequently return to the present one.

In the calculations given here, $U_{EM,\mathcal{S}-\mathcal{S}}$ and $U_{EM,\mathcal{S}-in}$ were first expanded as an integral over frequency, as can be seen in Eqs. (A25) and (A107). The quantities $E_{Ai;Bj}$ and $P^{T}_{Ai;Bj}$ in these two equations were then calculated, which in each case required the evaluation of a volume integral over $\mathcal{V}$ [see Eqs. (A24) and (A101)]. These integrals were evaluated by converting them into the sum of a volume integral and surface integral [see, for example, Eqs. (A28) and (A40)]. The volume integrals were carried out exactly, while the surface integrals were evaluated by only retaining terms proportional to $1/r^2$, where r is the distance from the approximate center of the N particles to a point on the surface $\mathcal{S}$. Thus, the assumption was made that the distance betwen any two particles was small compared to the distance from any particle to any point on $\mathcal{S}$.

However, this step of dropping terms in the surface integrals that were proportional to $1/r^n$, for $n \geq 3$, also appears to require the implicit assumption that $1 \ll kr$, as can be seen in the approximation made in Eq. (A42). For any nonzero value of k, this condition will be satisfied if the surface $\mathcal{S}$ is assumed to lie at infinity, but for any finite distance from the particles to $\mathcal{S}$, this condition cannot be met since $U_{EM,\mathcal{S}-\mathcal{S}}$ and $U_{EM,\mathcal{S}-in}$ were written as integrals over all frequency values.

Nevertheless, there are at least two reasons why we should expect that the approximation just mentioned is a reasonable one. First, if we assume that resonance conditions occur near the natural oscillating frequency ω_o of the oscillators, as discussed in Sec. VI.C, then our main concern in the above approximation is satisfying $1 \ll \omega_o r/c$. Our results then apply for any surface $\mathcal{S}$ at a distance from the particles that is large compared with the wavelength of light λ_o, where $\lambda_o = c/(2\pi\omega_o)$.

A second reason exists that essentially includes the first one: our justification of the dropping of the $1/r^n$ terms, for $n \geq 3$, can be equated with the assumption that when $1 \ll \omega r/c$ is <u>not</u> satisfied in the integrands of the surface integrals in question, such as in Eqs. (A40), (A117), and (A123), then we obtain a negligible contribution of these surface integrals to Eqs. (A25) and (A107), and ultimately to $\Delta U_{internal}$ from Eq. (20). To see why this condition should be true for reasonable choices of $\mathbf{h}_{in}$, where by "reasonable" it is meant here that $\mathbf{h}_{in}$ does not become large as $\omega \to 0$, we should note that for ℓ far removed from all the particles and for $1 \ll r/\lambda_o$, then $1 \ll \omega r/c$ is <u>not</u> satisfied only when there occurs <u>very</u> <u>small</u> values of ω in the surface integrals in question. Thus, we are questioning the validity of the above approximation in the very small frequency regime of the integral expressions for $U_{EM,\beta-\beta}$ and $U_{EM,\beta-in}$ in Eqs. (A25) and (A107). Consequently, the wavelengths we are concerned with are on the order of, or larger, than the approximate radius of the volume $\mathcal{V}$ enclosing the particles. The larger we make the approximate radius of $\mathcal{V}$, the smaller will be the frequency interval over which the above approximation is questionable.

The surface integrals do not exhibit any singular behavior in the low frequency regime. Moreover, one can show that the part of the integrands in Eqs. (A25) and (A107) that depends on these surface integrals is not singular as $\omega \to 0$. Consequently, the error in using this approximation to evaluate $U_{EM,\beta-\beta}$ and $U_{EM,\beta-in}$, so as to obtain $\Delta U_{internal}$, should decrease and become negligible as the size of $\mathcal{V}$ increases, since as $\mathcal{V}$ increases, the low frequency interval will become negligibly small over which this approximation is questionable.

2. Calculation for U_{PE}

From Eqs. (42)-(46),

$$U_{PE} \equiv \sum_{A=1}^{N} \left\langle \frac{m\omega_0^2}{2} |\delta \vec{z}_A|^2 \right\rangle$$

$$= \frac{m\omega_0^2}{2} \sum_{A=1}^{N} \sum_{i=1}^{3} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_1 e^{-i\omega_1 t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_2 e^{-i\omega_2 t} \frac{1}{C(\omega_1)C(\omega_2)} \left(\frac{e}{m}\right)^2 \cdot \tag{A1}$$

$$\cdot \sum_{B=1}^{N} \sum_{j=1}^{3} \sum_{D=1}^{N} \sum_{k=1}^{3} \left[M^{-1}(\omega_1)\right]_{Ai;Bj} \left[M^{-1}(\omega_2)\right]_{Ai;Dk} \left\langle \tilde{E}_{in\,j}(\vec{z}_B,\omega_1) \tilde{E}_{in\,k}(\vec{z}_D,\omega_2) \right\rangle .$$

From Eqs. (58) and (15) in Ref. 31,

$$\left\langle \tilde{E}_{in\,j}(\vec{z}_B,\omega_1) \tilde{E}_{in\,k}(\vec{z}_D,\omega_2) \right\rangle \tag{A2}$$

$$= 2\pi^2 \int_0^{\infty} d\omega \frac{\left[h_{in}(\omega)\right]^2}{\omega} \left[\delta(\omega_1-\omega)\delta(\omega_2+\omega) + \delta(\omega_1+\omega)\delta(\omega_2-\omega)\right] \mathrm{Im}\left[\eta^{0}_{jk}(\vec{z}_D-\vec{z}_B,\omega)\right] .$$

Substituting, we obtain

$$U_{PE} = \frac{m\omega_0^2}{2} \pi \left(\frac{e}{m}\right)^2 \sum_{A,i} \sum_{B,j} \sum_{D,k} \int_0^{\infty} d\omega \frac{h_{in}^2(\omega)}{\omega} \frac{1}{C(\omega)C(-\omega)} \cdot \tag{A3}$$

$$\cdot \left\{ \left[M^{-1}(\omega)\right]_{Ai;Bj} \left[M^{-1}(-\omega)\right]_{Ai;Dk} + \left[M^{-1}(-\omega)\right]_{Ai;Bj} \left[M^{-1}(\omega)\right]_{Ai;Dk} \right\} \mathrm{Im}\left[\eta^{0}_{jk}(\vec{z}_D-\vec{z}_B,\omega)\right] .$$

From Eqs. (40), (45), and (46), we can see that $C(-\omega)=C(\omega)^*$, $[M(-\omega)]=[M(\omega)]^*$, and likewise for $[M^{-1}(\omega)]$. Also, from Eqs. (40) and (46), one can see that both $[M(\omega)]_{Ai;Bj}$ and $[M^{-1}(\omega)]_{Ai;Bj}$ are symmetric in the indices A and B, and in i and j. Hence, we can reverse these indices at our convenience.

From Eqs. (34) and (63) in Ref. 31,

$$\mathrm{Im}\left[\eta^{D}_{jk}(\vec{Z}_D-\vec{Z}_B,\omega)\right] = -\frac{m}{e^2}\,\mathrm{Im}\left[C(\omega)\,M_{Bj;Dk}(\omega)\right] \quad . \tag{A4}$$

Hence, we obtain the following result after summing over matching indices and then relabeling dummy indices:

$$\begin{aligned} U_{PE} &= -\frac{\pi\omega_*^2}{2}\sum_{A,i}\sum_{B,j}\sum_{D,k}\int_0^\infty d\omega\,\frac{\mathcal{A}_{in}^2}{\omega}\frac{1}{|C|^2}\left\{\left[M^{-1}\right]_{Ai;Bj}\left[M^{-1}\right]^*_{Ai;Dk}+\left[M^{-1}\right]^*_{Ai;Bj}\left[M^{-1}\right]_{Ai;Dk}\right\}\times \\ &\qquad\qquad \times\left\{\frac{C\,[M]_{Bj;Dk}-C^*[M]^*_{Bj;Dk}}{2i}\right\} \qquad (A5) \\ &= +\pi\int_0^\infty d\omega\,\mathcal{A}_{in}^2(\omega)\,\mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bk}\left(\delta_{AB}\,\delta_{ij}\,\frac{\omega_*^2}{\omega}\right)\right] \quad . \end{aligned}$$

3. Calculation for U_{KE}

$$U_{KE} \equiv \sum_{A=1}^{N} \left\langle \frac{m}{2} \left| \frac{d\delta\vec{z}_A}{dt} \right|^2 \right\rangle$$

$$= \frac{m}{2} \sum_{A=1}^{N} \sum_{i=1}^{3} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_1 e^{-i\omega_1 t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_2 e^{-i\omega_2 t} \frac{1}{C(\omega_1)C(\omega_2)} \left(\frac{e}{m}\right)^2 (-i\omega_1)(-i\omega_2) \qquad (A6)$$

$$\cdot \sum_{B=1}^{N} \sum_{j=1}^{3} \sum_{D=1}^{N} \sum_{k=1}^{3} \left[M^{-1}(\omega_1)\right]_{Ai;Bj} \left[M^{-1}(\omega_2)\right]_{Ai;Dk} \left\langle \tilde{E}_{in\,j}(\vec{z}_B, \omega_1) \tilde{E}_{in\,k}(\vec{z}_D, \omega_2) \right\rangle .$$

For each of the two sets of delta functions in Eq. (A2), $(-i\omega_1)(-i\omega_2) \to +\omega^2$. The steps for U_{KE} then follow precisely the same steps as for U_{PE}. Hence,

$$U_{KE} = +\pi \int_0^{\infty} d\omega \, h_{in}(\omega) \, \mathrm{Im}\left[\frac{1}{C(\omega)} \sum_{A,B=1}^{N} \sum_{i,j=1}^{3} \left[M^{-1}(\omega)\right]_{Ai;Bj} \left(\delta_{AB}\delta_{ij}\,\omega\right)\right] . \qquad (A7)$$

4. Calculation for $U_{EM,\mathcal{D}a-\mathcal{D}a}$

$$U_{EM,\mathcal{D}a-\mathcal{D}a} \equiv \sum_{A=1}^{N} \frac{1}{8\pi} \int_V d^3x \left\langle \vec{E}_{\mathcal{D}a,A}(\vec{x},t) \cdot \vec{E}_{\mathcal{D}a,A}(\vec{x},t) + \vec{B}_{\mathcal{D}a,A}(\vec{x},t) \cdot \vec{B}_{\mathcal{D}a,A}(\vec{x},t) \right\rangle . \quad (A8)$$

Here, $\vec{E}_{\mathcal{D}a,A}(\vec{x},t)$ and $\vec{B}_{\mathcal{D}a,A}(\vec{x},t)$ are the parts of the fields of electric dipole A that are proportional to $|\vec{x}-\vec{Z}_A|^{-1}$ [see the brief remarks after Eq. 5, after Eq. (21), and before Eq. (38)]. Thus, these terms are given by the same form of expressions as in Eqs. (38) and (39), but with $\eta_{ij}^{\mathcal{D}}$ and $\rho_{ij}^{\mathcal{D}}$ replaced by $\eta_{ij}^{\mathcal{D}a}$ and $\rho_{ij}^{\mathcal{D}a}$, where

$$\eta_{ij}^{\mathcal{D}a}(\vec{R},\omega) = k^2\left(\delta_{ij} - \frac{R_i R_j}{R^2}\right)\frac{e^{ikR}}{R} , \qquad (A9)$$

$$\rho_{ij}^{\mathcal{D}a}(\vec{R},\omega) = -k^2 \sum_{\ell=1}^{3} \epsilon_{ij\ell} \frac{R_\ell}{R} \frac{e^{ikR}}{R} . \qquad (A10)$$

These expressions can easily be deduced from the 1/R terms resulting from Eqs. (40) and (41).

