

A NEW WAY OF OBTAINING ANALYTIC APPROXIMATIONS OF CHANDRASEKHAR'S H FUNCTION

by

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Applying the mean value theorem for definite integrals in the non-linear integral equation for Chandrasekhar's H function describing conservative isotropic scattering, we have derived a new, simple analytic approximation for it, with a maximal relative error below 2.5%. With this new function as a starting-point, after a single iteration in the corresponding integral equation, we have obtained a new, highly accurate analytic approximation for the H function. As its maximal relative error is below 0.07%, it significantly surpasses the accuracy of other analytic approximations.

Key words: H function, analytic approximation, isotropic scattering, monoenergetic transport

INTRODUCTION

H functions were first introduced by Ambartsumian [1] and later developed extensively by Chandrasekhar whose results were collected and presented in detail in his classical monograph [2]. These functions play a major role in the theory of radiative transfer in planetary and stellar atmospheres. Also, they have a key role in a number of problems in single speed, one-dimensional neutron transport theory with isotropic scattering as described in the monograph by Case and Zweifel [3]. Relatively recently, we have applied them to an entirely different field, in a detailed description of X-ray transfer relevant to medical diagnostics [4-5]. In all the mentioned applications, their accurate numerical values are needed.

First tabulations of H functions were made by Chandrasekhar and Breen [6] and later supplemented by similar calculations by Harris [7]. Valuable, though, these tabulations have been, there was still a

need for more detailed numerical data about H functions, especially for parameters close to unity, absent from these calculations. In the paper by Hiroi [8], the values of the H function for a much larger number of single particle albedo parameters and with a much higher accuracy were provided.

However, the various applications of these functions require values for any value of the single scatter albedo. Such requirements can be met by reliable and accurate analytic approximations for quick calculations. Useful approximations of the H function based on the Gauss-Legendre quadrature can be found in Chandrasekhar's book. More recent results for the approximate H function came out as a by-product from a variational treatment of the half-space problem by Pomraning [9]. Simović and Vukanić [10] have derived three approximate analytic expressions for the H function by using the ordinary and flux decomposition DPN method. The accuracy of the obtained approximations of the H function is examined in some detail and compared with analogous approximate results of Chandrasekhar, determined from table IX of ref. [2], as well as with Pomraning's approximations. Simović and Vukanić have found that their formulas are more accurate than Chandrasekhar's results for the same order of approximation. Their formulas are of similar accuracy as Pomraning's expressions, but simpler and more tractable. By using the approximative H function obtained from the flux decomposition DPO technique, the same authors treated analytically low-energy light ion reflection from solids [10-11]. This approach appears convenient for solving this energy-dependent

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albedo problem. Simović and Marković [12] have presented a novel approximative analytic solution for the H function obtained by the decomposition of the angular flux density of particles combined with the second modified DPN method.

Two approximations of Chandrasekhar's H function for isotropic scattering, one of which is very simple in form, the other extremely accurate, are presented in this work. Before describing them in detail in the next section, we shall first re-derive Chandrasekhar's integral equation in a simple and transparent way. In our opinion, this derivation is of some interest per se, although such derivations, in various forms, already exist in literature [2, 13, 14]. It is far from easy to follow the derivation of this formula, especially in pioneering works such as those by Kouganoff [14] or Chandrasekhar [2] and difficult to see clearly the origin of corresponding terms.

GENERAL CONSIDERATIONS

The H function describes the intensity of radiation scattered by a semi-infinite medium of independent scatterers. More precisely, when isotropic scattering is concerned, the angular distribution of particles backscattered from half space is given by an exact solution [2]

$$R(\mu_0, \mu) = \frac{\omega}{2} \frac{\mu}{\mu_0} H(\mu_0, \omega) H(\mu, \omega) \quad (1)$$

Here, μ_0 and μ are the directional cosines of the incident and reflected particles with respect to the target surface normal and $R(\mu_0, \mu)d\mu$ gives the probability for a projectile to be reflected with directional cosines between μ and $\mu + d\mu$, irrespective of the azimuthal angle. The scattering medium is characterized solely through the parameter ω which represents the single scatter albedo. This parameter is given by

$$\omega = \frac{\sigma_R}{\sigma_R + \sigma_a} \quad (2)$$

where σ_R and σ_a are the total cross-sections for scattering and absorption, respectively. Furthermore, $H(\mu, \omega)$ is the H function, which depends on the variable μ and parameter ω [2].

