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Theoretical developments on the optical properties of highly turbid waters and sea ice

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Abstract

The photon diffusion equation is derived in a direct manner from the radiative transfer equation and is shown to be an asymptotic equation that can be directly related to asymptotic radiative transfer theory. Diffusion theory predicts that the asymptotic diffuse attenuation coefficient, K_∞, is related to the beam attenuation coefficient, c, the single scattering albedo, ω_0, and the asymmetry parameter, g, of the scattering phase function by $K_\infty = c\sqrt{3[1 - \omega_0 - g(\omega_0 - \omega_0^2)]}$. Kirk has previously published a K relationship based entirely on Monte Carlo radiative transfer simulations that can be expressed in the form $K_\infty = c\sqrt{1 - 2\omega_0 + \omega_0^2 + G(\omega_0 - \omega_0^2)}$, where G is a regression parameter. Equating these two results gives $G = 3(1 - g) + 2(1/\omega_0 - 1)$, showing explicitly, as Kirk found numerically, how G is a function of ω_0 and g. These results are expected to be valid for highly turbid water where $\omega_0 > 0.95$. Comparison of the analytical expression for G with Kirk's regression value, using ω_0 of 0.99, differed by only 2%.

The forward problem in radiative transfer theory is considered solved in the sense that existing numerical models can accurately compute the light field propagating through an absorbing and scattering medium, given the inherent optical properties (IOPs) of the medium and appropriate boundary conditions (Mobley et al. 1993). Nonetheless, it is still quite useful to search for simple relationships between IOPs and apparent optical properties (AOPs), and also between IOPs and radiometric quantities such as radiance and irradiance from which AOPs are derived. Such relationships not only provide a means for quick calculations, but more importantly they lend insight to understanding light propagation and provide the basis for developing inversion algorithms. Forward numerical models are useful for searching for these simple relationships since they can generate an accurate database that is often difficult, if not impossible, to obtain through measurements. But relationships found in this fashion are often unsatisfying, both because they are not based on or verified by measurements and because they are not derived from or connected analytically to theory.

Relationships between AOPs and IOPs are historically one of the most intensively investigated areas of optical oceanography. To date, no exact analytic equation giving an AOP as a function strictly of IOPs and boundary conditions has been derived rigorously from radiative transfer theory. Even Gershun's (1939) famous result, $a = K\bar{\mu}$, where a is the absorption coefficient, K the net irradiance attenuation coefficient, and $\bar{\mu}$ the average cosine of the light field, does not meet this criterion because this equation involves two AOPs, namely K and $\bar{\mu}$.

Starting with the steady-state radiative transfer equation and applying the diffusion approximation of the light field, a differential equation is derived in terms of integrated radiance quantities (*see* Eq. 9 below). Similar differential equations can be found in the literature on diffusion theory (Ishimaru 1978; Morse and Feshbach 1953), although the notation and definitions of optical quantities differ considerably from those used in modern radiative transfer theory, and the derivations are done in various ways that do not directly illuminate the present discussion. The derivation below proceeds directly from the radiative transfer equation expressed in a form that is most commonly used in optical oceanography. It is then shown that a simple form of the steady-state diffusion equation, which includes absorption, can be derived from the rather formidable general expression of the diffusion equation as an asymptotic limit. Equating the solution to the diffusion equation to an equivalent expression derived from asymptotic radiative transfer theory (Preisendorfer 1959) produces an important relationship between the asymptotic attenuation coefficient K_∞ and certain IOPs.

K relationships

The first analysis of K as a function of IOPs appeared in a now declassified report by Sorenson et al. (1966). By examining a variety of ocean-optical measurements, they arrived at the simple relationship $K_\infty \cong a + b/6$, where b is the total scattering coefficient. This simple formula was based on data for clear ocean water and was considered valid only in the near-asymptotic regime, where $K \cong K_\infty$ is the asymptotic attenuation coefficient (Preisendorfer 1959). Wilson (1979) later showed that the Sorenson et al. functional form gave the best fit to the available data when compared with other published K relationships (Timofeeva and Gorobetz 1967; Preisendorfer 1976). Wilson's result can be expressed as $K_\infty = c(1 - 0.85\omega_0)$, where $c = a + b$ is the beam-attenuation coefficient and $\omega_0 = b/c$ is the single-scattering albedo. Drawing upon essentially the same database that Wilson analyzed, Zaneveld (1989) reported the three-term relationship $K_\infty = c(1 - 0.52\omega_0 - 0.44\omega_0^2)$. The ω_0^2 term takes into account the small curvature that appears when plotting K_∞/c vs. ω_0.

