A Modification of Block–Walker's Reaction Field for a Non-Ideal Dipole

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Block-Walker's reaction field derived from considering a distance-dependent relative permittivity for a point dipole in the center of a spherical cavity is modified for a non-ideal dipole directed along the radius vector. The reaction field energies of the non-ideal dipole for two special cases are compared with those of the point dipole in the center of the cavity. Thus, the validity of approximation of Block–Walker's reaction field is investigated.

The famous Onsager reaction field[1] of a non-polarizable point dipole in the center of a spherical cavity in a continuous dielectric has long been applied in many fields. The Onsager reaction field has a significant weak point: in the Onsager model, the local relative permittivity in the immediate neighborhood of a solute molecule is assumed to be equal to the bulk relative permittivity (ε_r) of the solvent. Block and Walker[2] have overcome the defect of the Onsager reaction field by introducing their parameter of $\varepsilon(r)=\varepsilon_r \exp(-\kappa/r)$ in which $\varepsilon(r)$ is the relative permittivity at a distance of r from the center of the spherical cavity and κ is the scaling constant. By solving the differential equation of $\nabla^2\phi_1(r)+\{1/\varepsilon(r)\}\nabla\varepsilon(r)\cdot\nabla\phi_1(r)=0$, they obtained the following expressions for the potentials of $\phi_1(r)$ and $\phi_2(r)$ outside and inside the cavity:

$$\phi_1(r)=\{A_1(\frac{2r}{\kappa}+1)+A_2(\frac{2r}{\kappa}-1)e^{\kappa/r}\}\cos\theta \quad (r>a), \tag{1}$$

$$\phi_2(r)=A_3 r\cos\theta+\frac{\mu\cos\theta}{(4\pi\varepsilon_0)r^2} \quad (r<a), \tag{2}$$

respectively, where ε_0 is the permittivity of a vacuum, θ the angle between the vector $\boldsymbol{r}$ and the positive z-axis, and A_1, A_2, and A_3 are arbitrary constants. Using the potential of Eqs. 1 and 2, Block and Walker presented the reaction field $\boldsymbol{R}$ given by

$$\boldsymbol{R}=\frac{2\boldsymbol{\mu}}{(4\pi\varepsilon_0)a^3}\times s, \tag{3}$$

where

$$s=\frac{3\varepsilon_r\ln\varepsilon_r}{2(\varepsilon_r\ln\varepsilon_r-\varepsilon_r+1)}-\frac{3}{\ln\varepsilon_r}-1. \tag{4}$$

This reaction field has been widely used. The potential of Eq. 1 is of course the solution of the differential equation shown above. The potential due to the dipole must be zero at infinity. Block and Walker probably obtained the reaction field of Eq. 3 by implicitly assuming $A_1=-A_2$.

It is not necessarily always adequate to apply the reaction field of the point dipole located in the center of the cavity, as described in a previous paper.[3] There has been no study concerning the difference between the reaction field energies of ideal and non-ideal dipoles in the case of Block–Walker's reaction field, except for the case of the Onsager reaction field.[3] In this paper, therefore, an attempt has been made to modify Block–Wakler's reaction field for calculation of the reaction field energy of the non-ideal dipole directed along the radius vector in a spherial cavity to compare with Block–Walker's reaction field energy of the ideal dipole in the center of the cavity.

Theoretical

In this case, we consider the non-ideal dipole directed along the radius vector in a spherical cavity, because the computation of the reaction field at an arbitrary position of the non-ideal dipole is very intricate.

The origin O is chosen in the center of the spherical cavity (of radius a) embedded in a continuous dielectric medium (of relative permittivity ε_r) and the positive z-axis is taken through the non-ideal dipole, whose moment is $\mu=q(r_A+r_B)$ in the direction of the positive z-axis, as shown in Fig. 1. In Fig. 1, the negative and positive charges ($-q$ and $+q$) of the dipole are at the point A ($z=r_A$) and at B ($z=-r_B$), respectively, on the z-axis. The distances from these charges to an arbitrary point P are written by $\overline{PA}$ and $\overline{PB}$. The distance from the origin to P is denoted by r and the angle between the vector $\boldsymbol{r}$ and the positive z-axis is denoted by θ. Then, assuming that $r>r_A$ and $r>r_B$, we obtain:[3]

$$\frac{1}{\overline{PA}}=\sum_{n=0}^{\infty}P_n(\cos\theta)\frac{r_A^n}{r^{n+1}}, \tag{5}$$

$$\frac{1}{\overline{PB}}=\sum_{n=0}^{\infty}(-1)^n P_n(\cos\theta)\frac{r_B^n}{r^{n+1}}. \tag{6}$$

Here $P_n(\cos\theta)$ is the Legendre polynomial.

