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A comparison of the Laplace and the alternative multipole expansion series for the Coulomb potential

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Multipole expansion is a powerful technique used in many-body physics to solve dynamical problems involving correlated interactions between constituent particles. The Laplace multipole expansion series of the Coulomb potential is well established in literature. We compare it with our recently developed perturbative and analytical alternative multipole expansion series of the Coulomb potential. In our working, we confirm that both expansion series are complete but quite different in the basis functions used. The analytical expansion, being the infinite limit of the perturbative expansion, is confirmed to be equivalent to the Laplace multipole expansion of the Coulomb potential. In terms of performance, the perturbative alternative multipole expansion series yields the lower bound while the Laplace and the analytical alternative multipole expansion series yield an upper bound of the expected results. The results show that only a finite number of terms in the series expansion of the basis functions for the perturbative alternative multipole expansion series are necessary for converged and accurate results. Our findings are likely to be useful in the perturbative treatment of the Coulomb potential in electronic structure calculations as well as in celestial mechanics.

I. INTRODUCTION

The Laplace multipole expansion series is established in the works of Laplace and Legendre in their search for solutions to the problem of attractions. The historical developments that led to the establishment of the expansion series and the introduction of the Legendre polynomials, for the first time, as the coefficients used in the Laplace expansion are captured in Laden's thesis[1]. The Laplace multipole expansion has become conventional knowledge in physics textbooks[2] and it is quite useful in solving the many-body physics problems in celestial mechanics, quantum physics and chemistry, nuclear physics, and condensed matter physics.

Naturally, the multipole expansion becomes convenient to use in solving physical problems in $3D$ if expressed in the spherical polar coordinates. This decomposes the problem as a product of both radial and angular parts. The radial part can be treated as a $1D$ case while the well defined angular algebra[3] can be used to simplify the angular parts. Several studies have employed multipole expansion techniques in the recent past in solving physical problems of interest[4–9].

In our alternative multipole expansion of the Coulomb potential[10,11], we stated that the Laplace multipole expansion series of the Coulomb repulsion term is incomplete, and therefore inaccurate. This statement was met with considerable criticism[12]. Because of the controversy, we feel obligated and motivated to give a comprehensive treatment to the problem with regards to the completeness of the Laplace multipole expansion series. We also compare the equivalence and the performance of the Laplace expansion method relative to our perturbative and analytical alternative multipole expansion methods. We have seen in literature that such a comparison, not exactly similar to the current study, is reported in ref.[13,14]. Comparison of different methods allows characterization of relative accuracy and capabilities, which is quite instrumental in guiding application[13].

In this study, we show that the Coulomb potential

$$\frac{1}{|\vec{r}_i - \vec{r}_j|} = \frac{1}{r_>} \sum_{s=0}^{\infty} f_s(x)\, \tilde{t}^s \tag{1}$$

is presented as the Laplace multipole expansion series, where $\tilde{t} = r_</r_>$, $r_> = \max\{r_i, r_j\}$, $r_< = \min\{r_i, r_j\}$, $x = \cos\theta$, with θ being the relative angle between the position vectors $\vec{r}_i$ and $\vec{r}_j$, s are integers, and $f_s(x)$ are the s^{th} order Laplace coefficients of $\tilde{t}^s$, also known as the Legendre polynomials.

In the alternative approach, the multipole expansion of the Coulomb potential

$$\frac{1}{|\vec{r}_i - \vec{r}_j|} = \frac{1}{r_>} \sum_{l=0}^{\infty} h_l(\tilde{t})\, P_l(x) \tag{2}$$

is expressed in the basis of Legendre polynomials,$P_l(x)$, where

$$h_l(\tilde{t}) = \frac{(2l+1)}{\sqrt{1+\tilde{t}^2}}\, \tilde{j}_l(\tilde{t}), \tag{3}$$

with $\tilde{j}_l(\tilde{t})$ as spherical Bessel-like functions which can be expanded in the perturbative polynomial form as[10,11]

$$j_0(\tilde{t}) = 1 + \textstyle\sum_{k=1}^{\infty} \frac{(4k-1)!!}{(2k)!!(2k+1)!!} \left(\frac{\tilde{t}}{1+\tilde{t}^2}\right)^{2k} \tag{4}$$