Consequently,

$$\left\langle \vec{E}_{\mathcal{D}a,A}(\vec{x},t) \cdot \vec{E}_{\mathcal{D}a,A}(\vec{x},t) \right\rangle \qquad (A11)$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_1 e^{-i\omega_1 t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_2 e^{-i\omega_2 t} \sum_{i,j,k=1}^{3} \eta_{ij}^{\mathcal{D}a}(\vec{x}-\vec{Z}_A,\omega_1)\eta_{ik}^{\mathcal{D}a}(\vec{x}-\vec{Z}_A,\omega_2) e^2 \left\langle \delta\tilde{z}_{Aj}(\omega_1)\delta\tilde{z}_{Ak}(\omega_2)\right\rangle ,$$

$$\left\langle \vec{B}_{\mathcal{D}a,A}(\vec{x},t) \cdot \vec{B}_{\mathcal{D}a,A}(\vec{x},t) \right\rangle \qquad (A12)$$
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_1 e^{-i\omega_1 t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\omega_2 e^{-i\omega_2 t} \sum_{i,j,k=1}^{3} \rho_{ij}^{\mathcal{D}a}(\vec{x}-\vec{Z}_A,\omega_1)\rho_{ik}^{\mathcal{D}a}(\vec{x}-\vec{Z}_A,\omega_2) e^2 \left\langle \delta\tilde{z}_{Aj}(\omega_1)\delta\tilde{z}_{Ak}(\omega_2)\right\rangle .$$

From Eqs. (44)-(46), and using Eqs. (A2) and (A4) in the following steps, yields

$$
\begin{aligned}
&\left\langle \delta\tilde{z}_{Aj}(\omega_1)\,\delta\tilde{z}_{Ak}(\omega_2)\right\rangle \\
&= \left(\frac{e}{m}\right)^2 \sum_{B,D=1}^{N} \sum_{m,n=1}^{3} \left[M^{-1}(\omega_1)\right]_{Aj;Bm} \left[M^{-1}(\omega_2)\right]_{Ak;Dn} \frac{1}{C(\omega_1)C(\omega_2)} \left\langle \tilde{E}_{in\,m}(\vec{z}_B,\omega_1)\,\tilde{E}_{in\,n}(\vec{z}_D,\omega_2)\right\rangle \\
&= -\frac{2\pi^2}{m} \sum_{B,D=1}^{N} \sum_{m,n=1}^{3} \int_0^\infty d\omega\, \frac{h_{in}^2(\omega)}{\omega}\, \mathrm{Im}\left[C(\omega)\left[M(\omega)\right]_{Dm;Bn}\right] \frac{1}{|C|^2}\, \cdot \\
&\quad \cdot \left\{ \left[M^{-1}(\omega)\right]_{Aj;Bm} \left[M^{-1}(\omega)\right]^*_{Ak;Dn} \delta(\omega_1-\omega)\,\delta(\omega_2+\omega) + \left[M^{-1}(\omega)\right]^*_{Aj;Bm} \left[M^{-1}(\omega)\right]_{Ak;Dn} \delta(\omega_1+\omega)\,\delta(\omega_2-\omega) \right\} .
\end{aligned}
\tag{A13}
$$

Substituting Eq. (A13) into Eq. (A11), summing over matching indices, and gathering terms, results in the following steps:

$$
\begin{aligned}
&\left\langle \vec{E}_{\Delta a,A}(\vec{x},t)\cdot\vec{E}_{\Delta a,A}(\vec{x},t)\right\rangle \\
&= -\pi\frac{e^2}{m} \int_0^\infty d\omega\, \frac{h_{in}^2(\omega)}{\omega} \frac{1}{|C|^2} \sum_{B,D=1}^{N} \sum_{\substack{i,j,k,\\ m,n}=1}^{3} \frac{1}{2i} \left\{ C[M]_{Dm;Bn} - C^*[M]^*_{Dm;Bn} \right\} \times \\
&\quad \times \left\{ [M^{-1}]_{Aj;Bm} [M^{-1}]^*_{Ak;Dn}\, n_{ij}^{\Delta a}(\vec{x}-\vec{z}_A,\omega)\, n_{ik}^{\Delta a *}(\vec{x}-\vec{z}_A,\omega) + [M^{-1}]^*_{Aj;Bm} [M^{-1}]_{Ak;Dn}\, n_{ij}^{\Delta a *}(\vec{x}-\vec{z}_A,\omega)\, n_{ik}^{\Delta a}(\vec{x}-\vec{z}_A,\omega) \right\} \\
&= +\pi\frac{e^2}{m} \int_0^\infty d\omega\, \frac{h_{in}^2}{\omega} \frac{1}{|C|^2} \sum_{i,j,k=1}^{3} \mathrm{Im}\left[C^* [M^{-1}]_{Aj;Ak}\, 2\,\mathrm{Re}\left\{ n_{ij}^{\Delta a}(\vec{x}-\vec{z}_A,\omega)\, n_{ik}^{\Delta a *}(\vec{x}-\vec{z}_A,\omega)\right\}\right] .
\end{aligned}
\tag{A14}
$$

If we now relabel the dummy indices by k->j, j->i, i->ℓ, then

$$
\begin{aligned}
&\frac{1}{8\pi}\int_V d^3x \left\langle \vec{E}_{\Delta a,A}(\vec{x},t)\cdot\vec{E}_{\Delta a,A}(\vec{x},t)\right\rangle \\
&= \pi \int_0^\infty d\omega\, h_{in}^2(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)} \sum_{i,j=1}^{3} \left[M^{-1}(\omega)\right]_{Ai;Aj} \left\{ \frac{e^2}{4\pi m} \frac{1}{\omega} \sum_{\ell=1}^{3} \mathrm{Re}\left(\int_V d^3x\, n_{\ell i}^{\Delta a}(\vec{x}-\vec{z}_A,\omega)\, n_{\ell j}^{\Delta a *}(\vec{x}-\vec{z}_A,\omega)\right)\right\}\right] .
\end{aligned}
\tag{A15}
$$

Repeating similar steps for the magnetic field correlation term, gives the same expressions as in Eqs. (A14) and (A15), but with $n_{ij}^{\mathcal{B}a}$ replaced by $\rho_{ij}^{\mathcal{B}a}$. Hence,

$$\frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{B}_{\mathcal{B}a,A}(\vec{x},t)\cdot\vec{B}_{\mathcal{B}a,A}(\vec{x},t)\right\rangle$$
$$= \pi\int_0^\infty d\omega\, h_{in}^2(\omega)\,\mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Aj}\left\{\frac{e^2}{4\pi m}\frac{1}{\omega}\sum_{\ell=1}^{3}\mathrm{Re}\left(\int_{\mathcal{V}} d^3x\,\rho_{\ell i}^{\mathcal{B}a}(\vec{x}-\vec{Z}_A,\omega)\,\rho_{\ell j}^{\mathcal{B}a*}(\vec{x}-\vec{Z}_A,\omega)\right)\right\}\right]. \quad (A$$

Let's now carry out the volume integration in Eqs. (A15) and (A16). From Eqs. (A9) and (A10), with $\vec{R}=\vec{x}-\vec{Z}_A$, gives

$$\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\, n_{\ell i}^{\mathcal{B}a}(\vec{x}-\vec{Z}_A,\omega)\,n_{\ell j}^{\mathcal{B}a*}(\vec{x}-\vec{Z}_A,\omega) = \sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\, k^4\left(\delta_{\ell i}-\frac{R_\ell R_i}{R^2}\right)\left(\delta_{\ell i}-\frac{R_\ell R_j}{R^2}\right)\frac{1}{R^2}$$

$$= k^4\int_{\mathcal{V}} d^3x\,\frac{\left[\delta_{ij}-\dfrac{(\vec{x}-\vec{Z}_A)_i(\vec{x}-\vec{Z}_A)_j}{|\vec{x}-\vec{Z}_A|^2}\right]}{|\vec{x}-\vec{Z}_A|^2}, \qquad (A17)$$

$$\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\,\rho_{\ell i}^{\mathcal{B}a}(\vec{x}-\vec{Z}_A,\omega)\,\rho_{\ell j}^{\mathcal{B}a*}(\vec{x}-\vec{Z}_A,\omega) = \sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\, k^4\sum_{m=1}^{3}\epsilon_{\ell i m}\frac{R_m}{R^2}\sum_{n=1}^{3}\epsilon_{\ell j n}\frac{R_n}{R^2}$$

$$= k^4\int_{\mathcal{V}} d^3x\sum_{m,n=1}^{3}\frac{R_m R_n}{R^4}\left(\delta_{ij}\delta_{mn}-\delta_{in}\delta_{mj}\right)$$

$$= k^4\int_{\mathcal{V}} d^3x\,\frac{\left[\delta_{ij}-\dfrac{(\vec{x}-\vec{Z}_A)_i(\vec{x}-\vec{Z}_A)_j}{|\vec{x}-\vec{Z}_A|^2}\right]}{|\vec{x}-\vec{Z}_A|^2}. \qquad (A18)$$

Thus, both quantities above are equal. If the volume $\mathcal{V}$ is a sphere with radius R and with $\vec{Z}_A$ at its center, then the above quantities equal

$$k^4\delta_{ij}(8\pi/3)R.$$

Also, the quantities in Eqs. (A17) and (A18) are real, so the "Re(...)" operation in Eqs. (A15) and (A16) are not necessary. We see that the electric and magnetic field energies in Eqs. (A15) and (A16) are equal; for a spherical volume $\mathcal{V}$, they are proportional to the radius of $\mathcal{V}$.

Our final result is

$$U_{EM,\mathcal{D}_a-\mathcal{D}_a} = \pi \int_0^\infty d\omega\, \lambda_{in}^2(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)} \sum_{A,B=1}^{N} \sum_{i,j=1}^{3} \left[M^{-1}(\omega)\right]_{Ai;Bj} \left(\delta_{AB} \frac{e^2}{m\omega} \mathcal{S}_{Aij}\right)\right], \quad (A19)$$

where

$$\mathcal{S}_{A\,ij} \equiv \frac{K^4}{2\pi} \int_{\mathcal{V}} d^3x \frac{\left(\delta_{ij} - \frac{(\vec{x}-\vec{Z}_A)_i (\vec{x}-\vec{Z}_A)_j}{|\vec{x}-\vec{Z}_A|^2}\right)}{|\vec{x}-\vec{Z}_A|^2} \quad . \quad (A20)$$

5. Calculation for $U_{EM,\mathcal{D}-\mathcal{D}}$

$$U_{EM,\mathcal{D}-\mathcal{D}} \equiv \sum_{\substack{A,B=1\\A\neq B}}^{N} \frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{\mathcal{D},B}(\vec{x},t) + \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{\mathcal{D},B}(\vec{x},t)\right\rangle . \tag{A21}$$

Here, $\vec{E}_{\mathcal{D},A}$ and $\vec{B}_{\mathcal{D},A}$ are given by Eqs. (38)-(41).

The first part of the above calculation follows very closely to the steps used in Eqs. (A11)-(A16), except that the two positions $\vec{z}_A$ and $\vec{z}_B$ are involved instead of just the single position $\vec{z}_A$, and of course the quantities $N_{ij}^{\mathcal{D}a}$ and $p_{ij}^{\mathcal{D}a}$ must be replaced by $N_{ij}^{\mathcal{D}}$ and $p_{ij}^{\mathcal{D}}$. Without a great deal of difficulty, one can show that

$$\frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{\mathcal{D},B}(\vec{x},t)\right\rangle \tag{A22}$$
$$= \pi\int_0^\infty d\omega\, h_{in}^2(\omega)\,\mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bj}\left\{\frac{e^2}{4\pi m}\frac{1}{\omega}\sum_{\ell=1}^{3}\mathrm{Re}\left(\int_{\mathcal{V}} d^3x\, n_{\ell i}^{\mathcal{D}}(\vec{x}-\vec{z}_A,\omega)\, n_{\ell j}^{\mathcal{D}*}(\vec{x}-\vec{z}_B,\omega)\right)\right\}\right],$$

$$\frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{\mathcal{D},B}(\vec{x},t)\right\rangle \tag{A23}$$
$$= \pi\int_0^\infty d\omega\, h_{in}^2(\omega)\,\mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bj}\left\{\frac{e^2}{4\pi m}\frac{1}{\omega}\sum_{\ell=1}^{3}\mathrm{Re}\left(\int_{\mathcal{V}} d^3x\, p_{\ell i}^{\mathcal{D}}(\vec{x}-\vec{z}_A,\omega)\, p_{\ell j}^{\mathcal{D}*}(\vec{x}-\vec{z}_B,\omega)\right)\right\}\right],$$

where $A\neq B$. The above results are very much analogous to Eqs. (A15) and (A16).

Combining the above, we see that the following quantity needs to be evaluated

$$E_{Ai;Bj} \equiv \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\left[n_{\ell i}^{\mathcal{D}}(\vec{x}-\vec{z}_A,\omega)\, n_{\ell j}^{\mathcal{D}*}(\vec{x}-\vec{z}_B,\omega) + p_{\ell i}^{\mathcal{D}}(\vec{x}-\vec{z}_A,\omega)\, p_{\ell j}^{\mathcal{D}*}(\vec{x}-\vec{z}_B,\omega)\right], \tag{A24}$$

for $A\neq B$, since $E_{Ai;Bj}$ appears in

$$\frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{\mathcal{D},B}(\vec{x},t) + \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{\mathcal{D},B}(\vec{x},t)\right\rangle$$

$$= \pi\int_0^\infty d\omega\, h_{in}^2(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bj}\left\{\frac{e^2}{m\omega}\mathrm{Re}\left[E_{Ai;Bj}\right]\right\}\right] . \qquad (A25)$$

As we'll soon see, $E_{Ai;Bj}$ is a fairly complicated quantity that depends on the precise shape and size of the volume $\mathcal{V}$. However, as shown in the following section on $U_{EM,\mathcal{D}-in}$, the $A\neq B$ terms of $E_{Ai;Bj}$ drop out completely in the sum of $U_{EM,\mathcal{D}-\mathcal{D}}$ plus $U_{EM,\mathcal{D}-in}$. Hence, if the reader is interested in only the sum of these energies, which is indeed the important quantity of interest for this article, then the remainder of this section on $U_{EM,\mathcal{D}-\mathcal{D}}$ can be skipped without loss.

