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Extension of the weak-line approximation and application to correlated-k methods



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# Extension of the weak-line approximation and application to correlated-k methods

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**abstract**

Global climate models require accurate and rapid computation of the radiative transfer through the atmosphere. Correlated-k methods are often used. One of the approximations used in correlated-k models is the weak-line approximation. We introduce an approximation $T_g$ which reduces to the weak-line limit when optical depths are small, and captures the deviation from the weak-line limit as the extinction deviates from the weak-line limit. This approximation is constructed to match the first two moments of the gamma distribution to the k-distribution of the transmission. We compare the errors of the weak-line approximation with $T_g$ in the context of a water vapor spectrum. The extension $T_g$ is more accurate and converges more rapidly than the weak-line approximation.

## 1. Introduction

Accurate treatments of the interactions of incident sunlight and emitted thermal radiation with Earth system components are essential for models of the climate system. While computations that resolve the line structure of the gases using line-by-line methods can provide a reference computation of radiative transfer for the known spectral characteristics of the known atmospheric composition, they are computationally too expensive—by several orders of magnitude—for routine use in global climate models. Band transmission models have been used in earlier generations of global climate models to estimate the radiative fluxes through the earth's atmosphere [1]. According to recent surveys of the climate modeling community (Q. Fu, private communication), correlated-k methods are currently the most widely used method of approximating the solution while maintaining acceptable accuracy and speed [2,3]. In these methods, the integrals over frequency required for broadband fluxes and heating rates are replaced via Laplace transforms with mathematically identical integrals over specific extinction.

A significant source of error in correlated-k methods is the quadrature error associated with the parameterization of the integration over the distribution of extinctions. The line strengths of radiatively active gases can vary over several orders of magnitude through a band; there are often many lines in a band, making accurate and fast integration through the corresponding range of extinctions difficult. Instead, the integration through the extinctions (or frequencies) is often parameterized by a weighted sum of exponentials [4–7]. This weighted sum is called the weighted sum of gray gases, or the exponential sum fitting of transmission.

A constructive method for approximating the transmission with a rigorous and predefined error constraint at all path lengths is found in [8]. This method appears to overestimate the terms required to construct an approximation satisfying the predefined error constraints. Furthermore, the number of terms required to meet the predefined error may be quite large.

The method described in this paper provides a higher order basis function, with a resulting faster convergence, but lack the necessary rigorous error bounds provided by the constructive method.

One of the gray gas approximations is the weak-line approximation [1] for the band transmission:

$$T(u) = \frac{1}{\Delta v}\int_{v_1}^{v_2} dv\ \exp(-k(v)u) \tag{1}$$

$$T(u) \approx \exp(-\langle k \rangle u) \tag{2}$$

where

$$\Delta v = v_2 - v_1 \tag{3}$$

$$\langle k \rangle = \frac{1}{\Delta v}\int_{v_1}^{v_2} dv\ k(v) \tag{4}$$

Here $\langle k \rangle$ is the mean absorption coefficient, $k(v)$ is the specific absorption, $u$ is the path length, and $v_1$ and $v_2$ are the frequency bounds of the band. This approximation is based on a number of assumptions that we will review, but despite the limited validity of these assumptions the weak-line approximation is commonly used to develop correlated-$k$ methods. Typically correlated-$k$ methods partition the range of extinctions and assign an effective extinction to each range. It is not clear *a priori* whether the weak-line limit is the optimal approximation for arbitrary partitioning and for arbitrary path lengths through the radiatively active medium.

We present an extension of the weak-line approximation that takes higher moments into account and provides a more accurate representation of the transmission. An analogue can be seen in the difference between the trapezoidal rule and Simpson's rule for numerical integration. In the case of transmission, the problem is complicated by the fact that the gray gas approximation has an exponential order error, i.e., the specific extinction appears in the exponent. In this paper, we approximate the $k$-distribution instead of approximating the argument of the exponential. We thereby obtain a parameterization that is more accurate and converges at higher order. The method is also easily constructed without reference to any numerical optimization. The only required information from the $k$-distribution is the first two moments of the distribution, although we present some alternatives in the appendices that require additional information.

