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Solution to the linear BGK equation via the principles of invariance

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Dedicated to the memory of S Chandrasekhar

Abstract. The solution to the linearized BGK equation of kinetic theory is obtained via the principles of invariance as formulated by Chandrasekhar. The solution represents an alternative to the singular eigenfunction method featuring regular integral equations which are more easily evaluated. Laplace transforms are obtained for the net flow velocity and velocity distribution for both the albedo and Milne problems with wall reflection. The transforms are then numerically inverted to a high degree of accuracy. Results are compared to those of Kainz and Titulaer.

1. Introduction

In the 1960s, Case and Zweifel [1] popularized the method of singular eigenfunctions, first developed by van Kampen [2], to the linear Boltzmann equation describing neutron transport in a medium. The method is very appealing owing to its similarity to the separation-of-variable approach, widely used for PDEs, and to its mathematical elegance. Because of this appeal, the method was applied to the linearized BGK equation of kinetic theory [3] characterizing the propagation of a disturbance into a gas bounded on one side resulting in analytical solutions. Recently, the method was revisited in a rather extensive analysis [4] in which exceptionally accurate results for selected quantities were found for the albedo and Milne problems of kinetic theory with and without partially reflecting boundaries. One major advantage of the singular eigenfunction method, shown for the range of problems considered, is that these problems can be cast into the same expansion formalism with the unknown coefficients determined from specific boundary conditions. By the same token, the method also has a major numerical drawback since the expansion coefficients for the (continuum) spectrum of the operator must be determined from singular integral equations which can be solved analytically for a non-reflecting boundary but cannot be for a reflecting boundary. Therefore, the singular eigenfunction method relies heavily on the solution to singular integral equations and the associated numerical evaluation of principal value integrals. While the analysis in [4] is flawless in its numerical presentation, considerable experience in dealing with principal-value integration is required. For this reason and for theoretical and numerical simplicity, a solution by application of principles of invariance combined with a numerical Laplace transform inversion is presented here as an alternative approach.

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While not as mathematically elegant as the singular eigenfunction method, the solution using the principles of invariance, first exploited by Chandrasekhar [5] in solving the equation of radiative transfer, has not enjoyed the popularity of the singular eigenfunction method. This is rather curious given the ease with which numerical solutions can be generated to a high degree of accuracy, as will be shown. For the reader who may not be familiar with the origin of the term 'principles of invariance', the phrase refers to the invariance of the emergent distribution from a half-space to the addition of material to the medium leading to a method of solution of the transport equation. This method of solution has several distinct advantages over the singular eigenfunction method. In particular, singular integral equations can be avoided. A nonlinear integral equation is encountered, however. Fortunately, with an appropriate quadrature, it can be efficiently evaluated through iteration. Also the solution for the spectrum of problems considered in [4] can be shown to be special cases of the albedo problem for a general source. In addition to theoretical simplicity, the expressions obtained by the principles of invariance lead to a straightforward and highly accurate numerical evaluation for a modest computational effort.

The theory of the principles of invariance approach is presented in section 2. We begin with the fundamental albedo problem solution at the free surface. The expression derived for the exiting velocity distribution at the wall is shown to serve as the image function for the Laplace transform inversion for the interior net flow velocity and the interior velocity distribution function. Next, the albedo problem for a reflecting boundary is solved in terms of the solution for the albedo problem. The section concludes with the solution of the Milne problem for a reflecting boundary in terms of the corresponding albedo solution. In all cases, the interior distributions are expressed as Laplace transform inversions which, as will be shown, can be most efficiently evaluated. In the final section, the numerical implementation and a demonstration is presented. The majority of the results found in [4] and more are presented.

2. Theory

2.1. Albedo problem without reflection

The linearized BGK transport equation for a flowing gas of interacting molecules in a half-space can be written as [4]

$$\left[u\frac{\partial}{\partial x}+1\right]f(x,u)=\phi_0(u)\int_{-\infty}^{\infty}\mathrm{d}u'\,f(x,u') \tag{1a}$$

where $f(x,u)$ is the perturbation of the molecular velocity distribution from an equilibrium Maxwellian distribution

$$\phi_0(u)=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-u^2/2}$$

at position x measured in mean free paths and velocity u measured in units of the thermal velocity. The fundamental albedo problem is defined for a source of the perturbation at the free boundary $(x=0)$ of the form

$$f(0,u)=g(u)\qquad u>0\,. \tag{1b}$$

Additional problems will be defined for a variety of boundary conditions with the requirement

$$\lim_{x\to\infty}f(x,u)<\infty\,. \tag{1c}$$

A more convenient form for (1) is obtained with the substitution

$$f(x,u) = \phi_0(u)h(x,u) \tag{2}$$

to give

$$\left[u\frac{\partial}{\partial x} + 1\right]h(x,u) = \int_{-\infty}^{\infty} \mathrm{d}u'\, \phi_0(u')h(x,u') \tag{3a}$$

$$h(0,u) = g(u)/\phi_0(u) \qquad u > 0 \tag{3b}$$

$$\lim_{x\to\infty} h(x,u) < \infty\,. \tag{3c}$$

The solution to (3) will now be found for several specific $g(u)$.