Regarding the two energy terms in Eqs. (A22) and (A23), each term depends upon the size and shape of $\mathcal{V}$, but the difference between them is essentially independent of $\mathcal{V}$, at least for large $\mathcal{V}$. Hence, instead of directly calculating $E_{Ai;Bj}$, we can obtain a little more insight into the energy terms by investigating the following two quantities:

$$Q_{Ai;Bj} \equiv \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x \left[\eta^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{z}_A,\omega)\,\eta^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{z}_B,\omega) - \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{z}_A,\omega)\,\rho^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{z}_B,\omega)\right] , \qquad (A26)$$

$$F_{Ai;Bj} \equiv \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\, \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{z}_A,\omega)\,\rho^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{z}_B,\omega) . \qquad (A27)$$

Thus

$$E_{Ai;Bj} = Q_{Ai;Bj} + 2F_{Ai;Bj} , \qquad (A28)$$

so that $Q_{Ai;Bj}$ represents the volume integral of interest if we subtracted the energy terms in Eqs. (A22) and (A23), while $F_{Ai;Bj}$

is the required volume integral in calculating the magnetic field energy term in Eq. (A23).

Let's first calculate $Q_{Ai;Bj}$. Substituting Eqs. (40) and (41) into Eq. (A26), multiplying out terms, and defining the quantity

$$Z_{xA} \equiv \frac{e^{iK|\vec{x}-\vec{Z}_A|}}{|\vec{x}-\vec{Z}_A|} , \qquad (A29)$$

yields that $Q_{Ai;Bj}$ equals the sum of six terms:

$$Q_{Ai;Bj} = \sum_{m=1}^{6} Q^{(m)}_{Ai;Bj} , \qquad (A30)$$

where

$$Q^{(1)}_{Ai;Bj} \equiv \frac{1}{4\pi} \sum_{\ell=1}^{3} \int_{V} d^3x \left(\nabla_\ell \nabla_i Z_{xA}\right)\left(\nabla_\ell \nabla_j Z^*_{xB}\right) , \qquad (A31)$$

$$Q^{(2)}_{Ai;Bj} \equiv \frac{K^2}{4\pi} \int_{V} d^3x \left(\nabla_i \nabla_j Z_{xA}\right) Z^*_{xB} , \qquad (A32)$$

$$Q^{(3)}_{Ai;Bj} \equiv \frac{K^2}{4\pi} \int_{V} d^3x \, Z_{xA} \left(\nabla_i \nabla_j Z^*_{xB}\right) , \qquad (A33)$$

$$Q^{(4)}_{Ai;Bj} \equiv \frac{\delta_{ij} K^4}{4\pi} \int_{V} d^3x \, Z_{xA} Z^*_{xB} , \qquad (A34)$$

$$Q^{(5)}_{Ai;Bj} \equiv \frac{-\delta_{ij} K^2}{4\pi} \sum_{\ell=1}^{3} \int_{V} d^3x \left(\nabla_\ell Z_{xA}\right)\left(\nabla_\ell Z^*_{xB}\right) , \qquad (A35)$$

$$Q^{(6)}_{Ai;Bj} \equiv \frac{K^2}{4\pi} \int_{V} d^3x \left(\nabla_j Z_{xA}\right)\left(\nabla_i Z^*_{xB}\right) . \qquad (A36)$$

In order to evaluate the above terms, we'll need the following identities, which can be obtained by integrating "by parts" and then converting volume integrals to surface integrals where possible:

$$Q^{(1)}_{Ai;Bj} = \frac{1}{4\pi}\int_{\mathcal{V}} d^3x\,(\nabla^2 Z_{xA})(\nabla_i\nabla_j Z^*_{xB})$$
$$+\frac{1}{4\pi}\oint_{\mathcal{S}} d^2x\left\{-\sum_{\ell=1}^{3}(\hat{n})_\ell(\nabla_\ell Z_{xA})(\nabla_i\nabla_j Z^*_{xB}) + (\hat{n})_i\sum_{\ell=1}^{3}(\nabla_\ell Z_{xA})(\nabla_\ell\nabla_j Z^*_{xB})\right\}, \qquad (A37)$$

$$Q^{(2)}_{Ai;Bj} + Q^{(6)}_{Ai;Bj} = \frac{K^2}{4\pi}\oint_{\mathcal{S}} d^2x\,(\hat{n})_i(\nabla_j Z_{xA})Z^*_{xB} \quad , \qquad (A38)$$

$$Q^{(5)}_{Ai;Bj} = \frac{\delta_{ij}K^2}{4\pi}\int_{\mathcal{V}} d^3x\,(\nabla^2 Z_{xA})Z^*_{xB} - \frac{\delta_{ij}K^2}{4\pi}\oint_{\mathcal{S}} d^2x\sum_{\ell=1}^{3}(\hat{n})_\ell(\nabla_\ell Z_{xA})Z^*_{xB} \quad . \qquad (A39)$$

Here, $\hat{\mathbf{n}}$ is the normal unit vector on the surface $\mathcal{S}$. We then have that

$$Q_{Ai;Bj} = \frac{1}{4\pi}\int_{\mathcal{V}} d^3x\left\{(\nabla^2 Z_{xA})(\nabla_i\nabla_j Z^*_{xB}) + \delta_{ij}K^2(\nabla^2 Z_{xA})Z^*_{xB}\right.$$
$$\left. + K^2 Z_{xA}(\nabla_i\nabla_j Z^*_{xB}) + \delta_{ij}K^4 Z_{xA}Z^*_{xB}\right\} \qquad (A40)$$
$$+\frac{1}{4\pi}\oint_{\mathcal{S}} d^2x\left\{(\hat{n})_i\sum_{\ell=1}^{3}(\nabla_\ell Z_{xA})\nabla_\ell\nabla_j Z^*_{xB} + (\hat{n})_i K^2(\nabla_j Z_{xA})Z^*_{xB}\right.$$
$$\left. -\sum_{\ell=1}^{3}(\hat{n})_\ell(\nabla_\ell Z_{xA})\nabla_i\nabla_j Z^*_{xB} - \sum_{\ell=1}^{3}(\hat{n})_\ell\,\delta_{ij}K^2(\nabla_\ell Z_{xA})Z^*_{xB}\right\}.$$

The above volume integral reduces to

$$\left\{\begin{matrix}\text{Volume integral}\\ \text{in Eq. A40}\end{matrix}\right\} = \frac{1}{4\pi}\int_{\mathcal{V}} d^3x\left[(\nabla^2+K^2)Z_{xA}\right]\left[(\nabla_i\nabla_j + \delta_{ij}K^2)Z^*_{xB}\right]$$
$$= \frac{1}{4\pi}\int_{\mathcal{V}} d^3x\left[-4\pi\delta^3(\vec{x}-\vec{Z}_A)\right]\left[\Omega^{D*}_{ij}(\vec{x}-\vec{Z}_B,\omega)\right] \qquad (A41)$$
$$= -\Omega^{D*}_{ij}(\vec{Z}_A-\vec{Z}_B,\omega) \quad .$$

Now we need to evaluate the surface integral in Eq. (A40). Here, we'll use the assumption described in Sec. 1 of this appendix, namely, that the surface $\mathcal{S}$ is far removed from any of the N dipole-particles. We'll ignore terms in the surface integral that become vanishingly small as the surface $\mathcal{S}$ is taken farther away from the particles. Further discussion on this approximation is given in Sec. 1.

Let the origin of our coordinate system be approximately near where the N particles are situated. Let $r=|\vec{x}|$ and $\hat{r}=\vec{x}/|\vec{x}|$. Retaining only the largest contributing terms in 1/r, yields the following approximation:

$$\nabla_i Z_{\rho A} = \frac{ik(\vec{x}-\vec{Z}_A)_i}{|\vec{x}-\vec{Z}_A|^2}\exp[ik|\vec{x}-\vec{Z}_A|] - \frac{(\vec{x}-\vec{Z}_A)_i}{|\vec{x}-\vec{Z}_A|^3}\exp[ik|\vec{x}-\vec{Z}_A|]$$
$$\approx \frac{ik(\vec{x})_i}{r^2}\exp[ik|\vec{x}-\vec{Z}_A|] \quad . \tag{A42}$$

Using this approximation, the first and second terms in the surface term in Eq. (A40) cancel, and we obtain

$$\begin{Bmatrix}\text{Surface integral}\\ \text{in Eq. A40}\end{Bmatrix} = \frac{ik^3}{4\pi}\oint_S d^2x\left\{(\hat{n}\cdot\hat{r})\left[(\hat{r})_i(\hat{r})_j-\delta_{ij}\right]\frac{e^{ik|\vec{x}-\vec{Z}_A|}\,e^{-ik|\vec{x}-\vec{Z}_B|}}{r^2} + O\left(\frac{1}{r^3}\right)\right\} . \tag{A43}$$

For future convenience, let

$$\vec{R}_{AB} \equiv \vec{Z}_B - \vec{Z}_A \quad , \tag{A44}$$

and, of course, $R_{AB}=|\vec{Z}_B-\vec{Z}_A|$.

A particularly convenient coordinate system to use in evaluating the surface integral in Eq. (A43) is the prolate spheroidal coordinate system.[39] To make use of this system, let's introduce primed coordinates $\vec{x}'$ via a translation vector $\vec{x}_o$ and a rotation matrix [O]:

$$\vec{x} = \vec{x}_o + [O]\,\vec{x}' \quad . \tag{A45}$$

Hence, we can define $\vec{Z}_A'$ and $\vec{Z}_B'$ via

$$\vec{Z}_A = \vec{x}_o + [O]\,\vec{Z}_A' \quad , \tag{A46}$$

$$\vec{Z}_B = \vec{x}_o + [O]\,\vec{Z}_B' \quad . \tag{A47}$$

Let us choose our origin and coordinate axes such that $\vec{Z}_A$'and $\vec{Z}_B$' are located at $-\hat{z}\cdot a$ and $+\hat{z}\cdot a$, respectively, so that $a \equiv \frac{1}{2}\cdot R_{AB}$. Adding and subtracting Eqs. (A46) and (A47) yields,

$$\vec{x}_o = \tfrac{1}{2}(\vec{Z}_A + \vec{Z}_B) \quad , \qquad (A48)$$

$$\vec{R}_{AB} = [O]\hat{z}(2a) \quad . \qquad (A49)$$

Thus, the primed coordinate system has its origin halfway along the line connecting $\vec{Z}_A$ to $\vec{Z}_B$, with its z axis along this direction.

As for the quantities in Eq. (A43),

$$\begin{aligned} |\vec{x} - \vec{Z}_A| &= |(\vec{x}_o + [O]\vec{x}') - (\vec{x}_o + [O](-\hat{z}a))| \\ &= |\vec{x}' + \hat{z}a| \quad , \qquad (A50) \end{aligned}$$

$$|\vec{x} - \vec{Z}_B| = |\vec{x}' - \hat{z}a| \quad . \qquad (A51)$$

Regarding the quantities $\hat{r}$ and $r=|\vec{x}|$ in Eq. (A43) that appear outside the quantities $\exp(ik|\vec{x}-\vec{Z}_A|)$ and $\exp(-ik|\vec{x}-\vec{Z}_B|)$, we can safely approximate them by

$$\hat{r} = \frac{\vec{x}_o + [o]\vec{x}'}{|\vec{x}_o + [o]\vec{x}'|} \approx \frac{[o]\vec{x}'}{|\vec{x}'|} \quad , \qquad (A52)$$

$$r = |\vec{x}_o + [o]\vec{x}'| \approx |\vec{x}'| \quad . \qquad (A53)$$

More specifically, we're assuming that the surface $\mathcal{S}$ is sufficiently far from all particles that the displacement $|\vec{x}_o|$ required to bring the origin of the primed coordinate system midway between two particles, is negligible compared to the distance $|\vec{x}'|$ to any point on the surface. Thus, for example, the $1/r^2$ term in Eq. (A43) becomes

$$\frac{1}{r^2} = \frac{1}{|\vec{x}_o + [O]\vec{x}'|^2} \approx \frac{1}{|\vec{x}'|^2}\left[1 - \frac{2\vec{x}_o\cdot[O]\vec{x}'}{|\vec{x}'|^2}\right] \quad . \tag{A54}$$

The correction term in Eq. (A54) just yields other $O(1/r^3)$ terms in Eq. (A43).

Consequently, Eq. (A43) becomes

$$\begin{Bmatrix}\text{Surface integral}\\ \text{in Eq. A40}\end{Bmatrix} \approx \frac{ik^3}{4\pi}\oint_{S'} d^2x'\left\{\left(\hat{n}'\cdot\frac{\vec{x}'}{|\vec{x}'|}\right)\left[\sum_{m=1}^{3}\sum_{n=1}^{3} O_{im}O_{jn}\left(\frac{\vec{x}'}{|\vec{x}'|}\right)_m\left(\frac{\vec{x}'}{|\vec{x}'|}\right)_n - \delta_{ij}\right]\frac{e^{ik|\vec{x}'+\hat{z}a|}\,e^{-ik|\vec{x}'-\hat{z}a|}}{|\vec{x}'|^2}\right\} . \tag{A55}$$

We can now introduce the prolate spheroidal coordinates (see Fig. 1 on the next page) via the following set of equations:

$$x' = a\sinh(u)\sin(v)\cos(\phi) \quad , \tag{A56}$$

$$y' = a\sinh(u)\sin(v)\sin(\phi) \quad , \tag{A57}$$

$$z' = a\cosh(u)\cos(v) \quad . \tag{A58}$$

We can then obtain the following relationships:

$$|\vec{x}' + \hat{z}a| = a\left(\cosh(u) + \cos(v)\right) \quad , \tag{A59}$$

$$|\vec{x}' - \hat{z}a| = a\left(\cosh(u) - \cos(v)\right) \quad , \tag{A60}$$

$$|\vec{x}'| = a\left[\sinh^2(u) + \cos^2(v)\right]^{1/2} \quad , \tag{A61}$$

$$d^3x' = h_u h_v h_\phi \, du\, dv\, d\phi \quad , \tag{A62}$$

$$h_u = h_v = a\left[\sin^2(v) + \sinh^2(u)\right]^{1/2} \quad , \tag{A63}$$

$$h_\phi = a\sinh(u)\sin(v) \quad , \tag{A64}$$

$$\vec{x}' = \frac{a^2}{h_u}\hat{e}_u\left[\cosh(u)\sinh(u)\right] - \frac{a^2}{h_u}\hat{e}_v\left[\cos(v)\sin(v)\right] \quad , \tag{A65}$$

where $\hat{e}_u$, $\hat{e}_v$, and $\hat{e}_\phi$ are unit directional vectors for the u, v, and ϕ coordinates. For a surface $\mathcal{S}$ far from the origin, we see from above that for points $\vec{x}$ on $\mathcal{S}$, $|\vec{x}'| \approx a\cdot\sinh(u) \approx a\cdot\frac{1}{2}\cdot\exp(u)$.