Maffione and Jaffe (1995) reported $K_8 = c(1 - 0.532\omega_0 - 0.379\omega_0^2)$ and $K_{11} = c(1 - 0.666\omega_0 - 0.280\omega_0^2)$ based on an analysis of data generated by Hydrolight, a numerical model that exactly solves the one-dimensional radiative

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transfer equation (Mobley 1994). The different coefficients in K_8 and K_{11} were due to two different volume scattering functions (VSF) that were used in the numerical simulations. The VSF for K_8 was that measured by Petzold (1972) at his reported station 8, and the VSF for K_{11} was measured at his reported station 11. The different coefficients in K_8 and K_{11} clearly show that K_∞ is a function not only of the IOPs c and ω_0, but also of the shape of the VSF.

In a series of papers, Kirk (1981, 1984, 1991, 1994) investigated the nature of the light field in turbid waters using a Monte Carlo radiative transfer model. For the case of an axially symmetric light field, e.g. sun at zenith, Kirk found that

$$K_d = \sqrt{a^2 + Gab} \tag{1}$$

best fit his numerically generated database. In this equation, K_d is the irradiance attenuation coefficient for downwelling irradiance, which approaches K_∞ far from boundaries, i.e. in the asymptotic limit; G is a free parameter found to depend on the shape of the scattering phase function, although no rigorous physical meaning to G was given. Kirk modeled the light field due to different water turbidities by varying the ratio b/a up to a value of 200 (Kirk 1994), which corresponds to $\omega_0 = 0.995$.

It is shown here that Eq. 1 can be derived from the radiative transfer equation under the diffusion (sometimes referred to as Eddington's) approximation. The derivation reveals that Kirk's parameter G is an explicit and simple function of ω_0 and g, the average cosine of the scattering angle of the phase function, namely

$$g \equiv 2\pi \int_{-1}^{1} \tilde{\beta}(\psi)\cos\psi \, d(\cos\psi), \tag{2}$$

where $\tilde{\beta}(\psi)$ is the scattering phase function. Because the derivation involves the diffusion approximation, it is generally valid only for highly turbid media, i.e. when ω_0 is close to one. How close to one ω_0 has to be for the diffusion approximation to be valid is a subject of current research, but it is generally thought that diffusion is applicable when $\omega_0 > 0.95$ (Ishimaru 1978; Mobley and Maffione 1996; Zege et al. 1991).

Kirk (1994) has pointed out that there are many interesting and important aquatic ecosystems where the turbidity, or single scattering albedo, of the water is exceptionally high, or, in other words, where $\omega_0 > 0.95$. These systems include areas of the ocean during coccolithophore blooms, and many estuaries, fjords, lakes, and rivers that receive large amounts of unconsolidated sediments. In these systems, ω_0 depends strongly on wavelength and will be largest in the region of the spectrum where absorption is lowest, which is generally in the blue-green region (~400–590 nm). At longer wavelengths (red and infrared), absorption rapidly increases so that a and b become comparable, even though b is still quite high. A natural optical medium for which ω_0 is generally close to unity throughout the visible spectrum is sea ice and snow (Maffione and Mobley 1997). Thus, the results presented here should be applicable to a limited set of aquatic ecosystems and in general to optical propagation in sea ice.

Theory

Derivation—For simplicity, the following derivation considers only changes in the vertical direction z, taken to be positive downward from the surface as is common in optical oceanography. Moreover, anticipating the application of the diffusion approximation, the medium is taken to be homogeneous, as was also done in the previously cited papers of Kirk. That is, IOPs are independent of spatial coordinates, although radiometric quantities such as radiance, as well as AOPs such as K_d, do change with depth. As will be shown, the diffusion approximation for radiative transfer theory is strictly valid only in the asymptotic limit of the light field. In the asymptotic limit, the light field is axially symmetric (Preisendorfer 1959) and therefore depends only on the polar angle θ and the depth z. The derivation is thus completely general for a homogeneous medium regardless of the boundary conditions, which are irrelevant in the asymptotic limit. Note that the derivation could have been done in three dimensions, but the final result, using somewhat more complicated vector equations, is easily shown to be identical to the one-dimensional derivation given here with the appropriate rotation of the Cartesian axes in the three-dimensional case. This is so because in the asymptotic limit there is one unique axis about which the light field is axially symmetric, except of course in the case where the light field is isotropic, in which case the two solutions are identical for any orientation of the axes.