$$j_{l>0}(\tilde{t}) = \textstyle\sum_{k=0}^{\infty} \frac{(2l+4k-1)!!}{(2k)!!(2l+2k+1)!!} \left(\frac{\tilde{t}}{1+\tilde{t}^2}\right)^{l+2k} \tag{5}$$

or analytically as a differential equation[11]

$$\tilde{j}_l(t) = (-1)^l \frac{t^l}{(2l+1)!!} \left[\frac{1}{t}\frac{\mathrm{d}}{\mathrm{d}t}\right]^l \left\{ \frac{1}{2t} \left[(1+2t)^{l+\frac{1}{2}} - (1-2t)^{l+\frac{1}{2}} \right] \right\}, \tag{6}$$

with

$$t = \frac{r_i r_j}{r_i^2 + r_j^2} = \frac{\tilde{t}}{1+\tilde{t}^2} \tag{7}$$

defined in terms of $\tilde{t}$ this case.

The coefficients of the Legendre polynomials in Eq. (2) can be shown to simplify to the conventional Laplace form, $f_l(t) \approx \tilde{t}^l$, using the lowest order approximation[10].

Our ultimate goal in this work is to highlight and emphasize the differences between the two exact forms of expansion of the Coulomb potential given by Eqs. (1) and (2), with the latter evaluated in both perturbative and exact expansions given by Eqs. (4) - (6) respectively. It is important to note that the form given by Eq. (1) is considered as the generating function for the Legendre polynomials[2,15].

II. THEORY

The Coulomb repulsion potential term can be expressed as

$$\frac{1}{|\vec{r}_i - \vec{r}_j|} = \frac{1}{r_>}\left(1 - 2x\tilde{t} + \tilde{t}^2\right)^{-\frac{1}{2}} \tag{8}$$

with a further expansion of the function

$$\begin{aligned}\left(1 - 2x\tilde{t} + \tilde{t}^2\right)^{-\frac{1}{2}} &= \sum_{k=0}^{\infty} \binom{n}{k} (\tilde{t}^2 - 2x\tilde{t})^k \\ &= \sum_{k=0}^{\infty}\sum_{\lambda=0}^{k} \binom{n}{k}\binom{k}{\lambda} (-2x)^{\lambda}\, \tilde{t}^{2k-\lambda}\end{aligned} \tag{9}$$

using the Binomial expansion series with $n = -1/2$, while k and λ being integers. Using the change of integer variable, $s = 2k - \lambda$, and some reorganization, Eq. (8) can further be expressed as

$$\begin{aligned}\frac{1}{|\vec{r}_i - \vec{r}_j|} &= \frac{1}{r_>}\sum_{k=0}^{\infty}\sum_{s=k}^{2k} \binom{n}{k}\binom{k}{2k-s} (-2x)^{2k-s}\,\tilde{t}^s \\ &= \frac{1}{r_>}\sum_{s=0}^{\infty} f_s(x)\,\tilde{t}^s\end{aligned} \tag{10}$$

where

$$f_s(x) = \sum_{k\geq\frac{s}{2}}^{s} \binom{n}{k}\binom{k}{2k-s} (-2x)^{2k-s} \tag{11}$$

is the desired Laplace coefficient. Since the Binomial coefficients are

$$\binom{n}{k} = \frac{(2k-1)!!}{(-2)^k k!}; \tag{12}$$

$$\binom{k}{2k-s} = \frac{k!}{(s-k)!(2k-s)!}, \tag{13}$$

where $n = -\frac{1}{2}$, the Laplace coefficients can, explicitly, be expressed as

$$f_s(x) = \sum_{k\geq\frac{s}{2}}^{s} (-2)^{k-s} \frac{(2k-1)!!}{(s-k)!(2k-s)!} x^{2k-s}. \tag{14}$$