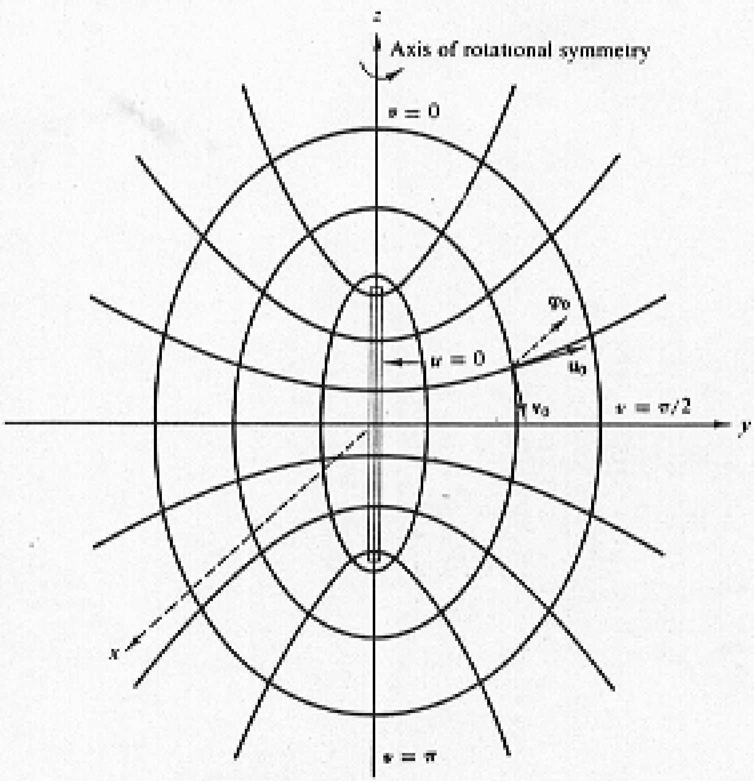

FIG. 1. Prolate spheroidal coordinates (u,v,ϕ). Figure reprinted with permission from Academic Press, out of Ref. 59, p. 104, Fig. 2.10.

Consider some volume $\mathcal{V}$ surrounding particles A and B, with a smooth surface $\mathcal{S}$ that can be described by the angles v and ϕ, so that the coordinate u on the surface can be described as $u_{max}(v,\phi)$. More specifically, let $\mathcal{S}$ be a surface such that the radius from the origin to each point on the surface varies continuously with v and ϕ.

As for the quantity $d^2x'\cdot\hat{n}'$ in Eq. (A55),

$$\hat{n}'d^2x' = \left(dv\,d\phi\,h_v h_\phi \hat{e}_u + du\,d\phi\,h_u h_\phi \hat{e}_v + du\,dv\,h_u h_v \hat{e}_\phi\right) \quad . \qquad (A66)$$

Here, du is related to dv and $d\phi$ by the function $u=u_{max}(v,\phi)$ that we are assuming describes the surface $\mathcal{S}$. Hence, the implicit assumption in Eq. (A66) is that

$$du = \frac{\partial u_{max}}{\partial v}dv + \frac{\partial u_{max}}{\partial \phi}d\phi \quad . \qquad (A67)$$

From above, for points on $\mathcal{S}$,

$$\frac{d^2x'\,\hat{n}'\cdot\vec{x}'}{|\vec{x}'|^3} = \frac{\left[\cosh(u_{max})\sinh^2(u_{max})\sin(v)dv\,d\phi - \sinh(u_{max})\cos(v)\sin^2(v)du\,dv\right]}{\left[\sinh^2(u_{max}) + \cos^2(v)\right]^{3/2}} \quad . \qquad (A68)$$

This quantity appears in Eq. (A55). For large u_{max}, the denominator above is approximately $\sinh^3(u_{max})$. The second term above contributes negligibly to the surface integral under our assumption of large $u_{max}(v,\phi)$. Hence,

$$\frac{d^2x'\,\hat{n}'\cdot\vec{x}'}{|\vec{x}'|^3} \approx \frac{\cosh(u_{max})}{\sinh(u_{max})}\sin(v)dv\,d\phi \approx \sin(v)dv\,d\phi \quad . \qquad (A69)$$

Equation (A55) now becomes

$$\left\{\begin{matrix}\text{Surface integral}\\ \text{in Eq. A40}\end{matrix}\right\} \approx \frac{ik^3}{4\pi}\sum_{m=1}^{3}\sum_{n=1}^{3} O_{im}O_{jn}\int_0^{2\pi}d\phi\int_0^{\pi}dv\sin(v)e^{ik2a\cos(v)}\left(\frac{\vec{x}'}{|\vec{x}'|}\right)_m\left(\frac{\vec{x}'}{|\vec{x}'|}\right)_n$$
$$-\frac{ik^3}{4\pi}\delta_{ij}\int_0^{2\pi}d\phi\int_0^{\pi}dv\sin v\, e^{ik2a\cos(v)} \quad . \qquad (A70)$$

From Eqs. (A56)-(A58),

$$\frac{\vec{x}'}{|\vec{x}'|} \approx \hat{x}\sin(v)\cos(\phi) + \hat{y}\sin(v)\sin(\phi) + \hat{z}\cos(v) \qquad (A71)$$

for large u_{max}. With $2a=R_{AB}$, one can now show that

$$\int_0^{2\pi} d\phi \int_0^{\pi} dv\,\sin(v)\, e^{ikR_{AB}\cos(v)} = \frac{4\pi\sin(kR_{AB})}{kR_{AB}} \quad , \qquad (A72)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} dv\,\sin(v) \left(\frac{\vec{x}'}{|\vec{x}'|}\right)_m \left(\frac{\vec{x}'}{|\vec{x}'|}\right)_n e^{ikR_{AB}\cos(v)}$$
$$= 4\pi\delta_{mn}\left\{ \left[-\frac{1}{(kR_{AB})^2}\cos(kR_{AB}) + \frac{1}{(kR_{AB})^3}\sin(kR_{AB})\right](\delta_{m1}+\delta_{m2}) \right. \qquad (A73)$$
$$\left. + \left[\frac{1}{kR_{AB}}\sin(kR_{AB}) + \frac{2}{(kR_{AB})^2}\cos(kR_{AB}) - \frac{2}{(kR_{AB})^3}\sin(kR_{AB})\right]\delta_{m3}\right\} \; .$$

Thus, the integral in Eq. (A73) equals zero unless m=n. Also, its m=n=1 and m=n=2 values are equal.

By now using the identity

$$\sum_{m=1}^{2} O_{im} O_{jn} = \delta_{ij} - O_{i3} O_{j3} \quad , \qquad (A74)$$

and realizing from Eq. (A49) that

$$O_{i3} = \frac{(\vec{R}_{AB})_i}{R_{AB}} \quad , \qquad (A75)$$

we can show that for A≠B,

$$\begin{Bmatrix} \text{Surface integral} \\ \text{in Eq. A40} \end{Bmatrix} \approx ik^3\,\mathrm{Im}\left[\left\{ -\frac{\left(\delta_{ij} - \frac{(\vec{R}_{AB})_i(\vec{R}_{AB})_j}{R_{AB}^2}\right)}{kR_{AB}} - i\,\frac{\left(\delta_{ij} - 3\frac{(\vec{R}_{AB})_i(\vec{R}_{AB})_j}{R_{AB}^2}\right)}{(kR_{AB})^2} \right.\right.$$
$$\left.\left. + \frac{\left(\delta_{ij} - 3\frac{(\vec{R}_{AB})_i(\vec{R}_{AB})_j}{R_{AB}^2}\right)}{(kR_{AB})^3} \right\} e^{ikR_{AB}}\right]$$
$$= -i\,\mathrm{Im}\left[\eta^{D}_{ij}(\vec{z}_B - \vec{z}_A, \omega)\right] \; . \qquad (A76)$$

The last step follows from Eq. (40) here, or Eq. (16) in Ref. 31.

Combining Eqs. (A26), (A40), (A41), and (A76) yields

$$Q_{Ai;Bj} \equiv \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x \left[n^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\, n^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{Z}_B,\omega) - \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\, \rho^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{Z}_B,\omega)\right]$$
$$\approx -\mathrm{Re}\, n^{\mathcal{D}}_{ij}(\vec{Z}_B-\vec{Z}_A,\omega) \quad , \qquad (A77)$$

for A≠B. The above relationship becomes exact as the surface $\mathcal{S}$ is removed to infinity.

Consequently, the difference in the electric and magnetic energy terms in Eqs. (A22) and (A23) is given by

$$\frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{\mathcal{D},B}(\vec{x},t) - \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{\mathcal{D},B}(\vec{x},t)\right\rangle$$
$$= \pi\int_0^\infty d\omega\, \mathcal{R}^2_{in}(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bj}\left\{-\frac{e^2}{m\omega}\,\mathrm{Re}\left[n^{\mathcal{D}}_{ij}(\vec{Z}_B-\vec{Z}_A,\omega)\right]\right\}\right] \quad , \qquad (A78)$$

for A≠B. Thus, the difference in these energies is essentially independent of the volume $\mathcal{V}$, at least for $\mathcal{V}$ sufficiently large.

Now let's turn to $F_{Ai;Bj}$ in Eq. (A27). Using Eq. (41), we obtain

$$F_{Ai;Bj} = -\left[Q^{(5)}_{Ai;Bj} + Q^{(6)}_{Ai;Bj}\right] \quad , \qquad (A79)$$

where these two terms are given in Eqs. (A35) and (A36). Using the identity of

$$\left(\nabla^2 + k^2\right)\left(\frac{e^{\pm ik|\vec{x}-\vec{x}_0|}}{|\vec{x}-\vec{x}_0|}\right) = -4\pi\delta^3(\vec{x}-\vec{x}_0) \quad , \qquad (A80)$$

for Z_{xA} in the first term in Eq. (A39), plus the approximation of Eq. (A42) for the surface term in Eq. (A39), yields

$$Q^{(5)}_{Ai;Bj} = \frac{\delta_{ij} k^2}{4\pi}\left[-k^2 \int_{\mathcal{V}} d^3x\, Z_{xA} Z^*_{xB} - \frac{4\pi e^{-ikR_{AB}}}{R_{AB}} - ik \oint_{\mathcal{S}} d^2x\, \hat{n}\cdot\hat{r}\, Z_{xA} Z^*_{xB} \right] . \qquad (A81)$$

As for $Q^{(6)}_{Ai;Bj}$,

$$Q^{(6)}_{Ai;Bj} = \frac{k^2}{4\pi} \nabla_{\vec{Z}_{Ai}} \nabla_{\vec{Z}_{Bj}} \left[\int_{\mathcal{V}} d^3x\, Z_{xA} Z^*_{xB} \right] , \qquad (A82)$$

where $\nabla_{Z_{Ai}}$ means to take the i^{th} component of the gradient with respect to $\vec{Z}_A$.

Thus, in order to evaluate $F_{Ai;Bj}$ in Eq. (A79), then we'll need to evaluate the following volume and surface integrals $I_{\mathcal{V}}$ and $I_{\mathcal{S}}$ that appear in Eqs. (A81) and (A82):

$$I_{\mathcal{V}} \equiv \int_{\mathcal{V}} d^3x\, Z_{xA} Z^*_{xB} , \qquad (A83)$$

$$I_{\mathcal{S}} \equiv \int_{\mathcal{S}} d^2x\, \hat{n}\cdot\hat{r}\, Z_{xA} Z^*_{xB} . \qquad (A84)$$

Turning to $I_{\mathcal{V}}$, the second line below was obtained by using the same translation vector and rotation matrix as in Eqs. (A45), (A48), and (A49). The third and fourth lines below follow from Eqs. (A56)-(A60) and (A62)-(A64):

$$\begin{aligned} I_{\mathcal{V}} &= \int_{\mathcal{V}} d^3x \frac{e^{ik|\vec{x}-\vec{Z}_A|}}{|\vec{x}-\vec{Z}_A|} \frac{e^{-ik|\vec{x}-\vec{Z}_B|}}{|\vec{x}-\vec{Z}_B|} \\ &= \int_{\mathcal{V}'} d^3x' \frac{e^{ik|\vec{x}'+\hat{z}a|}}{|\vec{x}'+\hat{z}a|} \frac{e^{-ik|\vec{x}'-\hat{z}a|}}{|\vec{x}'-\hat{z}a|} \\ &= \int_{\mathcal{V}'} du\,dv\,d\phi \cdot \frac{a^3(\sin^2(v)+\sinh^2(u))\sinh(u)\sin(v)\exp[2aik\cos(v)]}{a^2(\cosh(u)+\cos(v))(\cosh(u)-\cos(v))} \\ &= a \int_{\mathcal{V}'} du\,dv\,d\phi\, \sinh(u)\sin(v)\exp[2aik\cos(v)] , \end{aligned} \qquad (A85)$$

since $(\cosh^2 u - \cos^2 v) = (\sinh^2 u + \sin^2 v)$.