The relative permittivity within the cavity is assumed to be unity. For the distance-dependent relative permittivity outside the cavity we adopt Block–Walker's

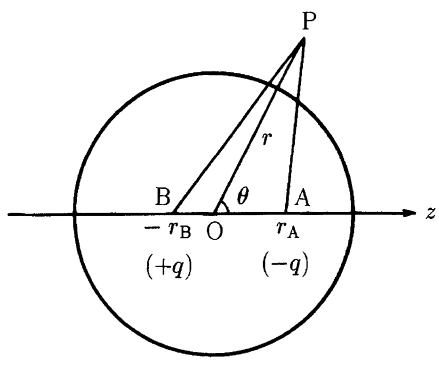

Fig. 1. Model.

parameter[2] given by

$$\varepsilon(r) = \varepsilon_r \exp(-\kappa/r). \tag{7}$$

The constant κ can be calculated as $\kappa = a \ln \varepsilon_r$ under the condition of $\varepsilon(r)=1$ for $r=a$. By differentiating Eq. 7 with respect to r, we obtain the following relationship:

$$\frac{r^2}{\varepsilon(r)} \times \frac{\mathrm{d}\varepsilon(r)}{\mathrm{d}r} = \kappa = a \ln \varepsilon_r. \tag{8}$$

We write the electric potential and field due to $\boldsymbol{\mu}$ as $\phi(r)$ and $\boldsymbol{E}$, respectively, at P. Following the treatment of Block and Walker,[2] we write the divergence of the electric displacement $\boldsymbol{D}$ from the differential form of Gauss's theorem of div $\boldsymbol{D}=\rho$ in the absence of the charge density ρ as follows: div $\boldsymbol{D}=$ div $\varepsilon(r)\boldsymbol{E} = \varepsilon(r)$ div $\boldsymbol{E} + \boldsymbol{E}$ grad $\varepsilon(r) = -\varepsilon(r)\nabla^2\phi(r) - \nabla\phi(r) \cdot \nabla\varepsilon(r) = 0$. If the unit vector of $\boldsymbol{r}$ is denoted by $\boldsymbol{e}_r$, we obtain $\nabla\varepsilon(r) = \boldsymbol{e}_r \mathrm{d}\varepsilon(r)/\mathrm{d}r$ and $\boldsymbol{e}_r \cdot \nabla\phi(r) = \partial\phi(r)/\partial r$. Therefore, we obtain

$$\nabla^2\phi(r) + \frac{1}{\varepsilon(r)} \times \frac{\mathrm{d}\varepsilon(r)}{\mathrm{d}r} \times \frac{\partial\phi(r)}{\partial r} = 0. \tag{9}$$

In this case of axial symmetry, the formula[4] already given for $\nabla^2\phi(r)$ was used in Eq. 9. Then, we assume $\phi(r)$ to be of the form:

$$\phi(r) = R(r) \times Y(\theta). \tag{10}$$

Thus, the partial differential equation of Eq. 9 can be reduced to two ordinary equations as follows:

$$r^2 \frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2} + (2r+\kappa)\frac{\mathrm{d}R(r)}{\mathrm{d}r} - CR(r) = 0, \tag{11}$$

$$\frac{\mathrm{d}^2Y(\theta)}{\mathrm{d}\theta^2} + \cot\theta \frac{\mathrm{d}Y(\theta)}{\mathrm{d}\theta} + CY(\theta) = 0, \tag{12}$$

where C is the separation constant. In the derivation of Eq. 11, the relationship of Eq. 8 was used. The solution of Eq. 12 is already given by[4]

$$Y(\theta) = A \times P_n(\cos\theta), \tag{13}$$

$$C = n(n+1), \tag{14}$$

where A is an arbitrary constant, and n an integer.

Inside the cavity, Eq. 11 is reduced to

$$r^2 \frac{\mathrm{d}^2R(r)}{\mathrm{d}r^2} + 2r\frac{\mathrm{d}R(r)}{\mathrm{d}r} - n(n+1)R(r) = 0, \tag{15}$$

because κ is zero for $\varepsilon_r = 1$. The solution of Eq. 15 is also given.[4] Inside the cavity, therefore, the potential $\phi_2(r)$ can be easily written as[4]

$$\phi_2(r) = \sum_{n=0}^{\infty}\left(C_n r^n + \frac{D_n}{r^{n+1}}\right) \times P_n(\cos\theta) \quad (r_A \text{ or } r_B < r < a), \tag{16}$$

where C_n and D_n are arbitrary constants.