Applying the first principle, we shall now derive the integral equation which describes the reflection of particles from half space assuming isotropic scattering and no energy loss. First, we extract a differentially thin layer Δz just below the target surface. The layer is so thin that a projectile may undergo at most one collision within it. Then we have the following five events, shown in fig. 1, which contribute to the angular distribution of reflected particles $R(\mu_0, \mu)$, whose probabilities are linear functions in Δz . All other cases are $O(\Delta z^2)$

Let us characterize physically these five cases (a) – (e).

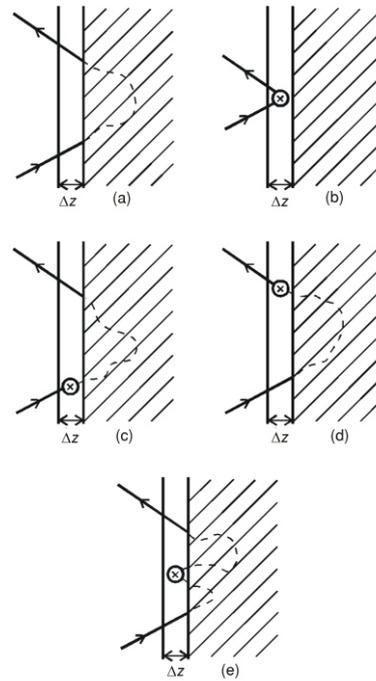


Figure 1. Possible events in the thin layer during the reflection of the projectile whose probabilities are linear functions of Δz . Crosses denote the scattering in the layer itself, while the broken line represents backscattering in the infinite medium

(a) A projectile passes the thin layer without scattering, is then reflected from the remaining half space and arrives back to the target surface, again without scattering in the thin layer.

(b) A backscattering event happens solely in the thin layer.

(c) The projectile is scattered inward in the thin layer and then reflected from the half space, with no scattering when leaving the thin layer.

(d) Entering, a projectile passes Δz without scattering, is then reflected from the half space and, finally, undergoes scattering in the thin layer, just before leaving the target surface.

(e) Entering, a projectile passes Δz without scattering, is then reflected from the half space and undergoes scattering in the thin layer, but this time inward, is again reflected and leaves the target without further scattering.

Writing the probabilities for elementary events from which these cases are composed and multiplying them, in the same order in which these elementary events occur, as depicted in fig. 1, we obtain the probabilities for our five cases, as follows:

$$(a) \quad 1 - \frac{\Delta z}{\mu_0} n\sigma_T \quad R(\mu_0, \mu) \quad 1 - \frac{\Delta z}{\mu} n\sigma_T$$

$$R(\mu_0, \mu) \quad \Delta z n\sigma_T \quad \frac{1}{\mu_0} \quad \frac{1}{\mu} \quad R(\mu_0, \mu)$$

where $\sigma_T \sigma_R \sigma_a$

$$(b) \quad \frac{\Delta z \sigma_R}{\mu_0 4\pi} 2\pi n \frac{\Delta z}{\mu_0} n \frac{\sigma_R}{2}$$

Factor 4 in denominator stems from the assumption that the scattering is isotropic, while factor 2 is the result of integration over the azimuthal angle.

$$(c) \quad \frac{\Delta z}{\mu_0} n \frac{\sigma_R}{2} R(\mu, \mu) d\mu$$

The integration extends over all inward directions μ .

$$(d) \quad R(\mu_0, \mu) \frac{\Delta z}{\mu} n \frac{\sigma_R}{2} d\mu$$

The integration extends over all outward directions μ .