Let us again assume that the surface $\mathcal{S}$ of volume $\mathcal{V}$ can be described by the angles v and ϕ, so that the coordinate u on the surface can be specified as $u_{max}(v,\phi)$. The volume integral $I_\mathcal{V}$ then becomes

$$I_\mathcal{V} = a\int_0^{2\pi} d\phi \int_0^{\pi} dv \sin(v) \exp[2aik\cos(v)] \int_0^{u_{max}(v,\phi)} du \sinh(u)$$
$$= a\int_0^{2\pi} d\phi \int_0^{\pi} dv \sin(v) \exp[2aik\cos(v)] \left\{\cosh(u_{max}(v,\phi)) - 1\right\}$$
$$= \frac{R_{AB}}{2}\int_0^{2\pi} d\phi \int_0^{\pi} dv \sin(v)\, e^{ikR_{AB}\cos(v)} \cosh(u_{max}(v,\phi)) - \frac{2\pi}{k}\sin(kR_{AB}) \;, \qquad (A86)$$

since $R_{AB}=2a$.

We can't proceed any further in evaluating $I_\mathcal{V}$ without knowing the precise shape and size of $\mathcal{V}$, or, more specifically, without knowing u_{max}. As an example, however, just to see how the energy term of Eq. (A27) can depend on the size of $\mathcal{V}$, let's evaluate $I_\mathcal{V}$ when $u_{max}(v,\phi)$ is a constant. Since we're assuming that the approximate diameter of $\mathcal{V}$ is much larger than R_{AB}, then treating $u_{max}(v,\phi)$ as being a constant implies that $\mathcal{V}$ will be nearly spherical in shape, as can be seen from Eq. (A61). From Eq. (A86), $I_\mathcal{V}$ then becomes

$$I_\mathcal{V} = \frac{2\pi}{k}\sin(kR_{AB})\left[\cosh(u_{max}) - 1\right] \;. \qquad (A87)$$

Thus, under the above condition, $I_\mathcal{V}$ is roughly proportional to the radius of $\mathcal{V}$, since from Eq. (A61) the radius of $\mathcal{V}$ is approximately equal to $\frac{1}{2}R_{AB}\cdot\sinh(u_{max})\approx\frac{1}{2}R_{AB}\cdot\cosh(u_{max})$ for large u_{max}.

Turning now to $I_\mathcal{S}$ in Eq. (A84), we can follow the same steps and approximations we used in evaluating the surface integral in

Eq. (A40). In particular, with the use of Eq. (A69), I_δ becomes equivalent to Eq. (A72):

$$I_\delta \approx \int_0^{2\pi} d\phi \int_0^{\pi} dv \sin(v)\, e^{ik2a\cos(v)} = \frac{4\pi \sin(kR_{AB})}{kR_{AB}} \quad , \qquad (A88)$$

Thus, I_δ is essentially independent of γ for large γ, which was not the case for I_γ in Eq. (A86).

Summarizing, we obtain that

$$F_{Ai;Bj} = \frac{k^2}{4\pi}\left[\left(k^2\delta_{ij} - \nabla_{\bar{z}_{Ai}}\nabla_{\bar{z}_{Bj}}\right) I_\gamma\right] + \delta_{ij} k^2 \frac{\cos(kR_{AB})}{R_{AB}} \quad , \qquad (A89)$$

where I_γ is given in Eq. (A86). Substituting this result into Eq. (A23), then yields an expression for this magnetic field energy term. Since I_γ depends strongly on the size of γ, then so will this magnetic energy term. Indeed, for an approximately spherical volume γ, this energy term will be roughly proportional to the radius of the volume. Moreover, the electric field energy term in Eq. (A22) will behave similarly due to our result of Eq. (A78).

6. Calculation for $U_{EM,\mathcal{D}-in}$

6.a. Initial Setup

$$U_{EM,\mathcal{D}\text{-}in} \equiv \sum_{A=1}^{N} \frac{1}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{in}(\vec{x},t) + \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{in}(\vec{x},t)\right\rangle \quad . \qquad (A90)$$

Proceeding to evaluate the electric field correlation part,

$$\left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{in}(\vec{x},t)\right\rangle$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega_1 e^{-i\omega_1 t}\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\omega_2 e^{-i\omega_2 t}\sum_{i,j=1}^{3} \eta^{\mathcal{D}}_{ij}(\vec{x}-\vec{Z}_A,\omega_1)\, e\left\langle \delta\tilde{z}_{A_j}(\omega_1)\tilde{E}_{in\,i}(\vec{x},\omega_2)\right\rangle \quad , \qquad (A91)$$

$$\left\langle \delta\tilde{z}_{A_j}(\omega_1)\tilde{E}_{in\,i}(\vec{x},\omega)\right\rangle = \frac{e}{mC(\omega_1)}\sum_{B=1}^{N}\sum_{k=1}^{3}\left[M^{-1}(\omega_1)\right]_{Aj;Bk}\left\langle \tilde{E}_{in\,k}(\vec{Z}_B,\omega_1)\tilde{E}_{in\,i}(\vec{x},\omega_2)\right\rangle \quad . \qquad (A92)$$

From Eq. (A2), we then obtain that

$$\left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{in}(\vec{x},t)\right\rangle$$
$$= 2\pi\frac{e^2}{m}\int_0^{\infty} d\omega\,\frac{\mathcal{A}^2_{in}}{\omega}\,\mathrm{Im}\left[\frac{i}{C(\omega)}\sum_{B=1}^{N}\sum_{i,j,k=1}^{3}\left[M^{-1}(\omega)\right]_{A\underset{j}{i};Bk}\eta^{\mathcal{D}}_{ij}(\vec{x}-\vec{Z}_A,\omega)\,\mathrm{Im}\,\eta^{\mathcal{D}}_{ki}(\vec{x}-\vec{Z}_B,\omega)\right] \quad . \qquad (A93)$$

The magnetic field correlation part follows similarly. However, instead of making use of Eq. (A2), the following relationship is needed:

$$\left\langle \tilde{E}_{in\,k}(\vec{Z}_B,\omega_1)\tilde{B}_{in\,i}(\vec{x},\omega_2)\right\rangle$$
$$= 2\pi^2\int_0^{\infty} d\omega\,\frac{\mathcal{A}^2_{in}(\omega)}{\omega}\frac{1}{i}\left[\delta(\omega_1+\omega)\delta(\omega_2-\omega)-\delta(\omega_1-\omega)\delta(\omega_2+\omega)\right]\mathrm{Re}\,\rho^{\mathcal{D}}_{ki}(\vec{Z}_B-\vec{x},\omega) \quad . \qquad (A94)$$

This identity can be deduced from Eqs. (20) and (21) in Ref. 31. Consequently,

$$\left\langle \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{in}(\vec{x},t)\right\rangle$$
$$= 2\pi\frac{e^2}{m}\int_0^{\infty} d\omega\,\frac{\mathcal{A}^2_{in}}{\omega}\,\mathrm{Im}\left[\frac{-1}{C(\omega)}\sum_{B=1}^{N}\sum_{i,j,k=1}^{3}\left[M^{-1}(\omega)\right]_{A\underset{j}{i};Bk}\rho^{\mathcal{D}}_{ij}(\vec{x}-\vec{Z}_A,\omega)\,\mathrm{Re}\,\rho^{\mathcal{D}}_{ki}(\vec{Z}_B-\vec{x},\omega)\right] \quad . \qquad (A95)$$

If we make the changes of k->j, j->i, and i->ℓ for the dummy variable sums, and note from Eqs. (40) and (41) that

$$\eta^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_B,\omega) = +\eta^{\mathcal{D}}_{i\ell}(\vec{x}-\vec{Z}_B,\omega) \quad , \qquad (A96)$$

$$\rho^{\mathcal{D}}_{\ell i}(\vec{Z}_B-\vec{x},\omega) = +\rho^{\mathcal{D}}_{i\ell}(\vec{x}-\vec{Z}_B,\omega) \quad , \qquad (A97)$$

then we obtain that

$$\frac{2}{8\pi}\int_{\mathcal{V}} d^3x \left\langle \vec{E}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{E}_{in}(\vec{x},t) + \vec{B}_{\mathcal{D},A}(\vec{x},t)\cdot\vec{B}_{in}(\vec{x},t)\right\rangle$$
$$= \pi\int_0^\infty d\omega\, \ell^2_{in}(\omega)\,\mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{B=1}^{N}\sum_{i,j=1}^{3}\left[M^{-1}(\omega)\right]_{Ai;Bj}\left\{\frac{e^2}{m\omega}\mathcal{P}_{Ai;Bj}\right\}\right] \quad , \qquad (A98)$$

where

$$\mathcal{P}_{Ai;Bj} \equiv \frac{1}{2\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\left[i\eta^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\,\mathrm{Im}\,\eta^{\mathcal{D}}_{\ell j}(\vec{x}-\vec{Z}_B,\omega) - \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\,\mathrm{Re}\,\rho^{\mathcal{D}}_{\ell j}(\vec{x}-\vec{Z}_B,\omega)\right] \quad . \qquad (A99)$$

Our task now reduces to evaluating $P_{Ai;Bj}$. Substituting in for the above imaginary and real parts in Eq. (A99), yields

$$\mathcal{P}_{Ai;Bj} = \mathcal{P}^{I}_{Ai;Bj} + \mathcal{P}^{II}_{Ai;Bj} \quad , \qquad (A100)$$

where

$$\mathcal{P}^{I}_{Ai;Bj} = \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\left[\eta^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\eta^{\mathcal{D}}_{\ell j}(\vec{x}-\vec{Z}_B,\omega) - \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\rho^{\mathcal{D}}_{\ell j}(\vec{x}-\vec{Z}_B,\omega)\right] \quad , \qquad (A101)$$

$$\mathcal{P}^{II}_{Ai;Bj} = -\frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x\left[\eta^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\eta^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{Z}_B,\omega) + \rho^{\mathcal{D}}_{\ell i}(\vec{x}-\vec{Z}_A,\omega)\rho^{\mathcal{D}*}_{\ell j}(\vec{x}-\vec{Z}_B,\omega)\right] \quad . \qquad (A102)$$

Thus, from Eq. (A24),

$$\mathcal{P}^{II}_{Ai;Bj} = -\,E_{Ai;Bj} \quad . \qquad (A103)$$

As mentioned in the previous section, we will show that the A≠B terms of $E_{Ai;Bj}$ drop out upon summing $U_{EM,\mathcal{D}-\mathcal{D}}$ and $U_{EM,\mathcal{D}-in}$.

Indeed, from Eq. (A103), we're close to proving this fact. However, Eq. (A25) contains only the real part of $E_{Ai;Bj}$, whereas Eqs. (A98), (A100), and (A103) deal with the whole of $E_{Ai;Bj}$. We can resolve this difference by (1) summing Eq. (A98) over A, and (2) using the fact that $[M^{-1}]_{Ai;Bj}$ is invariant upon switching the dummy variables A and B, and i and j. More specifically,

$$U_{EM,\mathcal{B}\text{-}in} = \pi\int_0^\infty d\omega\, \mathcal{A}^2_{in}(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}[M^{-1}]_{Ai;Bj}\left\{\frac{e^2}{m\omega}\mathcal{P}_{Ai;Bj}\right\}\right] \quad , \qquad \text{(A104)}$$

$$\begin{aligned}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}[M^{-1}]_{Ai;Bj}\mathcal{P}_{Ai;Bj} &= \frac{1}{2}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}\left([M^{-1}]_{Ai;Bj}\mathcal{P}_{Ai;Bj} + [M^{-1}]_{Bj;Ai}\mathcal{P}_{Bj;Ai}\right)\\ &= \sum_{A,B=1}^{N}\sum_{i,j=1}^{3}[M^{-1}]_{Ai;Bj}\,\frac{1}{2}\left(\mathcal{P}_{Ai;Bj} + \mathcal{P}_{Bj;Ai}\right) \quad . \qquad \text{(A105)}\end{aligned}$$

From Eqs. (A100)-(A102),

$$\frac{1}{2}\left(\mathcal{P}_{Ai;Bj} + \mathcal{P}_{Bj;Ai}\right) = \mathcal{P}^{I}_{Ai;Bj} + \mathrm{Re}\left[\mathcal{P}^{II}_{Ai;Bj}\right] \quad . \qquad \text{(A106)}$$

Hence, we indeed obtain

$$U_{EM,\mathcal{B}\text{-}in} = \pi\int_0^\infty d\omega\, \mathcal{A}^2_{in}(\omega)\, \mathrm{Im}\left[\frac{1}{C(\omega)}\sum_{A,B=1}^{N}\sum_{i,j=1}^{3}[M^{-1}]_{Ai;Bj}\left\{\frac{e^2}{m\omega}\left(\mathcal{P}^{I}_{Ai;Bj} - \mathrm{Re}\left[E_{Ai;Bj}\right]\right)\right\}\right] , \quad \text{(A107)}$$

thereby showing, via Eqs. (A21), (A25), and (A107), that the A≠B terms of $E_{Ai;Bj}$ do drop out of the sum of $U_{EM,\mathcal{B}-\mathcal{B}}$ and $U_{EM,\mathcal{B}-in}$.