This paper first provides a few definitions in Section 2. It reviews the weak-line approximation in Section 3. In Section 4 we introduce an extension of the weak-line approximation that is applicable to a larger range of extinctions and converges to the weak-line approximation when the range of extinctions is small. We test the approximation for a simple spectrum consisting of two Lorentz lines in Section 5. For a more rigorous test of the approximation, we study the approximation in the context of a realistic water vapor spectrum for a near-infrared band under stratospheric conditions in Section 6. Finally, we summarize the results in Section 7.

## 2. Definitions

For a frequency band $v \in [v_1, v_2]$, the band transmission is defined as

$$T(u) = \frac{1}{\Delta v}\int_{v_1}^{v_2} dv\ \exp(-k(v)u) \tag{5}$$

$$T(u) = \int_0^{\infty} dk\, f(k)\exp(-ku) \tag{6}$$

where $f(k)$ is the inverse Laplace transform of the transmission $T(u)$. The $k$-distribution $g(k)$ is defined in terms of $f(k)$ as follows:

$$f(k) = \mathcal{L}^{-1}(T(u); k) \tag{7}$$

$$g(k) = \int_{\underline{k}}^{k} dk\, f(k) \tag{8}$$

$$k(g) = g^{-1}(k) \tag{9}$$

where the minimum and maximum extinctions denoted by

$$\underline{k} = \min_{v \in [v_1, v_2]} k(v) \tag{10}$$

$$\overline{k} = \max_{v \in [v_1, v_2]} k(v) \tag{11}$$

are assumed to be positive, i.e. $\underline{k} > 0$. For some parts of this paper, the requirement of positivity is not required, but the development of the idea is clearest under the assumption that the extinction is positive in all parts of the band.

The coefficient of variation, defined as the ratio of standard deviation to mean value

$$V = \sqrt{\frac{\langle k^2 \rangle}{\langle k \rangle^2} - 1} \tag{12}$$

This coefficient will turn out to be a useful measure of the deviation of the $k$-distribution from a $\delta$-distribution. As $V \to 0$, the $k$-distribution becomes narrowly distributed around $k = \langle k \rangle$, and the transmission will be seen to be well approximated by the weak-line approximation. As $V$ increases, the range of path lengths for which the weak-line approximation is useful for band transmission will be seen to decrease.

The effective extinction for the transmission $T(u)$, used to compare transmission over a large range of paths, is defined as

$$k_e(u) = -\frac{1}{u}\log(T(u)) \tag{13}$$

The mean value of a function $h(k)$ is defined as follows

$$\langle h(k) \rangle = \int_{\underline{k}}^{\overline{k}} dk\, f(k)h(k) \tag{14}$$

$$\langle h(k) \rangle = \frac{1}{\Delta v}\int_{v_1}^{v_2} dv\ h(k(v)) \tag{15}$$

In addition, it is useful to refer to a partition $P_N$ of the range of extinctions into $N$ parts defined as

$$\{k_i \ni \underline{k} = k_0 < k_1 < \cdots < k_N = \overline{k}\} \tag{16}$$

and to define corresponding statistical measures on each part of the partition (where $i$ indexes the part)

$$g_i = g(k_i) \tag{17}$$

$$\delta_i g = g_i - g_{i-1} \tag{18}$$

$$\langle h(k) \rangle_i = \frac{1}{\delta_i g} \int_{g_{i-1}}^{g_i} dg \ h(k(g)) \tag{19}$$

$$V_i = \sqrt{\frac{\langle k^2 \rangle_i}{\langle k \rangle_i^2} - 1} \tag{20}$$

Lastly, to compare the transmission $T(u)$ with an approximation, say $T_a(u)$, we will graph the relative error of $k_e$ for $T_a(u)$. This relative error is defined as

$$R(T_a(u)) = \frac{|\ln(T(u)) - \ln(T_a(u))|}{|\ln(T(u))|} \tag{21}$$

This can be regarded as the relative error in effective extinction or as the relative error in band effective optical depth.