For homogeneous water illuminated by a zenith sun, or horizontal plane wave, the radiance distribution L is axially symmetric, i.e. is a function only of the polar angle θ which is measured from the z-axis. Moreover, L is a function of only one spatial coordinate, in this case depth z, so that $L = L(z, \theta)$. Considering elastic scattering only in a source free medium, the radiative transfer equation is then given by

$$\begin{aligned}\cos\theta \frac{\partial L(z,\theta)}{\partial z} &= -cL(z,\theta) + b \iint_{4\pi} \tilde{\beta}(\psi) L(z,\theta',\phi') \sin\theta' \, d\theta' \, d\phi' \\ &= -cL(z,\theta) + bL_s(z,\theta).\end{aligned} \tag{3}$$

The scattering angle ψ is the angle between directions (θ', ϕ') and (θ, ϕ), where ϕ can be any chosen azimuth angle since $L(z, \theta)$ is independent of ϕ. For example, taking $\phi = 0$ gives the relation $\cos\psi = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos\phi'$. The integral on the right-hand side of Eq. 3, denoted L_s, is called the source function because it adds radiance to the path due to scattering within the medium. It is common in oceanic optics to denote bL_s by L_*, the so-called path function. Integrating Eq. 3 over the complete 4π solid angle yields the one-dimensional form of Gershun's (1939) equation, viz.

$$\frac{\partial E(z)}{\partial z} = -aE_0(z), \tag{4}$$

where

$$E(z) \equiv 2\pi \int_0^{\pi} L(z, \theta)\cos\theta \sin\theta \, d\theta$$

$$= 2\pi\left[\int_0^{\pi/2} L(z, \theta)\cos\theta \sin\theta \, d\theta - \int_{\pi/2}^{\pi} L(z, \theta)|\cos\theta|\sin\theta \, d\theta\right]$$

$$= E_+(z) - E_-(z) \tag{5a}$$

is the net vertical irradiance and

$$E_0(z) \equiv 2\pi \int_0^{\pi} L(z, \theta)\sin\theta \, d\theta \tag{5b}$$

is the scalar irradiance.

The radiance distribution can be divided into the linear combination $L(z, \theta) = L_i(z, \theta) + L_d(z, \theta)$. The term $L_i(z, \theta)$ is referred to as the reduced incident radiance and represents that part of the radiance distribution which satisfies $\cos\theta \, \partial L_i(z, \theta)/\partial z = -cL_i(z, \theta)$. In other words, the reduced incident radiance is the radiance distribution that has been attenuated by absorption and scattering out of the path, but does not include the source radiance L_s. The diffuse radiance $L_d(z, \theta)$ is the radiance distribution that is created within the medium by scattering, and satisfies the following equation of transfer:

$$\cos\theta \frac{\partial L_d(z, \theta)}{\partial z} = -cL_d(z, \theta) + b \iint_{4\pi} \tilde{\beta}(\psi) L_d(z, \theta', \phi')\sin\theta' \, d\theta' \, d\phi' + b \iint_{4\pi} \tilde{\beta}(\psi) L_i(z, \theta', \phi')\sin\theta' \, d\theta' \, d\phi'$$

$$= -cL_d(z, \theta) + bL_{sd}(z, \theta) + bL_{si}(z, \theta), \tag{6}$$

where L_{sd} and L_{si} are the source functions due to the diffuse and incident radiances, respectively. Clearly, $L(z, \theta) = L_i(z, \theta) + L_d(z, \theta)$ satisfies Eq. 3. Analogous to obtaining Eq. 4, integration of Eq. 6 over the 4π solid angle gives

$$\frac{\partial E_d(z)}{\partial z} = -aE_{0d}(z) + bE_{0i}, \tag{7}$$

where the subscripts d and i denote the irradiances due to $L_d(z, \theta)$ and $L_i(z, \theta)$, respectively. (The subscript d should not be confused with downwelling, which in this paper is denoted by the "+" subscript.)