Thus, for the A≠B case, we only need to find $P^{I}_{Ai;Bj}$. This quantity looks very much like $Q_{Ai;Bj}$, as can be seen by comparing Eqs. (A26) and (A101). As was true with $Q_{Ai;Bj}$ for A≠B, $P^{I}_{Ai;Bj}$ will turn out to be essentially independent of γ, when γ is large. Let's turn to this A≠B case now, and then come back to the A=B situation later.

6.b. A≠B Calculation

From Eqs. (40) and (41),

$$\mathcal{P}^{I}_{Ai;Bj} = \sum_{m=1}^{6} \mathcal{P}^{I(m)}_{Ai;Bj} \quad , \qquad (A108)$$

where

$$\mathcal{P}^{I(1)}_{Ai;Bj} \equiv \frac{1}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x \left(\nabla_\ell \nabla_i Z_{xA}\right)\left(\nabla_\ell \nabla_j Z_{xB}\right) , \qquad (A109)$$

$$\mathcal{P}^{I(2)}_{Ai;Bj} \equiv \frac{K^2}{4\pi}\int_{\mathcal{V}} d^3x \left(\nabla_i \nabla_j Z_{xA}\right) Z_{xB} \quad , \qquad (A110)$$

$$\mathcal{P}^{I(3)}_{Ai;Bj} \equiv \frac{K^2}{4\pi}\int_{\mathcal{V}} d^3x \, Z_{xA}\left(\nabla_i \nabla_j Z_{xB}\right) \quad , \qquad (A111)$$

$$\mathcal{P}^{I(4)}_{Ai;Bj} \equiv \frac{\delta_{ij} K^4}{4\pi}\int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} \quad , \qquad (A112)$$

$$\mathcal{P}^{I(5)}_{Ai;Bj} \equiv +\frac{\delta_{ij} K^2}{4\pi}\sum_{\ell=1}^{3}\int_{\mathcal{V}} d^3x \left(\nabla_\ell Z_{xA}\right)\left(\nabla_\ell Z_{xB}\right) , \qquad (A113)$$

$$\mathcal{P}^{I(6)}_{Ai;Bj} \equiv -\frac{K^2}{4\pi}\int_{\mathcal{V}} d^3x \left(\nabla_j Z_{xA}\right)\left(\nabla_i Z_{xB}\right) \quad . \qquad (A114)$$

From Eq. (A113),

$$\mathcal{P}^{I(5)}_{Ai;Bj} = \frac{\delta_{ij} K^2}{4\pi}\left[\sum_{\ell=1}^{3}\oint_{\mathcal{S}} d^2x (\hat{n})_\ell \, Z_{xA} \nabla_\ell Z_{xB} - \int_{\mathcal{V}} d^3x \, Z_{xA} \nabla^2 Z_{xB}\right]$$

$$= \frac{\delta_{ij} K^2}{4\pi}\left[\sum_{\ell=1}^{3}\oint_{\mathcal{S}} d^2x (\hat{n})_\ell \, Z_{xA} \nabla_\ell Z_{xB} + 4\pi \frac{e^{iKR_{AB}}}{R_{AB}} + K^2 \int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB}\right] . \qquad (A115)$$

Hence,

$$\mathcal{P}^{I(4)}_{Ai;Bj} + \mathcal{P}^{I(5)}_{Ai;Bj} = \delta_{ij} K^2 \left(Y_{AB} + \frac{e^{iKR_{AB}}}{R_{AB}} \right) \quad , \qquad (A116)$$

where

$$Y_{AB} \equiv \frac{K^2}{2\pi}\int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} + \frac{1}{4\pi}\sum_{\ell=1}^{3}\oint_{\mathcal{S}} d^2x (\hat{n})_\ell \, Z_{xA} \nabla_\ell Z_{xB} \, . \qquad (A117)$$

As will be seen shortly, our main task of evaluating the sum of integrals in Eq. (A108) will reduce to evaluating Y_{AB}.

Turning to the remaining terms in Eq. (A109)-(A114),

$$\mathcal{P}^{I(1)}_{Ai;Bj} = \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{1}{4\pi} \sum_{\ell=1}^{3} \int_{\mathcal{V}} d^3x \left(\nabla_\ell Z_{xA}\right) \nabla_\ell Z_{xB} \right\}$$

$$= \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{1}{4\pi} \sum_{\ell=1}^{3} \oint_{\mathcal{S}} d^2x (\hat{n})_\ell Z_{xA} \nabla_\ell Z_{xB} + \frac{e^{i\kappa R_{AB}}}{R_{AB}} + \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} \right\}, \quad (A118)$$

$$\mathcal{P}^{I(2)}_{Ai;Bj} = \frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_j \left(\nabla_i Z_{xA}\right) Z_{xB} - \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, \nabla_i Z_{xA} \nabla_j Z_{xB}$$

$$= \frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_j \left(\nabla_i Z_{xA}\right) Z_{xB} - \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} \right\} , \quad (A119)$$

$$\mathcal{P}^{I(3)}_{Ai;Bj} = \frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_i Z_{xA} \nabla_j Z_{xB} - \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} \right\} , \quad (A120)$$

$$\mathcal{P}^{I(6)}_{Ai;Bj} = -\frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_j Z_{xA} \nabla_i Z_{xB} + \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, Z_{xA} \nabla_i \nabla_j Z_{xB}$$

$$= -\frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_j Z_{xA} \nabla_i Z_{xB} + \frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x (\hat{n})_i Z_{xA} \nabla_j Z_{xB} - \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{\kappa^2}{4\pi} \int_{\mathcal{V}} d^3x \, Z_{xA} Z_{xB} \right\} . \quad (A12$$

Adding the above quantities, we obtain one part where Y_{AB} appears, plus a term $\xi_{Ai;Bj}$ that is a sum of surface integrals:

$$\mathcal{P}^{I(1)}_{Ai;Bj} + \mathcal{P}^{I(2)}_{Ai;Bj} + \mathcal{P}^{I(3)}_{Ai;Bj} + \mathcal{P}^{I(6)}_{Ai;Bj}$$

$$= \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{e^{i\kappa R_{AB}}}{R_{AB}} - Y_{AB} \right\} + \xi_{Ai;Bj} , \quad (A122)$$

$$\xi_{Ai;Bj} = 2 \nabla_{\vec{z}_{Ai}} \nabla_{\vec{z}_{Bj}} \left\{ \frac{1}{4\pi} \sum_{\ell=1}^{3} \oint_{\mathcal{S}} d^2x (\hat{n})_\ell Z_{xA} \nabla_\ell Z_{xB} \right\}$$

$$+ \frac{\kappa^2}{4\pi} \oint_{\mathcal{S}} d^2x \left\{ (\hat{n})_j \left(\nabla_i Z_{xA}\right) Z_{xB} + 2 (\hat{n})_i Z_{xA} \nabla_j Z_{xB} - (\hat{n})_j Z_{xA} \nabla_i Z_{xB} \right\} . \quad (A123)$$

We can simplify $\xi_{Ai;Bj}$ somewhat. For $\mathcal{S}$ far away from the particles, we can use Eq. (A42) and show that the second term in

Eq. (A123) is approximately

$$\frac{ik^3}{4\pi}\oint_{\mathcal{S}} d^2x (\hat{n})_j (\hat{r})_i Z_{xA} Z_{xB} ,$$

while the fourth term yields its negative. The first and third terms in Eq. (A123) result in the first and second terms below, respectively:

$$\xi_{Ai;Bj} \approx \frac{ik^3}{2\pi}\oint_{\mathcal{S}} d^2x \left\{ \left[-(\hat{n}\cdot\hat{r})(\hat{r})_i(\hat{r})_j + (\hat{n})_i(\hat{r})_j \right] Z_{xA}\, Z_{xB} \right\} . \qquad (A124)$$

It should be noted that when the surface $\mathcal{S}$ is a sphere, then $\hat{\mathbf{n}}=\hat{\mathbf{r}}$, and $\xi_{Ai;Bj}$ vanishes. In general, though, the surface term is not equal to zero. However, it does become negligibly small when the surface $\mathcal{S}$ is taken to be far away from $\vec{Z}_A$ and $\vec{Z}_B$. Let's assume for the moment that $\xi_{Ai;Bj}$ is indeed negligible, and then return to prove this point at the end of this section.

Summarizing from Eqs. (A108), (A116), (A122), and neglecting $\xi_{Ai;Bj}$,

$$\mathcal{P}^{I}_{Ai;Bj} = k^2\delta_{ij}\left(Y_{AB} + \frac{e^{ikR_{AB}}}{R_{AB}} \right) + \nabla_{\vec{Z}_{Ai}} \nabla_{\vec{Z}_{Bj}} \left(-Y_{AB} + \frac{e^{ikR_{AB}}}{R_{AB}} \right) . \qquad (A125)$$

Thus, our problem reduces to finding Y_{AB} in Eq. (A117). Let's now turn to this task.

Again, let us introduce prolate spheroidal coordinates.[58] Following the same steps as in Eqs. (A85)-(A86) yields

$$\frac{k^2}{2\pi}\int_V d^3x\, Z_{xA} Z_{xB} = \frac{k^2}{2\pi}\int_V d^3x\, \frac{e^{ik|\vec{x}-\vec{z}_A|}}{|\vec{x}-\vec{z}_A|}\,\frac{e^{ik|\vec{x}-\vec{z}_B|}}{|\vec{x}-\vec{z}_B|}$$

$$= \frac{k^2}{2\pi}\int_{V'} du\,dv\,d\phi \cdot \frac{a^3\left(\sin^2(v)+\sinh^2(u)\right)\sinh(u)\sin(v)\exp\left[2aik\cosh(u)\right]}{a^2\left(\cosh(u)+\cos(v)\right)\left(\cosh(u)-\cos(v)\right)}$$

$$= \frac{k^2}{2\pi}a\int_0^{\pi} dv\sin(v)\int_0^{2\pi} d\phi\left\{\int_0^{u_{max}(v,\phi)} du\sinh(u)\exp\left[2aik\cosh(u)\right]\right\}$$

$$= \frac{k^2}{2\pi}a\int_0^{\pi} dv\sin(v)\int_0^{2\pi} d\phi\left\{\frac{\exp\left[2aik\cosh(u_{max}(v,\phi))\right]}{2aik} - \frac{\exp\left[2aik\right]}{2aik}\right\}$$

$$= ike^{ik2a} - \frac{ik}{4\pi}\int_0^{\pi} dv\sin(v)\int_0^{2\pi} d\phi\exp\left[2aik\cosh(u_{max}(v,\phi))\right] \quad . \qquad (A126)$$

Turning now to the surface integral in Y_{AB} in Eq. (A117), the first line below follows from Eq. (A42) and from retaining terms only proportional to $1/r^2$, as was done in Eq. (A43). The second line below follows from introducing the translation vector and rotation matrix in Eqs. (A48)-(A49), and from following the steps and approximations accompanying Eqs. (A50)-(A54). The third line comes from Eqs. (A59), (A60), and (A68):

$$\frac{1}{4\pi}\sum_{\ell=1}^{3}\oint_S d^2x\,(\hat{n}_\ell) Z_{xA}\nabla_\ell Z_{xB} \approx \frac{ik}{4\pi}\oint_S d^2x\,\frac{\hat{n}\cdot\vec{x}}{r^3}\exp\left[ik\left(|\vec{x}-\vec{z}_A|+|\vec{x}-\vec{z}_B|\right)\right]$$

$$\approx \frac{ik}{4\pi}\oint_{S'} d^2x'\,\frac{\hat{n}'\cdot\vec{x}'}{|\vec{x}'|^3}\exp\left[ik\left(|\vec{x}'+\hat{z}a|+|\vec{x}'-\hat{z}a|\right)\right] \qquad (A127)$$

$$= \frac{ik}{4\pi}\oint_{S'}\left\{\frac{\cosh(u)\sinh^2(u)\sin(v)\,dv\,d\phi - \sinh(u)\cos(v)\sin^2(v)\,du\,dv}{\left(\sinh^2(u)+\cos^2(v)\right)^{3/2}}\right\}\Bigg|_{u=u_{max}(v,\phi)} e^{ik2a\cosh(u_{max})} \; .$$

Since the denominator is approximately $\sinh^3(u_{max})$ for large u_{max}, then the second term in the surface integral above will be negligible compared to the first one and will go to zero as the minimum value of u on the surface S goes to infinity. Making the approximation that cosh(u)≈sinh(u) in the first integral above, then yields

$$\frac{1}{4\pi}\sum_{\ell=1}^{3}\oint_{\mathcal{S}} d^2x\,(\hat{n})_\ell\, Z_{xA}\nabla_\ell Z_{xB} \approx \frac{iK}{4\pi}\int_0^{\pi} dv\,\sin(v)\int_0^{2\pi} d\phi\,\exp\left[2aiK\cosh\left(u_{max}(v,\phi)\right)\right] \quad , \qquad (A128)$$

where correction terms to this result vanish as the minimum value of u on the surface becomes increasingly large.