$$(e) \quad R(\mu_0, \mu) \frac{\Delta z}{\mu} d\mu n \frac{\sigma_R}{2} R(\mu, \mu) d\mu$$

The angular distribution of reflected projectiles may be expressed, up to the terms linear in Δz , as the sum of these five probabilities. In such an expression, the term $R(\mu_0, \mu)$ appears on both sides of the equality and may be cancelled. By canceling the common linear factor $\Delta z n$ further, in respect to all remaining terms, and by neglecting the higher order terms, after simple rearrangements and factorization of the corresponding sum, we can form the following integral equation for $R(\mu_0, \mu)$

$$R(\mu_0, \mu) \frac{1}{2} \omega \frac{\mu}{\mu_0} [1 + R(\mu, \mu) d\mu] \times \frac{1}{\mu_0} \frac{R(\mu_0, \mu)}{\mu} d\mu \quad (3)$$

Writing $R(\mu_0, \mu)$ in the form given in eq. (1), one obtains the following integral equation for $H(\mu, \omega)$

$$H(\mu, \omega) = 1 - \frac{\omega}{2} \mu \int_0^1 \frac{H(\mu, \omega)}{\mu} d\mu \quad (4)$$

which is the starting point for all studies of the H function.

NEW ANALYTIC APPROXIMATIONS OF THE H FUNCTION

The integral eq. (4) which satisfies the H function can be written in the form of

$$\frac{1}{H(\mu, \omega)} = 1 - \frac{\omega}{2} \mu \int_0^1 \frac{H(\mu, \omega)}{\mu} d\mu \quad (5)$$

Applying the mean value theorem for definite integrals to this equation, instead of the function $1/(\mu + \mu')$ under the integral, we can write $1/[\xi(\omega, \mu) \mu]$ in front of it, so that we have

$$\frac{1}{H(\mu, \omega)} = 1 - \frac{\omega}{2} \mu \int_0^1 \frac{1}{\xi(\omega, \mu) \mu} H(\mu, \omega) d\mu \quad (6)$$

The new integral in this equation represents the zero order moment h_0 of Chandrasekhar's H function for which Chandrasekhar [2] found the exact value to be

$$h_0(\omega) = \int_0^1 H(\mu, \omega) d\mu = \frac{2}{\omega} (1 - \sqrt{1 - \omega}) \quad (7)$$

Now, inserting this expression in eq. (6), we can represent $H(\mu, \omega)$ in the form of

$$H(\mu, \omega) = \frac{\xi(\omega, \mu) \mu}{\xi(\omega, \mu) \sqrt{1 - \omega} \mu} \quad (8)$$

The simplicity of eq. (8) is somewhat deceiving, because the mean value theorem for the integrals is not constructive; it only guarantees the existence of $\xi(\omega, \mu)$, but does not provide the means to evaluate it.

However, this representation has some straightforward advantages. For example, if one takes the simplest approximation for ξ , namely $\xi = 1/2$, which means fixing μ' in the denominator of the integrand in eq. (5) to the middle value of the interval of integration over μ' , one obtains

$$H(\mu, \omega) = \frac{1}{1 - 2\sqrt{1 - \omega}} \frac{2\mu}{\omega \mu} \quad (9)$$

This expression is a well known approximation of Hapke [15] which gives a good approximation for multiple scattering phenomena, with the exception of the case when ω is close to unity.