The axially symmetric radiance distribution can be expanded in a Taylor series in $\cos\theta$. Thus, $L_d(z, \theta)$ can be written

$$L_d(z, \theta) = A_1 + A_2\cos\theta + \ldots .$$

If the diffuse light field is isotropic, then $L_d = E_{0d}/4\pi = A_1$. A necessary, though not sufficient condition for an isotropic light field is $\omega_0 = 1$ (i.e. $a = 0$). As ω_0 decreases from 1, $L_d(z, \theta)$ becomes less diffuse, i.e. more peaked about $\theta = 0°$. If $L_d(z, \theta)$ is not highly forward peaked, it can be accurately expressed by the first two terms in its Taylor expansion. The constant A_2 can be found by integrating the two-term expansion to obtain $E_d(z)$, viz.

$$E_d(z) = 2\pi \int_0^{\pi} L_d(z, \theta)\cos\theta \sin\theta \, d\theta$$

$$= 2\pi\left[\frac{E_0}{4\pi}\int_0^{\pi} \cos\theta \sin\theta \, d\theta + A_2 \int_{\pi/2}^{x} \cos^2\theta \sin\theta \, d\theta \, d\theta\right]$$

$$= \frac{4\pi A_2}{3},$$

giving $A_2 = 3E_d/4\pi$. The approximate expression for $L_d(z, \theta)$ is therefore

$$L_d(z, \theta) \cong \frac{1}{4\pi}[E_{0d}(z) + 3E_d(z)\cos\theta]. \tag{8}$$

Note that $E_{0d} \gg E_d = E_{+d} - E_{-d}$ since, for a diffuse light field, E_{+d} is only slightly greater than E_{-d}. The second term in Eq. 8 is therefore much smaller than the first term, justifying the accuracy of retaining only two terms in the Taylor expansion.

Substituting Eq. 8 into Eq. 6 gives

$$\cos\theta \frac{\partial E_{0d}(z)}{\partial z} + 3\cos^2\theta \frac{\partial E_d(z)}{\partial z} = -cE_{0d}(z) - 3cE_d(z)\cos\theta + bE_{0d} + 3bgE_d\cos\theta + 4\pi bL_{si}. \tag{9}$$

Multiplying Eq. 9 through by $\cos\theta \sin\theta \, d\theta \, d\phi$ and integrating over 4π leads directly to

$$\frac{\partial E_{0d}(z)}{\partial z} = 3(gb - c)E_d(z) + bE_{si}(z),$$

or

$$E_d(z) = -D\frac{\partial E_{0d}(z)}{\partial z} - \frac{b}{D}E_{*i}(z), \tag{10}$$

where

$$E_{*i}(z) = 4\pi \iint_{4\pi} L_{si}(z, \theta)\cos\theta \sin\theta \, d\theta \, d\phi, \tag{11}$$

and

$$D = \frac{1}{3(c - gb)}. \tag{12}$$

As will be seen below, D is interpreted as the diffusion coefficient. Substituting $E_d(z)$, given by Eq. 10, into Eq. 7 results in

$$D\frac{\partial^2 E_{0d}}{\partial z^2} - aE_{0d} + \frac{b}{D}\frac{\partial E_{si}}{\partial z} + bE_{0i} = 0, \tag{13}$$

which is the general form of the steady-state, one-dimensional diffusion equation.

As $z \to \infty$, the magnitudes of the last two terms in Eq. 13, which depend on the incident reduced radiance, decay much faster than do the first two terms, which depend on the diffuse radiance. This follows because, by its definition, $L_i(z, \theta)$ decays exponentially with a decay constant c, the beam attenuation coefficient. On the other hand, all $L_d(z, \theta)$-derived quantities will have an exponential decay constant that is a diffuse attenuation coefficient, similar to the well-known irradiance attenuation coefficients derived from the total radiance. If $b > 0$, then all diffuse attenuation coefficients, denoted generically as K_x, must be less than c. In the present context, ω_0 is close to 1, so that $b \gg a$ and therefore $K_x \ll c$. Thus, for large $\tau = cz$, where τ is the optical depth, the last two terms in Eq. 13 will be much smaller than the first two terms and can safely be neglected, leading to