To obtain the potential $\phi_1(r)$ that satisfies Eq. 11 and the boundary condition of $\{\phi_1(r)\}_{r\to\infty}=0$, we write $R(r)$ as

$$R_n(r) = \sqrt{2}z^{1/2}\mathrm{e}^z\rho(z), \tag{17}$$

where $z=\kappa/2r$ and $\rho(z)$ is a function of z. Putting Eq. 17 into Eq. 11, we finally obtain the following differential equation:

$$\frac{\mathrm{d}^2\rho(z)}{\mathrm{d}z^2} + \frac{1}{z}\frac{\mathrm{d}\rho(z)}{\mathrm{d}z} - \left\{1 + \frac{(n+1/2)^2}{z^2}\right\}\rho(z) = 0. \tag{18}$$

This is the modified Bessel differential equation and n is an integer. Therefore, $\rho(z)$ can be expressed as a linear combination of $I_{\pm(n+1/2)}(z)$. Accordingly, the general solutions of Eq. 11 are given by

$$R_n(r) = z^{1/2}\mathrm{e}^z \times \{a_n I_{n+1/2}(z) + b_n I_{-(n+1/2)}(z)\}, \tag{19}$$

where a_n and b_n are arbitrary constants. However, $I_{-(n+1/2)}(z)$ does not satisfy the boundary condition of $\{R_n(r)\}_{r\to\infty}=0$. Therefore, $b_n=0$, and thus $R_n(r) = z^{1/2}\mathrm{e}^z \times a_n I_{n+1/2}(z)$. It is more convenient to change the modified Bessel function of $I_{n+1/2}(z)$ by using Kummer's function of ${}_1F_1(n+1, 2n+2; 2z)$ for the subsequent calculation. Accordingly, we write the potential outside the cavity as

$$\phi_1(r) = \sum_{n=0}^{\infty}\frac{B_n}{2^{n+1/2}} \times \frac{z^{n+1}}{\Gamma(n+3/2)} \times {}_1F_1(n+1,\ 2n+2;\ 2z) \times P_n(\cos\theta) \quad (r > a), \tag{20}$$

where B_n is an arbitrary constant.

In the absence of the dielectric, the potential $\phi(r)$ due to the dipole is written by using Eqs. 5 and 6 as

$$\phi(r) = \frac{1}{4\pi\varepsilon_0}\left\{\frac{(-q)}{\overline{\mathrm{PA}}} + \frac{(+q)}{\overline{\mathrm{PB}}}\right\} = \frac{q}{4\pi\varepsilon_0}\sum_{n=0}^{\infty}\frac{\{(-1)^n r_B^n - r_A^n\}}{r^{n+1}} \times P_n(\cos\theta). \tag{21}$$

Then, we obtain $D_n = (q/4\pi\varepsilon_0)\{(-1)^n r_B^n - r_A^n\}$ in Eq. 16. Therefore, we can write Eq. 16 as

$$\phi_2(r) = \sum_{n=0}^{\infty}\left(C_n r^n + \frac{q\{(-1)^n r_B^n - r_A^n\}}{(4\pi\varepsilon_0)r^{n+1}}\right) \times P_n(\cos\theta). \tag{22}$$

The necessary boundary conditions are $\{\phi_1(r)\}_{r=a} = \{\phi_2(r)\}_{r=a}$ and $\{\varepsilon(r)(\partial\phi_1(r)/\partial r)\}_{r=a} = \{\partial\phi_2(r)/\partial r\}_{r=a}$. Applying these boundary conditions to Eqs. 20 and 22, we obtain

$$B_n = \frac{q\{(-1)^n r_B^n - r_A^n\}}{(4\pi\varepsilon_0)a^{n+1}} \times \frac{2^{2n+3/2}\Gamma(n+3/2)}{(\ln \varepsilon_r)^{n+1}} \times \frac{1}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_r)}, \tag{23}$$

$$C_n = \frac{q\{(-1)^n r_B^n - r_A^n\}}{(4\pi\varepsilon_0)a^{2n+1}} \times \left\{\frac{{}_1F_1(n+1,\ 2n+2;\ \ln\varepsilon_r)}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_r)} - 1\right\}. \tag{24}$$