## 3. Weak-line approximation

The weak-line approximation $T_W(u)$ can be derived as follows:

$$T(u) \tag{22}$$

$$= \frac{1}{\Delta \nu} \int_{\nu_1}^{\nu_2} d\nu \ \exp(-k(\nu)u) \tag{23}$$

$$\sim \frac{1}{\Delta \nu} \int_{\nu_1}^{\nu_2} d\nu \left(1 - k(\nu)u + \frac{1}{2}k^2(\nu)u^2\right) \tag{24}$$

$$= 1 - \langle k \rangle u + \frac{1}{2} \langle k^2 \rangle u^2 \tag{25}$$

$$\sim 1 - \langle k \rangle u + \frac{1}{2} \langle k \rangle^2 u^2 \tag{26}$$

$$\sim \exp(-\langle k \rangle u) \equiv T_W(u) \tag{27}$$

The approximation from (23) to (24) requires that the optical depth $\tau(\nu) = k(\nu)u$ is small compared to unity. From (25) to (26) requires that the coefficient of variation is small. And lastly, from (26) to (27) requires that $\langle k \rangle u \ll 1$ (which is implied by the optical depth being small).

The weak-line approximation can be summarized as follows:

$$\langle \exp(-ku) \rangle \sim \exp(-\langle k \rangle u) \tag{28}$$

Since the exponential function is convex, we know (using Jensen's inequality for measures of convex functions [9]) that the weak-line approximation will always underestimate the transmission. Thus, there is no reason to assume that, for an arbitrary extinction distribution, the weak-line approximation is the best one or that it is particularly valid for a large range of path lengths.

As an example, for an exponential $k$-distribution,

$$f(k) = \frac{1}{\beta} \exp(-k/\beta) \tag{29}$$

the transmission is the Padé function [10],

$$P_{0,1} = \frac{1}{1 + \langle k \rangle u} \tag{30}$$

and the coefficient of variation is

$$V = 1 \tag{31}$$

So while the simple algebraic form of $P_{0,1}$ is exact in this case, $T_W(u)$ is a poor approximation at large $u$. Of course, the $k$-distribution in this case has a significant weight at $k$=0, so the example is not particularly applicable for carefully chosen bands. Nevertheless, this example illustrates that for a band, a simple ratio of polynomials may be a better approximation than an exponential function.

In summary, if the optical depth is small compared to one for all frequencies then the weak-line limit is a good approximation. The coefficient of variation provides a measure of the error of the weak-line approximation as optical depths become larger. In the case of larger coefficient of variation, a different functional form may provide an approximation that provides a larger range of applicability or better error characteristics.

## 4. Extension of the weak-line approximation

Since the transmission has different algebraic forms for different $k$-distributions, we seek an approximation guaranteed to have the following properties:

1. Decreases monotonically from 1 to 0 as $u$ goes from 0 to $\infty$.
2. Matches the first two moments of the $k$-distribution.
3. Converges to $T_W(u)$ when $V \to 0$.

One such approximation is an extended weak-line approximation,

$$T_\gamma(u) = \frac{1}{(1 + \beta u)^\gamma} \tag{32}$$

where

$$\gamma = 1/V^2 \tag{33}$$

$$\beta = \langle k \rangle V^2 \tag{34}$$

$$V^2 = \frac{\langle k^2 \rangle}{\langle k \rangle^2} - 1 \tag{35}$$

$$k_{e\gamma} = \frac{\ln(1 + \langle k \rangle V^2 u)}{V^2 u} \tag{36}$$

are chosen so that the first three terms in the Taylor expansions near $u$=0 of $T(u)$ and $T_\gamma(u)$ match.

In the limit of small coefficient of variation ($V \ll 1$),

$$T_\gamma(u) = \exp\left(-\langle k \rangle u + \frac{V^2 \langle k \rangle^2 u^2}{2} + E(u)\right) \tag{37}$$

where

$$E(u) = O(V^4 \langle k \rangle^3 u^3) \tag{38}$$

indicating that the weak-line approximation is recovered for $\langle k \rangle^2 V^2 u^2 \ll 1$.