In Eq. (3) of ref.[10], we have shown that,

$$x^{2k-s} = \sum_{l=0\,\mathrm{or}\,1}^{2k-s} a_l^{2k-s} P_l(x), \tag{15}$$

can be expanded in terms of even or odd orders of the Legendre polynomials in ascending order for even and odd values of $2k - s$ respectively, where the coefficient

$$a_l^{2k-s} = \frac{(2l+1)\times(2k-s)!}{(2k-s-l)!!(2k-s+l+1)!!} \tag{16}$$

as per Eq. (20) of the same reference[10]. Substituting Eq. (15) into Eq. (11), we obtain the Laplace coefficient

$$f_s(x) = \sum_{k\geq\frac{s}{2}}^{s}\sum_{l=0\,\mathrm{or}\,1}^{2k-s} \binom{n}{k}\binom{k}{2k-s} (-2)^{2k-s} a_l^{2k-s} P_l(x) \tag{17}$$

expanded in terms of the Legendre polynonials. Eq. (17) can equivalently be expressed in terms of the Legendre basis functions as

$$f_s(x) = \sum_{l=0\,\mathrm{or}\,1}^{s} c_l^s P_l(x) \tag{18}$$

where the the sum runs over even or odd values of l respectively and the coefficients

$$c_l^s = \sum_{k=\frac{(l+s)}{2}}^{s} \left[\binom{n}{k}\binom{k}{2k-s} (-2)^{2k-s} a_l^{2k-s}\right] \tag{19}$$

are a series summed over k values. The coefficients for the Legendre polynomials in Eq. (15) therefore simplify to

$$c_l^s = \sum_{k=\frac{(l+s)}{2}}^{s} \left[(-1)^{k-s} \frac{(2l+1)2^{k-s}(2k-1)!!}{(s-k)!(2k-s-l)!!(2k-s+l+1)!!}\right] \tag{20}$$

when the constants in Eqs. (12), (13), and (15) are explicitly replaced.

III. RESULTS

We have expanded the Coulomb potential in the form of Eq. (1) in our investigation of the completeness of the Laplace multipole series. We obtain the Laplace coefficients explicitly in terms of the polynomials of order s and in terms of the Legendre polynomials as given by Eqs. (14) and (18) respectively. Using Eq. (14), the first six Laplace coefficients can be expressed in terms of x as

$$\begin{aligned} f_0(x) &= 1 \\ f_1(x) &= x \\ f_2(x) &= \frac{1}{2}[3x^2 - 1] \\ f_3(x) &= \frac{1}{2}[5x^3 - 3x] \\ f_4(x) &= \frac{1}{8}[35x^4 - 30x^2 + 3] \\ f_5(x) &= \frac{1}{8}[63x^5 - 35x^3 + 15x]. \end{aligned} \tag{21}$$

By inspection, these Laplace coefficients converge to the Legendre polynomials, $P_l(x)$, showing that Eqs. (1) and (2) are equivalent. It can also be confirmed that the series given by Eq. (20) converge to unity, that is,

$$c_l^s = \begin{cases} 1 & \text{if } \ l = s \\ 0 & \text{if } \ l \neq s \end{cases}. \tag{22}$$

The equivalence of the Laplace coefficients and the Legendre polynomials has a further implication that

$$\tilde{t}^l \stackrel{!}{=} \frac{(2l+1)}{\sqrt{1+\tilde{t}^2}} \sum_{k=0}^{k_{max}\to\infty} \frac{(2l+4k-1)!!}{(2k)!!(2l+2k+1)!!} \left(\frac{\tilde{t}}{1+\tilde{t}^2}\right)^{l+2k} \tag{23}$$

if the multipole expansion series are to converge locally for every order of the Legendre polynomials. In Eq. (23), we have defined $(-1)!! = 1$. In Fig. 1, we plot the convergence of the first two orders of the Laplace functions, $\tilde{t}^l$, relative to the alternative multipole expansion functions, $h_l(\tilde{t})$, as given by Eqs. (4) and (5). The domain $0 \leq \tilde{t} \leq 1$ has been chosen to coincide with the regime of convergence of the Laplace multipole expansion series. The convergence tests should confirm the validity of Eq. (23). If valid, the results would imply that the Laplace basis functions are equivalent to the alternative multipole expansion basis functions. Since $h_l(\tilde{t})$ is an infinite series function, it can be seen that only three terms (with $k_{max} = 2$) of the summation series already yield reasonable convergence. In subsequent figures, we use $h_l^{k_{max}=2}(\tilde{t})$ as our converged perturbative results.