According to Böttcher's book,[4] therefore, we obtain the reaction field potential $\phi^{\mathrm{R}}(r)$ for the whole cavity from the first term of Eq. 22 as

$$\phi^{\mathrm{R}}(r) = \sum_{n=0}^{\infty} \frac{q\{(-1)^n r_{\mathrm{B}}^n - r_{\mathrm{A}}^n\}}{(4\pi\varepsilon_0)a^{2n+1}} \times \left\{\frac{{}_1F_1(n+1,\ 2n+2;\ \ln\varepsilon_{\mathrm{r}})}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_{\mathrm{r}})} - 1\right\} \times r^n P_n(\cos\theta). \quad (25)$$

In Eq. 25, the values of $r=r_{\mathrm{A}}$ and $\cos 0=1$ (i. e., $P_n(1)=1$) and ones of $r=r_{\mathrm{B}}$ and $\cos\pi=-1$ (i. e., $P_n(-1)=(-1)^n$) should be used for the reaction potential of $\phi^{\mathrm{R}}(\mathrm{A})$ at the position of A and for the potential of $\phi^{\mathrm{R}}(\mathrm{B})$ at B, respectively. By using Eq. 25 in this way, the energy (E) of the non-ideal dipole $\boldsymbol{\mu}$ in its own reaction field is given as follows:

$$\begin{aligned} E &= \frac{1}{2}\{(-q)\phi^{\mathrm{R}}(\mathrm{A}) + (+q)\phi^{\mathrm{R}}(\mathrm{B})\} \\ &= -\frac{1}{2}\sum_{n=0}^{\infty} \frac{q^2\{(-1)^n r_{\mathrm{B}}^n - r_{\mathrm{A}}^n\}^2}{(4\pi\varepsilon_0)a^{2n+1}} \times \left\{1 - \frac{{}_1F_1(n+1,\ 2n+2;\ \ln\varepsilon_{\mathrm{r}})}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_{\mathrm{r}})}\right\} \\ &= -\frac{\mu^2}{(4\pi\varepsilon_0)a^3}\times t_1 - \sum_{n=2}^{\infty} \frac{q^2\{(-1)^n r_{\mathrm{B}}^n - r_{\mathrm{A}}^n\}^2}{(4\pi\varepsilon_0)a^{2n+1}}\times t_n, \end{aligned} \quad (26)$$

where

$$t_n = \frac{1}{2}\times\left\{1 - \frac{{}_1F_1(n+1,\ 2n+2;\ \ln\varepsilon_{\mathrm{r}})}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_{\mathrm{r}})}\right\}. \quad (27)$$

The term for $n=0$ in Eq. 26 is zero, because $\{(-1)^n r_{\mathrm{B}}^n - r_{\mathrm{A}}^n\}^2=0$ for $n=0$. The energy of Block–Walker's reaction field corresponds to the special case of $r_{\mathrm{A}}=0$ and $r_{\mathrm{B}}=0$ in Eq. 26. Therefore, the parameter t_1 corresponds to s of Block–Walker's reaction field for the point dipole in the center of the spherical cavity. In the Appendix, the identity of the parameter t_1 and Block–Walker's parameter s (Eq. 4) is proved. The calculation of s is easier than that of t_1 is. Hereafter, therefore, we use the parameter s instead of t_1.

Assuming that $r_{\mathrm{A}} > r_{\mathrm{B}}$, we adopt the following parameter u:

$$\frac{r_{\mathrm{B}}}{r_{\mathrm{A}}} = u. \quad (28)$$

Then, we obtain $\mu=qr_{\mathrm{A}}(1+u)$. Using Eq. 28, we can write Eq. 26 as

$$E = -\frac{\mu^2}{(4\pi\varepsilon_0)a^3}\times s\left(1+\frac{v}{s}\right). \quad (29)$$

Here

$$v = \frac{1}{(1+u)^2}\sum_{n=2}^{\infty}\left(\frac{r_{\mathrm{A}}}{a}\right)^{2(n-1)} \times\{(-1)^n u^n - 1\}^2\times t_n. \quad (30)$$

Equation 29 is the final equation.