Combining Eqs. (A117), (A126), and (A128), yields

$$Y_{AB} \approx iKe^{iKR_{AB}} \quad , \qquad (A129)$$

since $2a=R_{AB}$.

Now let us turn back to Eq. (A125). We obtain

$$\begin{aligned}\mathcal{P}^{II}_{Ai;Bj} &= K^2\delta_{ij}\left(iKe^{iKR_{AB}} + \frac{e^{iKR_{AB}}}{R_{AB}}\right) + \nabla_{\vec{Z}_{Ai}}\nabla_{\vec{Z}_{Bj}}\left(-iKe^{iKR_{AB}} + \frac{e^{iKR_{AB}}}{R_{AB}}\right)\\ &= \left(-1 + K\frac{d}{dK}\right)\left\{\left(-\nabla_{\vec{Z}_{Ai}}\nabla_{\vec{Z}_{Bj}} + K^2\delta_{ij}\right)\frac{e^{iK|\vec{Z}_B-\vec{Z}_A|}}{|\vec{Z}_B-\vec{Z}_A|}\right\}\\ &= \left(-1 + K\frac{d}{dK}\right)\left\{\left(\nabla_{\vec{Z}_{Bi}}\nabla_{\vec{Z}_{Bj}} + K^2\delta_{ij}\right)\frac{e^{iKR_{AB}}}{R_{AB}}\right\}\\ &= \left(-1 + K\frac{d}{dK}\right)\mathcal{R}^{D}_{ij}\left(\vec{R}_{AB},\omega\right) \quad . \end{aligned} \qquad (A130)$$

for A≠B.

Combining this result with Eq. (A107) shows that we've now verified the result given in Eq. (53) for the A≠B case, except for our required demonstration that $\xi_{Ai;Bj}$ in Eq. (A122) can indeed be neglected. Let's now complete this task.

As noted immediately following Eq. (A124), for a spherical surface $\mathcal{S}$, $\xi_{Ai;Bj}$ equals zero. Hence, we can add to our expression for $\xi_{Ai;Bj}$ the negative of the same integrand, but evaluated over a sphere that encloses $\mathcal{S}$. Let's call this sphere $\mathcal{S}_{outer}$. Rewriting Eq. (A124),

$$\xi_{Ai;Bj} \approx \frac{ik^3}{2\pi} \sum_{\ell=1}^{3} \oint_{\mathcal{S}} d^2x\, (\hat{n})_\ell \left\{ \left[-(\hat{r})_\ell (\hat{r})_i (\hat{r})_j + \delta_{i\ell} (\hat{r})_j \right] \frac{e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|}}{r^2} \right\}$$

$$= -\frac{ik^3}{2\pi} \sum_{\ell=1}^{3} \oint_{(\mathcal{S}_{outer} \& \mathcal{S})} d^2x\, (\hat{n})_\ell \left\{ \left[-(\hat{r})_\ell (\hat{r})_i (\hat{r})_j + \delta_{i\ell} (\hat{r})_j \right] \frac{e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|}}{r^2} \right\} . \quad (A131)$$

In the first line above, Z_{xA} was approximated by using $1/|\vec{x}-\vec{z}_A| \approx 1/|\vec{x}|$, and similarly for Z_{xB}. In the second line above, the unit normal vector was taken to be pointing inward instead of outward on $\mathcal{S}$, so the minus sign was added. Let $\hat{n}$ be defined to be along the outward direction on $\mathcal{S}_{outer}$. Via the divergence theorem, we can then rewrite the above surface integral as a volume integral over the volume enclosed between $\mathcal{S}_{outer}$ and $\mathcal{S}$, which we'll call $\Delta\mathcal{V}$:

$$\xi_{Ai;Bj} = -\frac{ik^3}{2\pi} \sum_{\ell=1}^{3} \int_{\Delta\mathcal{V}} d^3x\, \nabla_\ell \left\{ \left[-(\hat{r})_\ell (\hat{r})_i (\hat{r})_j + \delta_{i\ell} (\hat{r})_j \right] \frac{e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|}}{r^2} \right\} . \quad (A132)$$

Using the relationships of

$$\nabla_n (\hat{r})_m = \frac{\delta_{nm} - (\hat{r})_n (\hat{r})_m}{r} \quad , \quad (A133)$$

$$(\hat{r}\cdot\vec{\nabla})(\hat{r})_m = 0 \quad , \quad (A134)$$

one can show that

$$\sum_{\ell=1}^{3} \nabla_\ell \left\{ \left[-(\hat{r})_\ell (\hat{r})_i (\hat{r})_j + \delta_{i\ell} (\hat{r})_j \right] \frac{e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|}}{r^2} \right\}$$

$$= e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|} (\hat{r})_j \frac{ik}{r^2} \left\{ -(\hat{r})_i \frac{(\vec{x}-\vec{z}_A)\cdot\hat{r}}{|\vec{x}-\vec{z}_A|} - (\hat{r})_i \frac{(\vec{x}-\vec{z}_B)\cdot\hat{r}}{|\vec{x}-\vec{z}_B|} + \frac{(\vec{x}-\vec{z}_A)_i}{|\vec{x}-\vec{z}_A|} + \frac{(\vec{x}-\vec{z}_B)_i}{|\vec{x}-\vec{z}_B|} \right\}$$

$$+ e^{ik|\vec{x}-\vec{z}_A|} e^{ik|\vec{x}-\vec{z}_B|} \frac{\left(\delta_{ij} - 3(\hat{r})_i (\hat{r})_j\right)}{r^3} . \quad (A135)$$

The quantity in brackets in the first term on the RHS is equal to
$$\left\{ \frac{(\hat{r})_i(\vec{Z}_A\cdot\hat{r})-(\vec{Z}_A)_i}{|\vec{x}-\vec{Z}_A|} + \frac{(\hat{r})_i(\vec{Z}_B\cdot\hat{r})-(\vec{Z}_B)_i}{|\vec{x}-\vec{Z}_B|} \right\} .$$
For the integrand in Eq. (A132) integrated over ΔV, we can safely approximate the above quantity in brackets by using $1/|\vec{x}-\vec{Z}_A| \approx 1/|\vec{x}-\vec{Z}_B| \approx 1/|\vec{x}|$. Consequently,

$$\xi_{Ai;Bj} \approx \frac{-ik^3}{2\pi}\int_{\Delta V} d^3x \frac{e^{ik|\vec{x}-\vec{Z}_A|}\,e^{ik|\vec{x}-\vec{Z}_B|}}{r^3}\left\{ \left[ik(\vec{Z}_A+\vec{Z}_B)\cdot\hat{r}\right](\hat{r})_i - ik(\vec{Z}_A+\vec{Z}_B)_i + (\delta_{ij}-3(\hat{r})_i(\hat{r})_j)\right\} . \qquad (A136)$$

We wish to show that $\xi_{Ai;Bj} \to 0$ as the minimum radius of $\mathcal{S}$ becomes large. We can demonstrate this result, without carrying out the full integrations above, by noting that the quantity in brackets in Eq. (A136) depends on $\vec{x}$ only through the directional vector $\hat{r}$. If we ignore this dependence, then we'll be concerned with the quantity
$$\int_{\Delta V} d^3x \frac{e^{ik|\vec{x}-\vec{Z}_A|}\,e^{ik|\vec{x}-\vec{Z}_B|}}{r^3} .$$
The $1/r^3$ factor, plus the oscillatory behavior with radius of the exponential factors, are what make this quantity go to zero as $\mathcal{S}$ is removed far from the particles. More specifically, the above quantity behaves similarly to

$$\int_{\Delta V} d^3x \frac{e^{ik2|\vec{x}|}}{|\vec{x}|^3} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_{r_{max}(\theta,\phi)}^{r_{outer}} dr\, r^2 \frac{e^{ik2r}}{r^3} , \qquad (A137)$$

where spherical coordinates have been used, the radius of the surface $\mathcal{S}$ has been written as a function of Θ and ϕ, and the radius of $\mathcal{S}_{outer}$ has been denoted as r_{outer}. The integral

$$\mathcal{J}(\theta,\phi) \equiv \int_{r_{max}(\theta,\phi)}^{r_{outer}} dr \cdot \left\{ \frac{e^{ik2r}}{r} \right\} \quad , \qquad (A138)$$

goes to zero as $r_{max}(\theta,\phi)\to\infty$ and for $r_{max}<r_{outer}$, as can been seen from Ref. 60 via the following: (a) entries # 2.6322 and 2.6324 on p. 183 with $\mu=0$ and $a=2k$, (b) entry # 8.3502 on p. 940 with $\alpha=0$, and (c) entry # 8.357 on p. 942 with $\alpha=0$ and, for example, $M=1$.

Thus, if we examine the magnitude of the quantity in Eq. (A137), then

$$\begin{aligned} \left| \int_{\Delta V} d^3x \, \frac{e^{ik|\vec{x}|}}{|\vec{x}|^3} \right| &= \left| \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \, \mathcal{J}(\theta,\phi) \right| \\ &\le \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \left| \mathcal{J}(\theta,\phi) \right| \qquad (A139) \\ &\le 4\pi J_{max} \quad , \end{aligned}$$

where J_{max} is the maximum value of $|\mathcal{J}(\theta,\phi)|$. Since $J_{max}\to 0$, then we've shown that the magnitude of Eq. (A137) also goes to zero. The quantity $\mathcal{E}_{Ai;Bj}$ in Eq. (A136) will behave similarly.

6.c. <u>A=B Calculation</u>

We now need to evaluate the A=B term in the curly brackets in either Eq. (A104) or Eq. (A107). First, it's helpful to note that

$$\mathcal{P}_{Ai;Bj} = \mathcal{P}^{I}_{Ai;Bj} - \mathcal{R}e\left[E_{Ai;Bj}\right] \quad , \text{ for A=B,} \qquad (A140)$$

as can be verified from Eqs. (A99)-(A103). Now, let's break the calculation of $P_{Ai;Aj}$ into two parts: namely, $\mathrm{Im}(P_{Ai;Aj})$ and $\mathrm{Re}(P_{Ai;Aj})$. To find $\mathrm{Im}(P_{Ai;Aj})$, we can use the result of the last section and let $R_{AB}\to 0$, since $\mathrm{Im}(\eta^{D}_{ij}(R_{AB},w)$ is not singular as $R_{AB}\to 0$. More specifically, by expanding exp(ikR) in a Taylor's series in Eq. (40), one can show that

$$\lim_{R\to 0} \mathrm{Im}\, \eta^{D}_{ij}(\hat{R}R,\omega) = \delta_{ij}\frac{2}{3}k^3 \quad . \qquad (A141)$$

Consequently, from Eqs. (A140), (A141), and (A130),

$$\begin{aligned}\mathrm{Im}(P_{Ai;Aj}) &= \lim_{R_{AB}\to 0} \mathrm{Im}\left(P^{I}_{Ai;Bj} - \mathrm{Re}[E_{Ai;Bj}]\right) \\ &= \left(-1 + k\frac{d}{dk}\right)\delta_{ij}\frac{2}{3}k^3 \qquad (A142) \\ &= \delta_{ij}\frac{4}{3}k^3 \quad .\end{aligned}$$

Turning now to $\mathrm{Re}(P_{Ai;Aj})$, from Eqs. (A99), (40) and (41),

$$\begin{aligned}&\mathrm{Re}(P_{Ai;Aj}) \\ &= -\frac{1}{2\pi}\sum_{l=1}^{3}\int_{V} d^3x\left\{\mathrm{Im}\,\eta^{D}_{li}(\vec{x}-\vec{z}_A,\omega)\,\mathrm{Im}\,\eta^{D}_{lj}(\vec{x}-\vec{z}_A,\omega) + \mathrm{Re}\,\rho^{D}_{li}(\vec{x}-\vec{z}_A,\omega)\,\mathrm{Re}\,\rho^{D}_{lj}(\vec{x}-\vec{z}_A,\omega)\right\} \\ &= -\frac{1}{2\pi}\int_{V} d^3x\left\{\sum_{l=1}^{3}(\nabla_l\nabla_i\mathcal{J})(\nabla_l\nabla_j\mathcal{J}) + 2k^2\mathcal{J}\nabla_i\nabla_j\mathcal{J} + k^4\delta_{ij}\mathcal{J}^2\right. \\ &\qquad\left. + k^2\delta_{ij}\sum_{l=1}^{3}(\nabla_l\mathcal{J})\nabla_l\mathcal{J} - k^2(\nabla_j\mathcal{J})\nabla_i\mathcal{J}\right\} \quad , \qquad (A143)\end{aligned}$$

where

$$\mathcal{J} = \frac{\sin(k|\vec{x}-\vec{z}_A|)}{|\vec{x}-\vec{z}_A|} \quad . \qquad (A144)$$