The unknown function $\xi(\omega, \mu)$ can be found only approximately. Another advantage of our approach is that one can find an analytic approximation for ξ without the iteration procedure. Taking into account the behavior of the H function as a function of ω , we have, by trial and error, found that a highly suitable approximation is of the form

$$\xi(\omega, \mu) = a(\omega) + b\mu \frac{a_0}{1 - a_1 \sqrt{1 - \omega}} + b\mu \quad (10)$$

where the unknown constants a_0 , a_1 , and b will be determined by matching the zero order moment of the H function as accurately as possible. Inserting this expression in eq. (8), we obtain the approximate expression for the H function in the form of

$$H_{\text{app}}^1(\mu, \omega) = \frac{a(\omega) + (b - 1)\mu}{a(\omega) + (b - \sqrt{1 - \omega})\mu} \quad (11)$$

With this function, the expression for the zero order moment is given by

$$h_{0,app}(\omega) = \int_0^1 H_{app}^1(\mu, \omega) d\mu = \frac{b}{a(\omega)} \frac{1}{\sqrt{1-\omega}} \ln \left[\frac{a(\omega)(1-\sqrt{1-\omega})}{(b-\sqrt{1-\omega})^2} \right] \quad (12)$$

Making a dense, three-dimensional grid for parameters a_0 , b , and a_1 we have found that their best values are $a = 0.431$, $b = 0.105$, and $a_1 = 0.316$. In this case, the values of the zero order moment obtained from eq. (12) have the accuracy of 0.1% for the whole range of ω . With this approximation, the relative error of the H function is within 2.5%. In this manner, we have managed to obtain an analytical approximation of the H function, very simple in form and with a fairly high accuracy.

At the cost of the simplicity of the structure, the accuracy of the approximation can be enormously improved if we insert solution (12) into the integral eq. (6) and make a first order analytic iteration. This procedure gives the improved approximate formula

$$H_{app}(\mu, \omega) = \frac{1}{2} \frac{\omega}{\mu} \frac{1}{a(\omega) (b - \sqrt{1-\omega}) \mu} \ln \left[\frac{a(\omega) (1 - \sqrt{1-\omega})}{b - \sqrt{1-\omega}} \right] + [a(\omega) (b - 1)\mu] \ln \left[\frac{1}{\mu} \right] \quad (13)$$

The estimation of its accuracy is given in the next section.

DISCUSSION

We have compared our newly obtained results with the best known previously published results. Hapke [15] approximated the H function as an analytical form

$$H(\mu, \omega) = \frac{1}{1 - 2\sqrt{1-\omega}\mu} \quad (14)$$

A while later, Hapke [16] proposed an even better approximation

$$H(\mu, \omega) = \frac{1}{1 - (1 - \sqrt{1-\omega}) r_0} \frac{r_0}{2} r_0 \mu \ln \frac{1}{\mu} + r_0 \frac{2}{1 - \sqrt{1-\omega}} \quad (15)$$

The errors of our approximate functions were found to be, in comparison to Hiroi's [8] numerical re-

sults which have an accuracy of at least five decimal points, even more accurate than Chandrasekhar's and our own, highly accurate (up to ten decimal points) numerical results, not published yet. The comparison of the accuracy of our analytical approximations with the accuracy of the analytical approximations quoted by Hiroi, shows that our respective approximations are more accurate than all others. Figure 2 shows the relative error δH

$$\delta H = \frac{H(\mu, \omega) - H_{app}^1(\mu, \omega)}{H(\mu, \omega)} \quad (16)$$

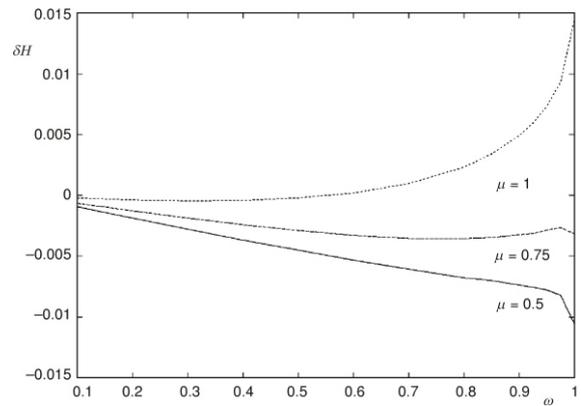


Figure 2. The relative error δH of the H function, calculated from our first approximate formula (11), shown as a function of the parameter ω for the three characteristic values of the variable μ