$$D\frac{\partial^2 E_{0d}}{\partial z^2} - aE_{0d} = 0. \tag{14}$$

Eq. 14 has the simple bounded solution

$$E_{0d}(\Delta z) = E_{0d}(z_0)\exp(-\sqrt{a/D}\,\Delta z), \tag{15}$$

where $\Delta z = z - z_0$ and $z_0 \gg 1/c$, since the solution is not valid near the boundary. For a highly scattering medium, or turbid water with a high ω_0, Eq. 15 becomes increasingly more accurate as the depth (i.e. distance from the boundary) increases. At the same time, the light field is approaching its asymptotic state, and does so relatively rapidly in a highly scattering medium. In the asymptotic state, all photons have scattered at least once, so that $L_d(z, \theta) = L_\infty(z, \theta)$, where $L_\infty(z, \theta)$ is the asymptotic radiance distribution, which is constant in shape and decays exponentially according to (Preisendorfer 1959):

$$L_\infty(\Delta z, \theta) = L_\infty(z_0, \theta)\exp(-K_\infty \Delta z). \tag{16}$$

In the asymptotic state, all exponential decay coefficients are constant and equal, so that the form of Eq. 16 applies equally well for any light field quantity, including $E_{0d}(z)$ in Eq. 15. This implies that, far from the boundary of a highly scattering medium,

$$\begin{aligned} K_\infty &= \sqrt{a/D} \\ &= \sqrt{3a(c - gb)} \\ &= c\sqrt{3[1 - \omega_0 - g(\omega_0 - \omega_0^2)]} \end{aligned} \tag{17}$$

Comparison with Kirk's results—Kirk expressed his results in terms of the ratio b/a. In what follows, ω_0 is used in place of b/a, as is customary in radiative transfer theory. The two quantities are related by

$$\frac{b}{a} = \frac{\omega_0}{1 - \omega_0}$$

and

$$\omega_0 = \frac{b/a}{1 + b/a}.$$

One advantage of using ω_0 instead of b/a as a descriptor for the relative degree of scattering, or turbidity, of a medium is that it is bounded by $0 \le \omega_0 \le 1$, whereas b/a is unbounded. Rewriting Kirk's result, Eq. 1, in terms of ω_0, gives

$$K_\infty = c\sqrt{1 - 2\omega_0 + \omega_0^2 + G(\omega_0 - \omega_0^2)}. \tag{18}$$

Equating Eq. 17 and 18 and solving for G yields

$$G = 3(1 - g) + 2(1/\omega_0 - 1). \tag{19}$$

Eq. 19 explains rather well the results of Kirk for highly turbid water. He found that G was a weak function of ω_0, or in his case of b/a (Kirk 1994), but exhibited a somewhat stronger dependence on the shape of the phase function, as described by g (Kirk 1991). This can be explained in Eq. 19 by noting that large changes in b/a for highly turbid water, where Eq. 19 is valid, correspond to relatively small changes in ω_0 and hence in G. Small changes in g, however, correspond to relatively large changes in the shape of the phase function.

In the most highly turbid case that Kirk (1994) investigated, namely $\omega_0 = 0.995$, he reported a value of $G = 0.233$. In his simulation, Kirk used a phase function measured by Petzold (1972) in San Diego Harbor, considered to be turbid water. Computing g by Eq. 2 for Petzold's measured phase function gives $g = 0.924$. Substituting these values for g and ω_0 into Eq. 19 gives $G = 0.238$, which differs only 2% from Kirk's numerically simulated value of $G = 0.233$.

From his Monte Carlo calculations, Kirk reported that G varied from 0.233 to 0.264, with an average value of 0.245 over the range $b/a = 2$ to 200, or $\omega_0 = 0.667$ to 0.995. Morever, Kirk found that, when comparing K/a from his Monte Carlo calculations with K/a computed with his analytical expression using the average value $G = 0.245$, they differed by at most 2.5% over the entire range b/a range he was considering. Thus, Kirk's analytical expression, using $G = 0.245$, should provide an accurate means to easily investigate the lower bounds of ω_0 for which the diffusion result is valid. Figure 1 shows calculations of K/c computed with Eq. 17 (diffusion) and Eq. 18 (Kirk) for ω_0 from 0.95 to 1.0. The divergence of the two curves as ω_0 decreases illustrates how the diffusion result breaks down as the optical medium becomes less turbid. At $\omega_0 = 0.95$, the percent difference in the two results is 14%, which is probably the upper limit for acceptable errors in most applications where Eq. 17 might be used. At $\omega_0 = 0.98$, which is probably the lower bound for most types of sea ice, the percent error is ~4%. At higher values of ω_0, the differeces fluctuate around 2%, which is approximately the error that Kirk reports in his equation for K.