Discussion

The special expression of Eq. 19 for $n=1$ is given by

$$R_1(r) = \frac{1}{\sqrt{2\pi}}\left\{(a_1-b_1)\left(\frac{2r}{\kappa}+1\right) -(a_1+b_1)\left(\frac{2r}{\kappa}-1\right)\mathrm{e}^{\kappa/r}\right\}. \quad (31)$$

This equation leads to Eq. 1, if $A_1=(a_1-b_1)/\sqrt{2\pi}$ and $A_2=-(a_1+b_1)/\sqrt{2\pi}$. In this case of the non-ideal dipole, Eq. 31 cannot be used, because Eq. 31 is due to the point dipole in the center of the cavity.

From Eq. 25, we can write the reaction field $\boldsymbol{R}$ in the cavity as

$$\boldsymbol{R} = -\mathrm{grad}\,\phi^{\mathrm{R}}(r). \quad (32)$$

On the z-axis, the components of $\boldsymbol{R}$ in the x- and y-direction will be zero due to the symmetry in this case. Thus, we have for the component of $\boldsymbol{R}(z)$ on the z-axis:

$$\begin{aligned} \boldsymbol{R}(z) &= -\boldsymbol{k}\frac{\mathrm{d}}{\mathrm{d}z}\{\phi^{\mathrm{R}}(r=z;\ \cos\theta=1)\} \\ &= -\boldsymbol{k}\sum_{n=0}^{\infty}\frac{q\{(-1)^n r_{\mathrm{B}}^n - r_{\mathrm{A}}^n\}}{(4\pi\varepsilon_0)a^{2n+1}} \times\left\{\frac{{}_1F_1(n+1,\ 2n+2;\ \ln\varepsilon_{\mathrm{r}})}{{}_1F_1(n+1,\ 2n+1;\ \ln\varepsilon_{\mathrm{r}})} - 1\right\} \times nz^{n-1}. \end{aligned} \quad (33)$$

Here $\boldsymbol{k}$ is the unit vector in the direction of the z-axis. Remembering the expression of $\boldsymbol{\mu}=(-q)\boldsymbol{r}_{\mathrm{A}}+q\boldsymbol{r}_{\mathrm{B}}=\boldsymbol{k}(-q)(r_{\mathrm{A}}+r_{\mathrm{B}})$ in this case, we can write the following E value by using Eqs. 32 and 33:

$$\begin{aligned} E &= -\frac{1}{2}\times(-q)\int_{\mathrm{B}}^{\mathrm{A}} R(z)\mathrm{d}z \\ &= \frac{1}{2}\{(-q)\phi^{\mathrm{R}}(\mathrm{A}) + (+q)\phi^{\mathrm{R}}(\mathrm{B})\}, \end{aligned} \quad (34)$$

because the reaction field acts on the line from B to A on the z-axis in this case. Then, Eq. 34 is identical with Eq. 26.

Applications

The first term of $-\{\mu^2/(4\pi\varepsilon_0)a^3\}t_1$ for $n=1$ in Eqs. 26 and 29 is Block–Walker's reaction field energy, because $t_1\equiv s$ as described above. Therefore, the value of $(1+v/s)$ in Eq. 29 indicates the degree of difference in the E values between the non-ideal dipole and the point dipole (in the center of the cavity). In this section, we apply Eq. 29 to two special cases.

In the Case of $r_{\mathrm{A}}=r_{\mathrm{B}}$ (u=1). In this case, we can write $\mu=q\times(2r_{\mathrm{A}})$. Putting $u=1$ into Eq. 30, we obtain

$$v = \frac{1}{4}\sum_{n=2}^{\infty}\left(\frac{r_{\mathrm{A}}}{a}\right)^{2(n-1)}\times\{(-1)^n - 1\}^2\times t_n. \quad (35)$$

The values of $(1+v/s)$ for several values of r_{A}/a and ε_{r} are given in Table 1. The table shows that the $(1+v/s)$ value does not change very much from unity at the range of r_{A}/a smaller than 0.5. In the case of $r_{\mathrm{A}}=r_{\mathrm{B}}$, therefore, Block–Walker's reaction field of the point dipole may be satisfactorily used for the r_{A}/a value smaller than 0.5.