We can rewrite the first term in Eq. (A143) as

$$\sum_{l=1}^{3}\int_{V} d^3x(\nabla_l\nabla_i\mathcal{J})(\nabla_l\nabla_i\mathcal{J}) = \sum_{l=1}^{3}\oint_{S} d^2x(\hat{n})_l(\nabla_i\mathcal{J})(\nabla_l\nabla_j\mathcal{J}) - \sum_{l=1}^{3}\int_{V} d^3x\,\nabla_i\mathcal{J}\,\nabla_j(\nabla^2\mathcal{J}) \quad , \qquad (A145)$$

and use the relationship

$$\nabla^2 \vartheta = -k^2 \vartheta \quad . \qquad (A146)$$

Likewise, the fourth term in Eq. (A143) can be rewritten via

$$\sum_{\ell=1}^{3} \int_V d^3x (\nabla_\ell \vartheta)(\nabla_\ell \vartheta) = \sum_{\ell=1}^{3} \oint_S d^2x (\hat{n})_\ell \vartheta \nabla_\ell \vartheta + k^2 \int_V d^3x \vartheta^2 . \qquad (A147)$$

Also, we can rewrite the second term in (A143) as

$$\int_V d^3x \vartheta \nabla_i \nabla_j \vartheta = \oint_S d^2x (\hat{n})_i \vartheta \nabla_j \vartheta - \int_V d^3x (\nabla_i \vartheta)(\nabla_j \vartheta) . \qquad (A148)$$

Combining the above,

$$R_e(P_{Ai;Aj}) = -\frac{K^2}{\pi}\int_V d^3x \left\{ -(\nabla_i \vartheta)(\nabla_j \vartheta) + \delta_{ij} k^2 \vartheta^2 \right\}$$
$$-\frac{1}{2\pi}\oint_S d^2x \left\{ (\hat{n})_\ell (\nabla_i \vartheta)(\nabla_\ell \nabla_j \vartheta) + \delta_{ij} (\hat{n})_\ell k^2 \vartheta \nabla_\ell \vartheta + 2k^2 (\hat{n})_i \vartheta \nabla_j \vartheta \right\} . \qquad (A149)$$

Substituting in Eq. (A144), and again dropping terms that will vanish with large radius in the surface term, results in:

$$R_e(P_{Ai;Aj}) = -\frac{K^2}{\pi}\int_V d^3x \left\{ \frac{r_i r_j}{r^2}\left[-\frac{K^2\cos^2(kr)}{r^2} + \left\{ \frac{2Kr\cos(kr)\sin(kr) - \sin^2(kr)}{r^4} \right\} \right] + k^2 \delta_{ij} \frac{\sin^2(kr)}{r^2} \right\}$$
$$-\frac{K^3}{2\pi}\oint_S d^2x \frac{\sin(kr)\cos(kr)}{r^2}\Big((\hat{n}\cdot\hat{r})\big(\delta_{ij} - (\hat{r})_i (\hat{r})_j\big) + 2(\hat{n})_i (\hat{r})_j \Big) , \qquad (A150)$$

where we've let $\vec{r} \equiv \vec{x} - \vec{Z}_A$.

Let's first evaluate the volume integral term above, which will be called T_V. We can substitute

$$\left\{ \frac{2Kr\cos(kr)\sin(kr) - \sin^2(kr)}{r^4} \right\} = \frac{1}{r^2}\frac{d}{dr}\left(\frac{\sin^2(kr)}{r} \right) , \qquad (A151)$$

plus $\cos^2(kr) = \frac{1}{2}[1+\cos(2kr)]$ and $\sin^2(kr) = \frac{1}{2}[1-\cos(2kr)]$ into this expression. We obtain:

$$T_\gamma = -\frac{K^4}{2\pi}\int_\gamma d^3x\,\frac{\left(\delta_{ij}-(\hat{r})_i(\hat{r})_j\right)}{r^2} + \frac{K^2}{\pi}\int_\gamma d^3x\left\{\frac{K^2}{2}\left(\delta_{ij}+(\hat{r})_i(\hat{r})_j\right)\frac{\cos(2kr)}{r^2} + \frac{1}{r^2}\frac{d}{dr}\left(\frac{\sin^2(kr)}{r}\right)\right\}. \quad (A152)$$

Since $\vec{r}\equiv\vec{x}-\vec{Z}_A$, the first term above is just $-\mathcal{S}_{Aij}$ from Eq. (A20). As for the second term, let us evaluate it by using spherical polar coordinates, with the surface of γ defined by $r=r_{max}(\theta,\phi)$. Thus,

$$T_\gamma = -\mathcal{S}_{Aij} + \frac{K^2}{\pi}\int_0^\pi d\theta\sin\theta\int_0^{2\pi} d\phi\int_0^{r_{max}(\theta,\phi)} dr\left\{\frac{K^2}{2}\left(\delta_{ij}+(\hat{r})_i(\hat{r})_j\right)\cos(2kr) + \frac{d}{dr}\left(\frac{\sin^2(kr)}{r}\right)\right\}$$

$$\approx -\mathcal{S}_{Aij} + \frac{K^3}{4\pi}\int_0^\pi d\theta\sin\theta\int_0^{2\pi} d\phi\left\{\left(\delta_{ij}+(\hat{r})_i(\hat{r})_j\right)\sin\left(2kr_{max}(\theta,\phi)\right) + \frac{4\sin^2(kr_{max})}{kr_{max}}\right\}. \quad (A153)$$

We can neglect the last term above since

$$\frac{\sin^2(kr_{max})}{kr_{max}}$$

becomes negligible for large r_{max}. Noting that

$$d^2x\,\hat{n}\cdot\hat{r} = d\phi\, d\theta\sin\theta\left(r_{max}(\theta,\phi)\right)^2, \quad (A154)$$

for an area element on $\mathcal{S}$, then T_γ becomes

$$T_\gamma = -\mathcal{S}_{Aij} + \frac{K^3}{4\pi}\oint_{\mathcal{S}} d^2x\,(\hat{n}\cdot\hat{r})\left(\delta_{ij}+(\hat{r})_i(\hat{r})_j\right)\frac{\sin(2kr)}{r^2}. \quad (A155)$$

Combining this term with the surface term in Eq. (A150), with $\sin(kr)\cdot\cos(2kr)=\frac{1}{2}\sin(2kr)$, yields

$$R_e\left(\mathcal{P}_{Ai;Aj}\right) = -\mathcal{S}_{Aij} + \frac{K^3}{2\pi}\oint_{\mathcal{S}} d^2x\,\frac{\sin(2kr)}{r^2}\left\{(\hat{n}\cdot\hat{r})(\hat{r})_i(\hat{r})_j - (\hat{n})_i(\hat{r})_j\right\}. \quad (A156)$$

When the surface $\mathcal{S}$ is a sphere about $\vec{\mathbf{Z}}_A$, then the surface term above vanishes, since then $\hat{\mathbf{n}}=\hat{\mathbf{r}}$. In general, though, the surface term is not equal to zero, although it does become negligibly small when the surface $\mathcal{S}$ is taken to be far away from $\vec{\mathbf{Z}}_A$. To see that this statement is true, we simply need to note that the surface term in Eq. (A156) is equal to $\mathrm{Re}(\xi_{Ai;Aj})$ from Eq. (A124).

Consequently, we've finally shown that

$$\mathrm{Re}(\mathcal{P}_{Ai;Aj}) \simeq -\mathcal{S}_{Aij} \quad , \qquad (A157)$$

when the surface $\mathcal{S}$ is far from the point $\vec{\mathbf{Z}}_A$. Combining Eqs. (A142) and (A157) yields

$$\mathcal{P}_{Ai;Aj} \approx -\mathcal{S}_{Aij} + i\delta_{ij}\tfrac{4}{3}K^3 \quad . \qquad (A158)$$

6.d. Summary

By combining Eqs. (A130), (A140), and (A158), we obtain:

$$\mathcal{P}^{I}_{Ai;Bj} - \mathrm{Re}\left[E_{Ai;Bj}\right]$$

$$= \delta_{AB}\left(-\mathcal{S}_{Aij} + i\delta_{ij}\tfrac{4}{3}K^3\right) + (1-\delta_{AB})\left(-\mathrm{Re}\left[E_{Ai;Bj}\right] - \Omega^{\theta}_{ij}(\vec{Z}_A-\vec{Z}_B,\omega) + \omega\frac{d}{d\omega}\Omega^{\theta}_{ij}(\vec{Z}_A-\vec{Z}_B,\omega)\right). \quad (1$$

Together with Eq. (A107), this result yields the quantity reported in Eq. (53).

APPENDIX B: CHECK ON EQ. (66) FOR RJ, ZPP AND ZP RADIATION

Here we wish to show that RJ, ZPP, as well as ZP radiation, satisfies Eq. (66). (Of course, ZP radiation is just the T->0 limit of ZPP radiation.) To prove this result, we'll need to examine the dependence of Im(ln(Det[M])) upon ω for small and large values of ω. Now, Im(ln(Det[M])) depends on ω through $M_{Ai;Bj}$ in Eq. (46), which in turn depends on ω through η_{ij}^{θ} in Eq. (40) and $C(\omega)$ in Eq. (45).

From Eqs. (40) and (45), one can prove that for $\omega \to 0$, and for $|\vec{\mathbf{R}}| \neq 0$ below, then

$$\frac{\eta_{ij}^{\theta}(\vec{R},\omega)}{C(\omega)} \approx \left[-\frac{(\delta_{ij}-3R_iR_j/R^2)}{\omega_0^2 R^3} + \mathcal{O}(\omega^2)\right] + i\left[+\frac{\omega^3}{\omega_0^2}\frac{2}{3c^3}\delta_{ij} + \mathcal{O}(\omega^5)\right] . \quad \text{(B1}$$

Consequently, in the limit of $\omega \to 0$, the imaginary part of $M_{Ai;Bj}$ vanishes. Hence, Det[M], as well as ln(Det[M]) are real quantities for $\omega \to 0$, so

$$\lim_{\omega\to 0}\left[\operatorname{Im}\ln \operatorname{Det}[M]\right] = 0 \quad . \qquad \text{(B2)}$$

Thus,

$$\lim_{\omega\to 0}\left[(h_{in})^2 \operatorname{Im}\ln \operatorname{Det}[M]\right] = 0 \quad , \qquad \text{(B3)}$$

for RJ, ZPP, and ZP radiation, since as $\omega \to 0$, $(h_{in})^2$ has limiting values of kT/π^2, kT/π^2, and 0, respectively, for these three cases.

Now turning to the $\omega \to \infty$ case, from Eqs. (40) and (45) one can show that for $|\vec{\mathbf{R}}| \neq 0$,

$$\frac{\eta^{D}_{ij}(\vec{R},\omega)}{C(\omega)} \approx \frac{1}{\omega\Gamma}\frac{(\delta_{ij}-R_iR_j/R^2)}{c^2R}ie^{i\kappa R} + \Theta\left(\frac{1}{\omega^2}\right) . \quad (B4)$$

Since the A≠B terms in $M_{Ai;Bj}$ equal $-e^2\eta^{D}_{ij}/(mC)$, then they go to zero as $1/\omega$ for large ω. The remaining matrix elements in $M_{Ai;Bj}$ are either unity for A=B and i=j, or zero for A=B and i≠j.

Of course, Det[M] consists of a linear combination of all products of the matrix elements, provided that only one element from each column and row is present in each product. For large ω, clearly the largest product term in Det[M] will be the product of the diagonal matrix elements, which equals unity. The next largest terms in Det[M] result from when all the diagonal terms in $M_{Ai;Bj}$, except for two of them, are multiplied together, with the remaining two factors being the A≠B off-diagonal terms, $-e^2\eta^{D}_{ij}/(mC)$. (To see this fact, note that if, say, the diagonal term from row α is missing in one of the product terms in Det[M], so as to allow in the product a matrix element from row α and some column β, where $\alpha\neq\beta$, then the diagonal term from column β and row β must also be absent and another off-diagonal term present.)

Hence,

$$\mathrm{Det}[M] \approx 1 + \frac{(\mathcal{A} + i\mathcal{B})}{\omega^2} , \qquad (B5)$$

where $\mathcal{A}$ and $\mathcal{B}$ are real numbers. Writing Det[M] as $\mathcal{M}e^{i\Theta}$, where $\mathcal{M}$ and Θ are real numbers, then we obtain that $\mathcal{M}\approx 1+\mathcal{A}/\omega^2$ and $\Theta\approx\mathcal{B}/\omega^2$ for large ω. Consequently,

$$\mathrm{Im}\,\ln \mathrm{Det}[M] \approx \frac{\mathcal{B}}{\omega^2} . \qquad (B6)$$

We then have that

$$\lim_{\omega \to \infty} \left[(\hbar_{in})^2 \, \mathrm{Im} \ln \mathrm{Det}[M] \right] = 0 \quad , \qquad \text{(B7)}$$

provided that as $\omega \to \infty$, $(\hbar_{in})^2$ remains either finite, or else diverges to ∞ slower than as ω^2. From Eqs. (27)-(29), we see that this condition is obeyed for RJ, ZPP, and ZP radiation.

spectrum $\chi\left(\frac{\omega}{c}\right)^3\coth\left(\frac{\pi^2\chi\omega}{k_B T}\right)$ yields the RJ and ZPP spectrums for arbitrary values of T when $\chi\to 0$ and when $\chi=\frac{\hbar}{2\pi^2}$, respectively.

[59]See, for example, G. Arfken, <u>Mathematical Methods for Physicists</u>, 2nd ed. (Academic Press, New York, 1970), Sec. 2.10.

[60]I.S. Gradshteyn and I. M. Ryzhik, <u>Table of Integrals, Series, and Products</u> (Academic Press, New York, 1980).