$T_\gamma(u)$ has a $k$-distribution (density) known as the gamma distribution

$$f_\gamma(k) = \frac{1}{\Gamma(\gamma)k}\left(\frac{k}{\beta}\right)^\gamma \exp(-k/\beta) \tag{39}$$

Other possible extensions are discussed in Appendix A.

For comparison, the $k$-distribution corresponding to $T_W(u)$ is the Dirac-delta function

$$f_W(k) = \delta(k - \langle k \rangle) \tag{40}$$

Comparison of $T_W(u)$ and $T_\gamma(u)$ with $T(u)$ for a range of path lengths is illustrative of the applicability of this extension of the weak-line approximation. We evaluate the accuracy of $T_\gamma(u)$ relative to $T_W(u)$ for idealized and realistic spectra in the next two sections.

## 5. Two Lorentz lines

As our first example, consider transmission through two Lorentz lines. The $k$-distribution (Fig. 1) corresponds to the extinction $k(\nu)$ defined by a sum of two Lorentz lines,

$$k(\nu) = \frac{S_1\alpha_1}{\pi(\alpha_1^2 + (\nu-\nu_1)^2)} + \frac{S_2\alpha_2}{\pi(\alpha_2^2 + (\nu-\nu_2)^2)} \tag{41}$$

where $S_1 = 3, \alpha_1 = .3, \nu_1 = 2, S_2 = 3, \alpha_2 = .5$, and $\nu_2 = 3$. The band is defined as the frequencies $\nu \in [1,4]$. Fig. 2 compares the effective extinction for the band transmission through the two lines with the effective extinctions for $T_W(u)$ and $T_\gamma(u)$. As this figure shows, the effective extinction for $T_\gamma(u)$ is much closer to the effective extinction of $T(u)$ than is the effective extinction of $T_W(u)$. Note that the relative error in the transmission is proportional to the exponential of the differences of the effective extinction,

$$\frac{T(u) - T_\gamma(u)}{T(u)} = 1 - \exp((k_e - k_{e\gamma})u) \tag{42}$$

So even small differences in the effective extinction can lead to large relative errors for the transmission for large $u$.

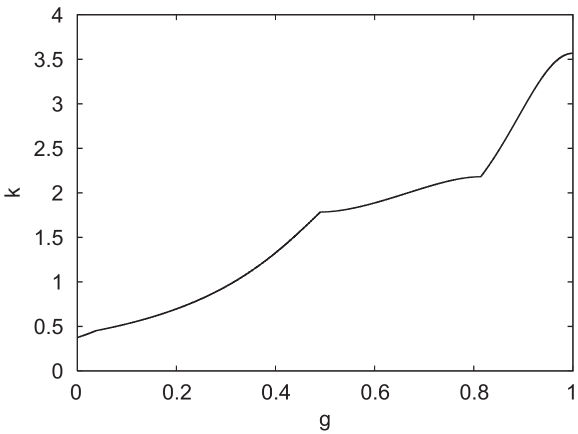


**Fig. 1.** The $k$-distribution of double line spectrum defined in Eq. (41). Cusps in the distribution of extinctions exist at maxima and minima of $k(\nu)$.

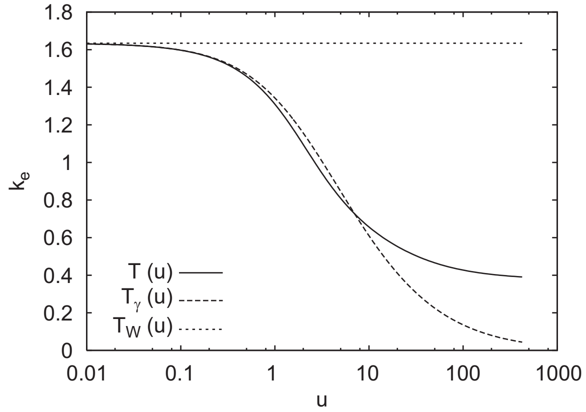


**Fig. 2.** Effective extinction of double line spectrum in Eq. (41). Also shown are the effective extinction of the weak-line approximation $T_W(u)$ and the extended-weak-line approximation $T_\gamma(u)$.