In Fig. 2a, we compare the converged perturbative results with the corresponding analytical, $h_l(\tilde{t}) = h_l^{k_{max}\to\infty}$, functions as given by Eq. (6) and the Laplace basis functions for the first six orders of l. Except at lower values of $\tilde{t}$, the corresponding perturbative basis functions diverge from each other in all the cases considered. The analytical basis functions, on the other hand, show excellent agreement with the Laplace basis functions. In Fig. 2b, we show the relative deviation between the analytical and the Laplace basis functions. The relative deviation are calculated as the absolute difference between the analytical $h_l(\tilde{t})$ and the Laplace $f_l(\tilde{t}) = \tilde{t}^l$ functions divided by the Laplace functions. The observed relative deviations can be attributed to numerical noise as well as the divergences due to singularities in the analytical function as $\tilde{t} \to 0$.

The convergence of the corresponding analytical and Laplace basis functions imply that the Laplace multipole expansion method is exactly equivalent to the present alternative multipole expansion method. The analytical functions given by Eqs. (3) and (6) can be considered as the infinite limit of the perturbative expansions given by Eqs.(4) and (5). The equivalence of Eq. (23) implies that:

$$\sum_{k=0}^{k_{max}\to\infty} \frac{(2l+4k-1)!!}{(2k)!!(2l+2k+1)!!} \left(\frac{\tilde{t}}{1+\tilde{t}^2}\right)^{2k} = \frac{(1+\tilde{t}^2)^{l+\frac{1}{2}}}{2l+1}, \tag{24}$$

$$\frac{(2l+1)}{\sqrt{1+\tilde{t}^2}} \tilde{j}_l(\tilde{t}) = \tilde{t}^l, \tag{25}$$

$$\tilde{j}_l(\tilde{t}) = \left(\tfrac{2l-1}{2l+1}\right) \tilde{t}\, \tilde{j}_{l-1}(\tilde{t}). \tag{26}$$

The use of the recurrence relation given by Eq. (26) can be useful in eliminating singularities associated with the analytical expression of the spherical Bessel-like functions, $\tilde{j}_l(\tilde{t})$,[11] as $\tilde{t} \to 0$.

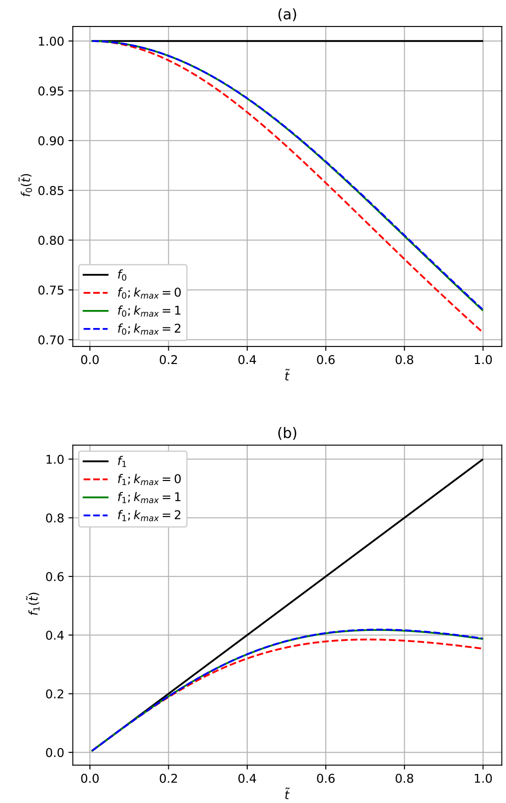

FIG. 1. (Color online) Comparison of the functions (a)$f_0(\tilde{t}) = 1$ and $h_0(\tilde{t}) = f_0^{k_{max}}(\tilde{t})$ and (b) $f_1(\tilde{t}) = \tilde{t}$ and $h_1(\tilde{t}) = f_1^{k_{max}}(\tilde{t})$, summed up to the maximum value (k_{max}), plotted using left and right hand side of Eq. (23) respectively. The black solid line corresponds to the Laplace basis functions, $\tilde{t}^l$.

Because of the divergence with the perturbative functions, it became of importance to test the performance of the expansions in repreducing the function given by Eq. (9) for various values of $\tilde{t}$ across the angular spectrum, with the maximum value of $l = 5$ used in all the series. The performance results are summarized in Fig. 3 for all values of $x = \cos\theta$. As expected, at lower values of $\tilde{t}$, there is a good agreement between all set of results, although the descrepancy with the perturbative results is still visible between the approximation methods used. At large values, $\tilde{t} > 0.5$, the perturbative results of the alternative multipole expansion series are significantly better in comparison with the Laplace series and the analytical functions, which overestimates the expected actual results. The discrepancy with the expected results show that not all terms in the infinite series expansion of the basis functions are necessary to accurately approximate the desired function. From the results presented, it can be observed that the perturbative alternative multipole expansion series sets the lower bound while the Laplace and the analytical alternative multipole expansion series sets an upper bound to the expected results.