where for $H(\mu, \omega)$, numerical values from the tables are used, while $H_{app}^1(\mu, \omega)$ is calculated from our approximate formula (11). The relative error is given as a function of single scatter albedo ω , for the three chosen μ values $\mu = 0.5, 0.75$, and 1 . The relative error is within 2.5% for all μ values, as shown in fig. 2. In this way, we have obtained the analytical approximation of a very simple form which has a fairly high accuracy. Figure 3 shows the relative error of our improved approximate formula (13) as a function of the single scatter albedo ω , for the three values of the directional cosine $\mu = 0.5, 0.75$, and 1 . The relative error is within 0.07% and decreases as μ increases. Figures 4 and 5 show the relative error of Hapke's approximations (14) and (15). The first approximation is within a 4.1% margin. Hapke's improved approximation gives results within a relative error of 0.8%.

CONCLUSION

It is evident that our first approximation is more accurate than the first approximation of Hapke. Our improved approximation also shows better agreement with the exact H function than that of Hapke's im-

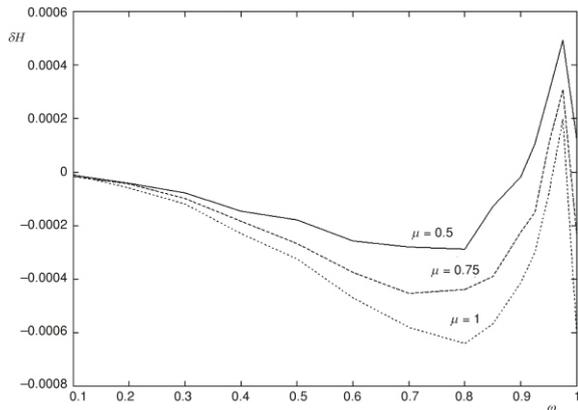


Figure 3. The relative error δH of the H function, calculated from our improved approximative formula (13), shown as a function of the parameter ω for the three characteristic values of the variable μ

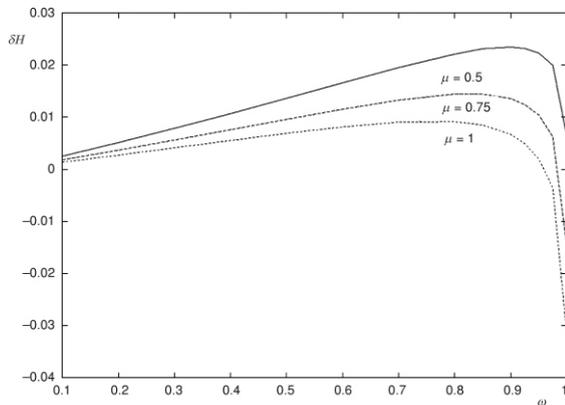


Figure 4. The relative error δH of the H function, calculated from Hapke's first approximative formula (14), shown as a function of the parameter ω for the three characteristic values of the variable μ

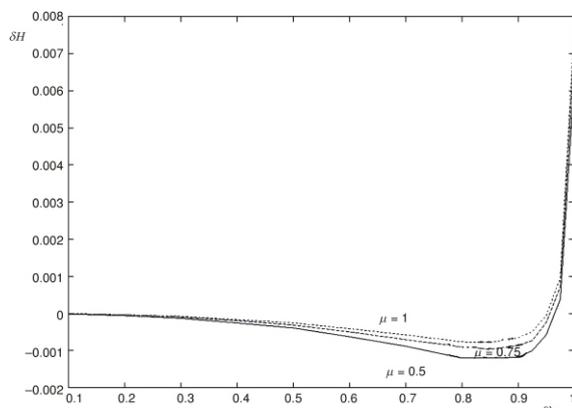


Figure 5. The relative error δH of the H function, calculated from Hapke's improved approximative formula (15), shown as a function of the parameter ω for the three characteristic values of the variable μ

proved formula. Note that we have chosen parameters a_0 , b , and a_1 so as to minimize the supremum of relative errors and not their mean value. However, in spite of the achieved high accuracy, it seems that, for close to unity, further improvement of analytical approximation is called for.