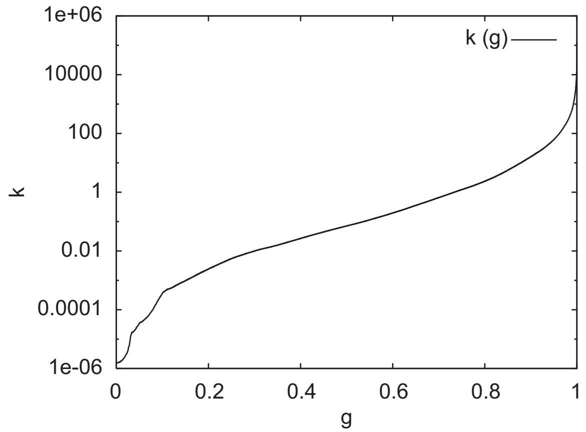


**Fig. 3.** The $k$-distribution for water vapor in the stratosphere between 0.7 and 5 μm. The cusps in the curve near $g$=0 are numerical artifacts of the sampling of far-wing shapes.

## 6. Water vapor spectrum

As another comparison, consider the transmission through water vapor in the stratosphere. The water vapor spectrum in the stratosphere in the near-IR has a large number of lines and these lines are much narrower than in the lower troposphere. As a result the extinction spectrum spans nearly 12 orders of magnitude (Fig. 3). We study the approximation of this spectrum for all path lengths. Typical water vapor paths do not saturate all parts of the frequency spectrum from 0.7 to 5 μm, so the longest path lengths studied here are an extreme test. Nevertheless, the comparisons provide insight into the applicability of $T_W$ and $T_\gamma$ for bands and gases with a large range of extinction.

The effective extinction decreases as a function of path length as can be seen in Fig. 4. The band is saturated for path lengths larger than $10^6$.

For bands such as the near-IR stratospheric water vapor where the extinction varies over many orders of

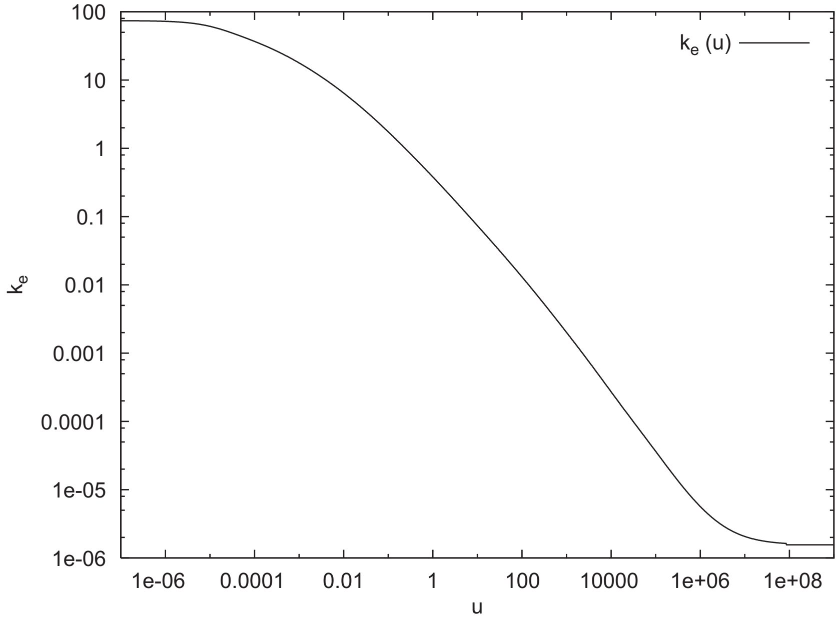


**Fig. 4.** Effective extinction as a function of path for the water vapor spectrum in Fig. 3. As the path length increases from zero, the effective extinction decreases from the average extinction $\langle k \rangle$ to the minimum extinction.