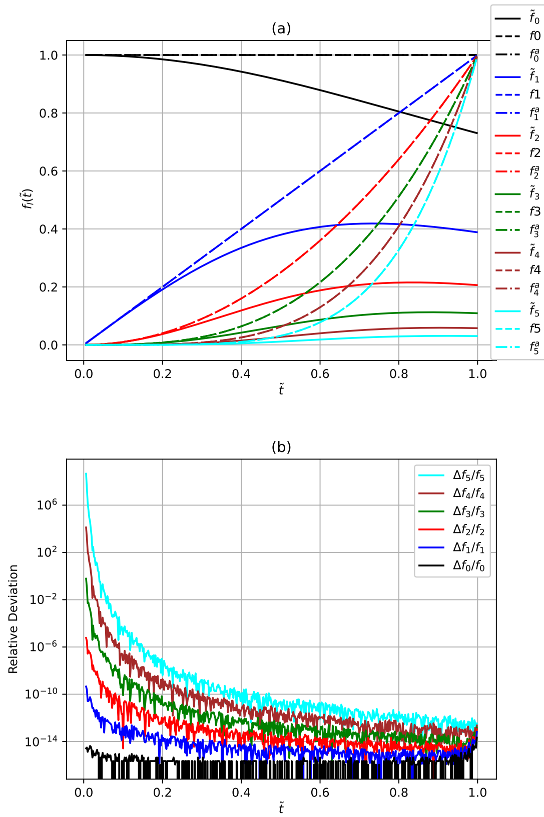

FIG. 2. (Color online) (a) Comparison of the six functions of $f_l(\tilde{t}) = t^l$, $h_l(\tilde{t}) = \tilde{f}_l^{k_{max}}(\tilde{t})$ with the value $k_{max} = 2$, and the analytical $h_l(\tilde{t}) = \tilde{f}_l(\tilde{t})$, plotted using left and right hand side of Eq. (23) respectively. The solid and the dash-dot lines represent the perturbative and the analytical $h_l(\tilde{t})$ functions, as given by Eqs. (3) - (6), while the dashed lines represent the Laplace basis functions, $f_l(\tilde{t}) = \tilde{t}^l$, respectively. (b) The relative deviation given as the absolute difference between the analytical $h_l(\tilde{t})$ and the Laplace $f_l(\tilde{t}) = \tilde{t}^l$ functions divided by the Laplace functions.

IV. CONCLUSION

The completeness as well as the performance of the Laplace multipole expansion of the Coulomb potential, in comparison with our recently developed alternative multipole expansion series, is investigated in this study. We have confirmed that the Laplace expansion series are in deed complete as opposed to our claim in ref.[10,11]. However, because of the difference in the basis functions used, the expansions yield complementary set of results with the Laplace and the analytical alternative multipole expansion series being an upper bound while the perturbative alternative multipole expansion being the lower bound of the expected results. In general, it can be seen that the alternative multipole expansion series is convergent in all the regimes, that is $0 < \tilde{t} < \infty$, as opposed to the Laplace expansion series which is only valid for $0 < \tilde{t} < 1$. Accurate results can be obtained using only a finite number of terms in the perturbative treatment of the spherical Bessel-like functions used in the alternative multipole expansion series of the Coulomb potential.