Conclusions

The derivation of the steady-state photon diffusion equation, Eq. 14, shows that it is the asymptotic limit of the more general diffusion equation, Eq. 13. Solutions to Eq. 14 are therefore strictly valid only in the asymptotic limit, as $z \to \infty$. Although the general solution, Eq. 15, includes absorption, it is a fundamental requirement that $a \ll b$, or ω_0 is close to one, i.e. the medium is highly scattering. At what minimum value of ω_0 Eq. 15 significantly breaks down is a

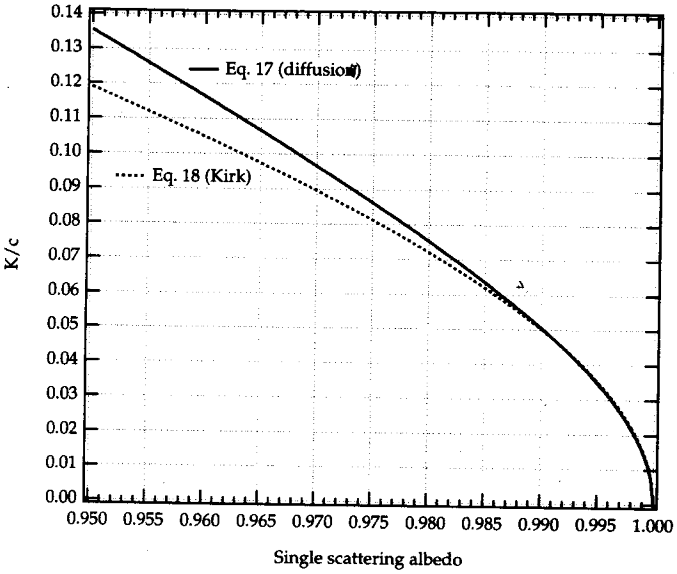

Fig. 1. Comparison of K/c using the diffusion result, Eq. 17, and Kirk's reported result, Eq. 18 in the text. In computing K with Kirk's equation, his reported average value of $G = 0.245$ was used.

subject of current research, but it is generally accepted that $\omega_0 = 0.95$ is a lower limit (Ishimaru 1978; Mobley and Maffione 1996; Zege et al. 1991). In highly turbid water and sea ice, where in general $\omega_0 > 0.95$, the diffusion approximation is expected to be valid for describing light propagation in the asymptotic limit. Moreover, the asymptotic state is more rapidly approached as ω_0 increases, implying that the boundary layer where the diffusion approximation breaks down should be relatively thin.

Kirk has published a K relationship, Eq. 1, that was arrived at by analyzing a numerically generated dataset with a Monte Carlo radiative transfer model. The equation contains a regression parameter, G, that was found by Kirk to vary when he varied the IOPs in his simulations. Although Kirk showed that his equation was valid over a wide range of optical properties, including highly turbid water, his equation has a surprisingly similar form to the K equation derived from diffusion theory, Eq. 17. Equating Kirk's equation with the diffusion K equation resulted in a simple relationship for G as a function of ω_0 and g, given by Eq. 19. Substitution of Kirk's values for ω_0 and g in his simulations for highly turbid water into Eq. 19 yielded a value of G that was within 2% of Kirk's reported value. This gratifying result shows that, for highly turbid water and sea ice, Kirk's numerically derived K relationship can be interpreted and understood within the context of photon diffusion theory. Conversely, applying Kirk's result to investigate the validity of the diffusion result reveals that the latter is accurate to within a few percent of the true value of K down to $\omega_0 = 0.98$, with errors gradually increasing as ω_0 decreases. At $\omega_0 = 0.95$, the estimated percent error in using Eq. 17 is ~14%. Below $\omega_0 = 0.95$, the diffusion approximation rapidly breaks down, as expected.

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