magnitude, the weak-line limit is not applicable, so in many correlated-$k$ codes the extinction is partitioned and the weak-line approximation is used on each part. By partitioning the extinction spectrum so that the log of the extinction is evenly divided

$$k_{i+1}/k_i = \text{constant}, \quad i = 0,1,2,\ldots,N \tag{43}$$

a weak-line approximation of the transmission function can be specified as

$$T_W^N(u) = \sum_{i=1}^{N} \delta_i g \exp(-\langle k \rangle_i u) \tag{44}$$

Similarly, an extended weak-line approximation (Section 4) can be specified as

$$T_\gamma^N(u) = \sum_{i=1}^{N} \frac{\delta_i g}{(1+\beta_i u)^{\gamma_i}} \tag{45}$$

where

$$\gamma_i = 1/V_i^2 \tag{46}$$

$$\beta_i = \langle k \rangle_i V_i^2 \tag{47}$$

As the partition is refined, the coefficient of variation $V_i$ on each partition goes to zero and the extended weak-line approximation converges to the weak-line approximation. This illustrates how $V_i$ is one measure of the error associated with the weak-line limit. Fig. 5 shows that the relative error in the effective extinction for $T_W(u)$ is much larger than $T_\gamma(u)$. When the partition has 20 parts, the magnitudes of the relative errors have both decreased toward zero, but the error of $T_W(u)$ is approximately 10 times that of $T_\gamma(u)$ for all values of $u$ (Fig. 6).

We graph the relative error of the effective extinction at two different path lengths for $T_W$ and $T_\gamma$ in Fig. 7. Noting that the relative errors are approximately linear, we can define an order of convergence, $\alpha$, as

$$\ln\left(\frac{k_e - k_{e\gamma}}{k_e}\right) = \beta - \alpha \ln(N) \tag{48}$$

or, equivalently, as

$$\frac{k_e - k_{e\gamma}}{k_e} = \left(\frac{N_0}{N}\right)^{\alpha} \tag{49}$$

In other words, $\alpha$ is the slope of each line in Fig. 7. As can be seen the order of convergence of $T_\gamma(u)$ is larger than $T_W(u)$.

## 7. Discussion

Correlated-$k$ methods typically parameterize the frequency quadrature of the transmission. Matching the first two moments of the gamma distribution to the $k$-distribution provides a parameterization $T_\gamma(u)$ that offers a significant improvement when compared to the weak-line approximation. The extension is more accurate for a larger range of path lengths.

This method also provides a measure $V_i$ of the error on each part of the partition. It remains to be seen if this measure of the error could be used to improve the choice of the partition boundaries, $k_i$.

While this paper has considered extensions to the weak-line limit in the context of correlated-$k$ methods, these extensions could be quite useful in other contexts where an estimate of a Laplace transform of a distribution of positive values is required.

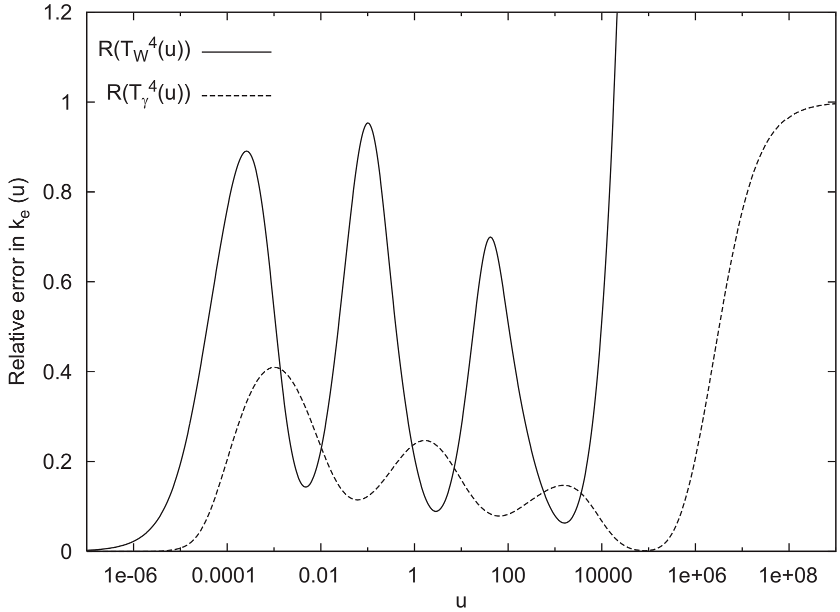


**Fig. 5.** With a coarse partition of only 4 parts, the weak-line limit typically used in correlated-$k$ methods is (on average) a factor of two larger than $T_\gamma^4(u)$.