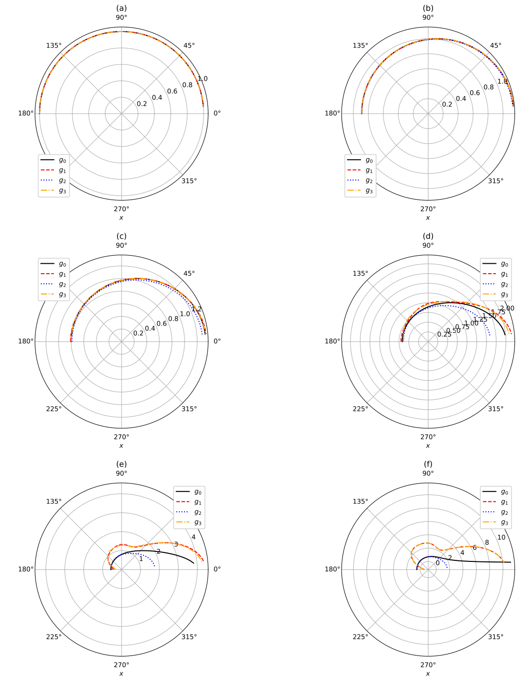

FIG. 3. (Color online) Comparison of the convergence of the different multipole expansion series to the expected actual value of the function $g(x,\tilde{t}) = (1 - 2x\tilde{t} + \tilde{t}^2)^{-\frac{1}{2}}$ given by Eq. (9) for various values of $\tilde{t}$: (a) $\tilde{t} = 0.00$, (b) $\tilde{t} = 0.125$, (c) $\tilde{t} = 0.25$, (d) $\tilde{t} = 0.50$, (e) $\tilde{t} = 0.75$, and (f) $\tilde{t} = 1.00$, and for all values of $x = \cos\theta$. The series is summed up to $l_{max} = 5$ for all the expansions. The black solid curve is the actual curve, the red dashed line correspond to the Laplace multipole expansion series approximation, the blue dotted line correspond to our alternative multipole expansion series approximation with up to second-order perturbatively evaluated functions, and the orange dash-dot line corresponding to the analytical alternative multipole expansion method.

DATA AVAILABILITY STATEMENT

All the data generated in the work are embedded as figures in the manuscript.

REFERENCES

[1] H. N. Laden, *An Historical and Critical Development of the Theory of Legendre Polynomials before 1900, MA thesis* (University of Maryland, 1938).
[2] G. B. Arfken, H. J. Weber, and F. Haris, *Mathematical methods for physicists*, vol. 7th Edition (Elsevier Academic Press, New York, 2013).
[3] A. Messiah, *Quantum Mechanics*, vol. I (North Holland Publishing Company, Amsterdam, 1961).
[4] H. Kusunose and S. Hayami, Journal of Physics: Condensed Matter **34**, 464002 (2022), URL `https://dx.doi.org/10.1088/1361-648X/ac9209`.
[5] Y. Zhou, Y. Meng, W. Huang, and K. Li, Results in Physics **39**, 105742 (2022), ISSN 2211-3797, URL `https://www.sciencedirect.com/science/article/pii/S2211379722004156`.

[6]J. L. Hernández–Pastora, The European Physical Journal C **82**, 224 (2022), URL https://doi.org/10.1140/epjc/s10052-022-10190-7.
[7]S. D. Chao, J. D. Kress, and A. Redondo, The Journal of Chemical Physics **120**, 5558 (2004), https://doi.org/10.1063/1.1649727, URL https://doi.org/10.1063/1.1649727.
[8]Romano, S. and Sommacal, D., Eur. Phys. J. D **32**, 45 (2005), URL https://doi.org/10.1140/epjd/e2004-00174-3.
[9]A. V. Nikolaev, Phys. Rev. B **71**, 165102 (2005), URL https://link.aps.org/doi/10.1103/PhysRevB.71.165102.
[10]E. O. Jobunga and S. O. Okeyo, Scientific Reports **10**, 20126 (2020).
[11]E. O. Jobunga, J. K. Mutembei, and K. O. Awuor, AIP Advances **12**, 075301 (2022), https://doi.org/10.1063/5.0097029, URL https://doi.org/10.1063/5.0097029.
[12]G. Vaman, Hal Open Science pp. ha–03582029 (2022).
[13]M. Motta, D. M. Ceperley, G. K.-L. Chan, J. A. Gomez, E. Gull, S. Guo, C. A. Jiménez-Hoyos, T. N. Lan, J. Li, F. Ma, et al. (Simons Collaboration on the Many-Electron Problem), Phys. Rev. X **7**, 031059 (2017), URL https://link.aps.org/doi/10.1103/PhysRevX.7.031059.
[14]J. P. Wikswo and K. R. Swinney, Journal of Applied Physics **56**, 3039 (1984), https://doi.org/10.1063/1.333885, URL https://doi.org/10.1063/1.333885.
[15]J. Vanderlinde, *Classical Electromagnetic Theory*, vol. 2nd Edition (Kluwer Academic Publishers, New York, 2005).