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REFERENCES

- [1] Ambarzumian, V. A., Uber Die Beziehung Zwischen Der Loesung des Strahlungs-Gleichgewicht, *Z. Phys A.*, 52 (1929), 3-4, pp. 263-267
- [2] Chandrasekhar, S., Radiative Transfer, Oxford University Press, London, 1950
- [3] Case, K. M., Zweifel, P. F., Linear Transport Theory, Addison-Wesley, Reading, MA, 1967
- [4] Davidović, D. M., Vukanić, J., Arsenović, D., Simplified Model of Low Energy X-Ray Backscattering, *Phys. Med. Biol.*, 48 (2003), pp. N213-N221
- [5] Davidović, D. M., Vukanić, J., Arsenović, D., Influence of Anisotropy of Compton Scattering on Low Energy X-Ray Backscattering, *Journal of Phys. D: Appl. Phys.*, 37 (2004), pp. 2314-2317
- [6] Chandrasekhar, S., Breen, F. H., On the Radiative Equilibrium of a Stellar Atmosphere XIX, *Astrophys. J.*, 106 (1947), pp. 143-144
- [7] Harris, D. J., Diffuse Reflection from Planetary Atmospheres, *Astrophys. J.*, 126 (1957), pp. 408-412
- [8] Hiroi, T., Recalculation of Isotopic H Functions, *ICARUS*, 109 (1994), pp. 313-317
- [9] Pomraning, G. C., A Variational Treatment of the Asymptotic Flux Behavior in a Half Space, *Transport Th. Statist. Phys.*, 19 (1990), 6, pp. 515-525
- [10] Simović, R., Vukanić, J., Analytic Approximations of the H-Function Based on Different DPN Procedures, *J. Quant. Spectrosc. Radiat. Transfer*, 61 (1998), 1, pp. 59-71
- [11] Vukanić, J., Simović, R., Analytical Solutions of the Boltzmann Transport Equation for Light Ion Reflection, *Fusion Technol.*, 30 (1996), 3, pp. 372-382
- [12] Simović, R., Marković, S., A Note on the Analytic Approximations of the H-Function, *Nuclear Technology & Radiation Protection*, 19 (2004), 2, pp. 47-51
- [13] Mingle, J. O., Applications of the Invariant Imbedding Method to Monoenergetic Neutron Transport Theory in Slab Geometry, *Nuclear Science and Engineering*, 28 (1967) pp. 177-189
- [14] Kourganoff, V., Basic Methods in Transfer Problems, Clarendon Press, Oxford, UK, 1952
- [15] Hapke, B., Bidirectional Reflectance Spectroscopy 1. Theory, *J. Geophys. Res.*, 86 (1981), B4, pp. 3039-3054
- [16] Hapke, B., In Theory of Reflectance and Emittance Spectroscopy, Cambridge University Press, Cambridge, UK, 1993

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**ЈЕДАН НОВ НАЧИН ЗА ДОБИЈАЊЕ АНАЛИТИЧКИХ
АПРОКСИМАЦИЈА ЧАНДРАСЕКАРОВЕ X_a -ФУНКЦИЈЕ**

Примењујући у нелинеарној интегралној једначини за Чандрасекарову X_a -функцију, која описује конзервативно изотропно расејање, теорему о средњој вредности одређених интеграла, извели смо нову једноставну аналитичку апроксимацију за X_a -функцију, чија је максимална релативна грешка испод 2.5%. Полазећи од ове нове функције као почетне апроксимације у одговарајућој интегралној једначини, после само једне итерације, која може да се изврши аналитички, добили смо нову врло тачну аналитичку апроксимацију за X_a -функцију. Максимална релативна грешка наше друге апроксимације је испод 0.07%, тако да ова апроксимација далеко превазилази тачност других аналитичких апроксимација познатих у литератури.

Кључне речи: X_a -функција, аналитичка апроксимација, изотропно расејање, моноенергетски трансјори