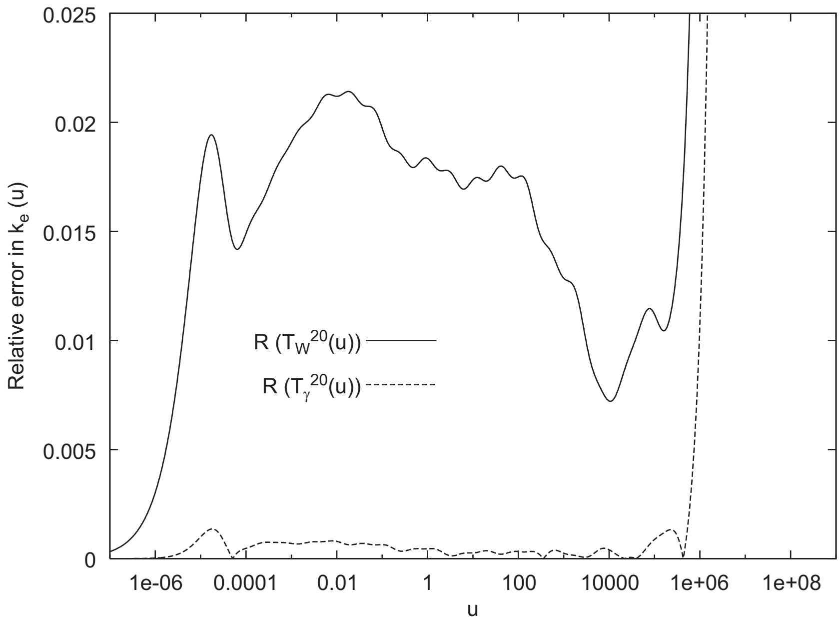


**Fig. 6.** With a refined partition of 20 parts, the error associated with the weak-line limit is typically more than 10 times the error of $T_\gamma^{20}(u)$.

The extension $T_\gamma(u)$ of the weak-line approximation (Section 4) is applicable for a large range of $k$-distributions, in the sense that it can be constructed for a generic $k$-distribution, without having to worry about any constraints on the range of validity. For example, it is guaranteed that $V \geq 0$. While the error is not guaranteed to be small in general, the approximation will at least be a decreasing (from 1 to 0) function of the path length. Furthermore, the Taylor expansion near $u=0$ matches for the first two terms of the approximation.

In general there are a large class of possible models. $T_\gamma(u)$ was constructed to match the first two moments and thus be asymptotic (for small $u$) to order $O(u^2)$. Some alternatives are provided in Appendix A.

The ease with which this approximation can be constructed, its robustness, its easy algebraic representation,