In the Case of r_{B}=0 (u=0). In this case, we can write $\mu=qr_{\mathrm{A}}$, because the positive charge of the B point is at the origin. Putting $u=0$ into Eq. 30, we obtain:

Table 1. Values of $(1+v/s)$ for $r_A=r_B$

	Values of $(1+v/s)$					
	ε_r=2	ε_r=10	ε_r=20	ε_r=30	ε_r=50	ε_r=80
(s:	0.0550	0.1596	0.1951	0.2136	0.2345	0.2517)
r_A/a						
0	1	1	1	1	1	1
0.1	1.0000	1.0001	1.0001	1.0001	1.0001	1.0001
0.2	1.0007	1.0008	1.0008	1.0008	1.0009	1.0009
0.3	1.0036	1.0040	1.0042	1.0043	1.0044	1.0045
0.4	1.0116	1.0127	1.0133	1.0136	1.0140	1.0144
0.5	1.0290	1.0319	1.0333	1.0341	1.0351	1.0361
0.6	1.0629	1.0694	1.0724	1.0742	1.0765	1.0786

Table 2. Values of $(1+v/s)$ for $r_B=0$

	Values of $(1+v/s)$					
	ε_r=2	ε_r=10	ε_r=20	ε_r=30	ε_r=50	ε_r=80
(s:	0.0550	0.1596	0.1951	0.2136	0.2345	0.2517)
r_A/a						
0	1	1	1	1	1	1
0.1	1.0062	1.0067	1.0069	1.0070	1.0071	1.0072
0.2	1.0254	1.0272	1.0281	1.0285	1.0291	1.0296
0.3	1.0594	1.0637	1.0657	1.0668	1.0682	1.0694
0.4	1.1117	1.1201	1.1238	1.1260	1.1287	1.1311
0.5	1.1889	1.2034	1.2100	1.2139	1.2186	1.2229
0.6	1.3028	1.3272	1.3383	1.3447	1.3528	1.3601

$$v = \sum_{n=2}^{\infty} \left(\frac{r_A}{a}\right)^{2(n-1)} \times t_n. \tag{36}$$

The values of $(1+v/s)$ for several values of r_A/a and ε_r are shown in Table 2. The table shows that the $(1+v/s)$ value considerably increases with the increasing value of r_A/a from unity and slightly depends on the ε_r value for the same r_A/a value. From Table 2, it is known that Block–Wakler's reaction field energy for the point dipole at the origin gives considerably smaller values than Eq. 29 does above the r_A/a value of 0.3. The use of Block–Walker's reaction field energy is, therefore, inappropriate for the case where the center of the non-ideal dipole is considerably shifted from the center of the spherical cavity.

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Appendix

Proof of $t_1 \equiv s$. We can express ε_r as

$$\varepsilon_r = e^{\ln \varepsilon_r} = 1 + \sum_{n=1}^{\infty} \frac{(\ln \varepsilon_r)^n}{n!}. \tag{A1}$$

Using this relation, we can write ${}_1F_1(2,\ 3;\ \ln \varepsilon_r)$ as

$$\begin{aligned} {}_1F_1(2,\ 3;\ \ln \varepsilon_r) &= 1 + \sum_{j=1}^{\infty} \frac{2 \cdot 3 \cdot 4 \cdots (1+j)}{3 \cdot 4 \cdot 5 \cdots (2+j)} \times \frac{(\ln \varepsilon_r)^j}{j!} \\ &= 1 - 2\sum_{j=2}^{\infty} \left\{ \frac{1}{(n+1)!} - \frac{1}{n!} \right\} (\ln \varepsilon_r)^{n-1} \\ &= \frac{2}{(\ln \varepsilon_r)^2} \times (\varepsilon_r \ln \varepsilon_r - \varepsilon_r + 1). \end{aligned} \tag{A2}$$

From Eq. 27, therefore, we obtain

$$\begin{aligned} t_1 &= \frac{1}{2} \times \left\{ 1 - \frac{\Gamma(1+3/2) e^{(\ln \varepsilon_r)/2} (\ln \varepsilon_r/4)^{-3/2} I_{1+1/2}(\ln \varepsilon_r/2)}{{}_1F_1(2,\ 3;\ \ln \varepsilon_r)} \right\} \\ &= \frac{\varepsilon_r (\ln \varepsilon_r)^2 - 4\varepsilon_r \ln \varepsilon_r - 2 \ln \varepsilon_r + 6\varepsilon_r - 6}{2 \ln \varepsilon_r (\varepsilon_r \ln \varepsilon_r - \varepsilon_r + 1)} \\ &= \frac{3\varepsilon_r \ln \varepsilon_r}{2(\varepsilon_r \ln \varepsilon_r - \varepsilon_r + 1)} - \frac{3}{\ln \varepsilon_r} - 1 \\ &= s. \end{aligned} \tag{A3}$$

Thus, we obtain $t_1 \equiv s$ (Eq. 4).

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