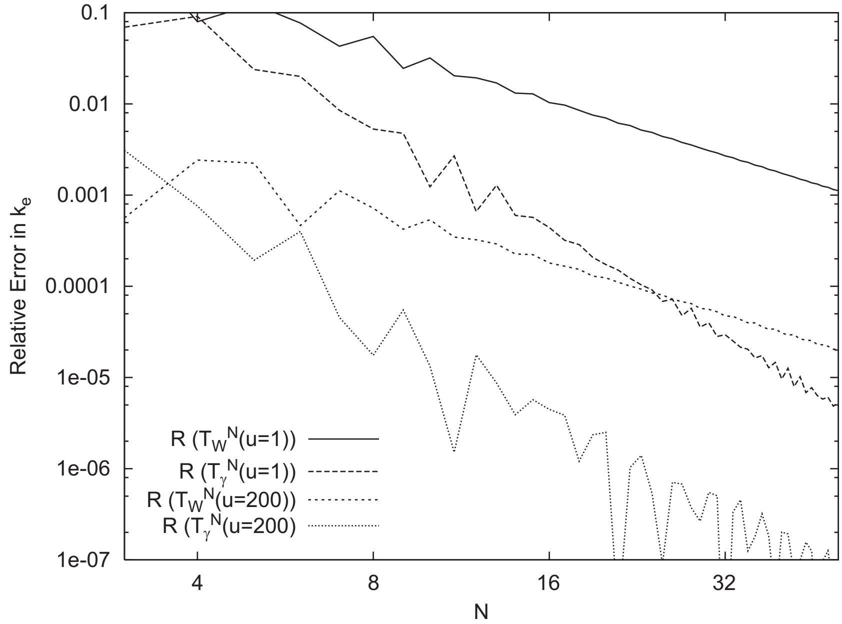


**Fig. 7.** The order of convergence is higher for the extended approximation, $T_\gamma$ than for the weak-line approximation typically used in correlated-$k$. This increased order is shown at both $u$=1 and $u$=200.

and its higher order convergence indicate that it should be tested in a correlated-$k$ method for a realistic atmospheric profile and compared with results from existing correlated-$k$ codes.

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## Appendix A. Other extensions

We list here some other approximations that could be valuable. These methods also require the $k$-distribution to be known, a priori. But additional constraints on the $k$-distribution are required, beyond those necessary for the construction of $T_\gamma(u)$.

### *A.1. Truncated exponential*

Choosing an exponential model for the $k$-distribution,

$$f_a(k) = \frac{1}{\alpha}\exp(-(k-\kappa)\alpha)\Theta(k-\kappa) \tag{A.1}$$

$$\kappa = \langle k \rangle (1-V) \tag{A.2}$$

$$\alpha = \langle k \rangle V \tag{A.3}$$

where $\Theta(x)$ is the unit step function, yields an approximation that also matches the first two moments $\langle k \rangle$ and $\langle k^2 \rangle$ as follows:

$$T_a(u) = \frac{\exp(-\kappa u)}{1+\alpha u} \tag{A.4}$$

This approximation has the advantage that it is easy to compute the transmission through a sequence of two materials. If the pencil of radiation has path $u_1$ through material with $\kappa_1$ and $\alpha_1$, followed by path $u_2$ through material with $\kappa_2$ and $\alpha_2$, it is easily derived that for correlated extinctions,

$$T(u) = \frac{\exp(-\kappa u)}{1+\alpha u} \tag{A.5}$$

$$u = u_1 + u_2 \tag{A.6}$$

$$\kappa = \frac{\kappa_1 u_1 + \kappa_2 u_2}{u} \tag{A.7}$$

$$\alpha = \frac{\alpha_1 u_1 + \alpha_2 u_2}{u} \tag{A.8}$$

In this approximation, $\kappa$ can become negative when $\langle k^2 \rangle > 2\langle k \rangle^2$ as can be seen from Eq. (A.2). Under these conditions the exponential is no longer decreasing. So band boundaries or partition boundaries would have to be chosen so that the coefficient of variation meets the criterion $\langle k^2 \rangle < 2\langle k \rangle^2$ for this approximation to be useful.

### *A.2. Padé forms*

Padé approximations [10] are often more accurate for a larger range of path length than the corresponding Taylor approximation. The following Padé approximations (with an additional exponential factor) are constructed to have an effective extinction that is asymptotic to $\underline{k}$ for large $u$, and to have an effective extinction asymptotic to $\langle k \rangle$ for small $u$.

$$P_{0,1} = \exp(-\frac{\underline{k}u)}{1+s} \tag{A.9}$$

$$P_{1,2} = (1+s)\exp(-\frac{\underline{k}u)}{1+2s+rs^2} \tag{A.10}$$

$$s = (\langle k \rangle - \underline{k})u \tag{A.11}$$

$$r = \frac{1}{2}\left(4 - \langle (k - \frac{\underline{k})^2 \rangle}{(\langle k \rangle - \underline{k})^2}\right) \tag{A.12}$$

Both of these approximations are quite useful when $\underline{k} \sim \langle k \rangle$, but as the coefficient of variation becomes large these will have regions where $T'(u) > 0$.

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