2.1.1. Standard albedo problem. The solution procedure begins by temporarily specifying $g(u)$ to be

$$g(u) = \phi_0(u_0)\delta(u-u_0) \qquad u_0 > 0$$

and reformulating (3) into an integral form by following the disturbance along its trajectory. Thus, from integral transport theory for $u > 0$

$$h(x,u;u_0) = \delta(u-u_0)\mathrm{e}^{-x/u_0} + \frac{1}{u}\int_0^x \mathrm{d}x'\, \mathrm{e}^{-(x-x')/u} q(x';u_0) \tag{4a}$$

and for $u < 0$

$$h(x,u;u_0) = -\frac{1}{u}\int_x^{\infty} \mathrm{d}x'\, \mathrm{e}^{-(x'-x)/u} q(x';u_0) \tag{4b}$$

where the net flow velocity in the direction of flow for this case is defined as

$$q(x;u_0) \equiv \int_{-\infty}^{\infty} \mathrm{d}u'\, \phi_0(u')h(x,u';u_0)\,. \tag{5}$$

The explicit dependence on u_0 is indicated since h now represents a Green function in the velocity variable. Special note is made of the expression for the exiting perturbation at the wall (to be used later)

$$h(0,-u;u_0) = \frac{1}{u}\int_0^{\infty} \mathrm{d}x'\, \mathrm{e}^{-x'/u} q(x';u_0) \qquad u > 0\,. \tag{6}$$

Explicit solution for h at the wall ($x = 0$). An expression for the exiting perturbation is obtained in the following analysis as outlined by Busbridge [6] for the equation of radiative transfer and adapted here for kinetic theory.

(i) *Integral equation for $q(x;u_0)$.* By forming an equation for $q(x;u_0)$, we obtain

$$(1 - L_x)q(x';u_0) = \phi_0(u_0)\mathrm{e}^{-x/u_0} \tag{7a}$$

where the operator L_x is defined by

$$L_x \equiv \int_0^{\infty} \mathrm{d}x'\, k(|x-x'|)(\cdot) \tag{7b}$$

with

$$k(x) \equiv \int_0^{\infty} \mathrm{d}u\, \phi_0(u)\frac{\mathrm{e}^{-x/u}}{u}\,. \tag{7c}$$

(ii) *Differentiation with respect to* x. By differentiation of (7*a*) with respect to x, there results

$$(1 - L_x)\frac{\partial q(x'; u_0)}{\partial x'} = -\phi_0(u_0)\frac{\mathrm{e}^{-x/u_0}}{u_0} + k(x)q(0; u_0) \tag{8}$$

which is obtained by a change of variable and interchanging the differentiation and integral operators.

(iii) *Alternative expression for* $k(x)$. From a division of (7*a*) by $u_0(u_0 > 0)$, integration over u_0, and noting the form of $k(x)$ in (7*c*), we conveniently find

$$k(x) = (1 - L_x)\int_0^\infty \frac{\mathrm{d}u'}{u'} q(x'; u')\,. \tag{9}$$

(iv) Integro-differential equation for $q(x; u_0)$. With the substitution of (9) and (7*a*) for $\phi_0(u_0)\mathrm{e}^{-x/u_0}$, equation (8) becomes

$$(1 - L_x)\left\{\left[\frac{\partial}{\partial x'} + \frac{1}{u_0}\right]q(x'; u_0) - q(0; u_0)\int_0^\infty \frac{\mathrm{d}u'}{u'} q(x'; u')\right\} = 0\,.$$

From an analysis similar to that found in [6], one can show that the expression in the curly brackets is in the null space of the operator $1 - L_x$ for the anticipated function space of the solution; thus,

$$\left[\frac{\partial}{\partial x} + \frac{1}{u_0}\right]q(x; u_0) = q(0; u_0)\int_0^\infty \frac{\mathrm{d}u'}{u'} q(x; u')\,. \tag{10}$$

(v) *Integration over* x. Multiplying (10) by $\mathrm{e}^{-x/u}$, integrating over x on $[0, \infty)$ and making liberal use of (6) yields

$$h(0, -u; u_0) = \frac{u_0}{u + u_0} q(0; u_0)\left[1 + \int_0^\infty \mathrm{d}u' \,\frac{u}{u'} h(0, -u; u')\right]. \tag{11}$$

(vi) *Reciprocity*. Since the operator L_x is self-adjoint, shown by considering (7*a*) for u and u' separately, integrating over x on $[0, \infty)$ and subtracting, the following reciprocity relation holds:

$$u\phi_0(u)h(0, -u; u') = u'\phi_0(u')h(0, -u'; u)\,. \tag{12}$$

(vii) *Final expression for* $h(0, -u; u_0)$. When the reciprocity relation is introduced into (11), we obtain

$$h(0, -u; u_0) = \frac{u_0}{u + u_0} q(0; u_0)q(0; u)/\phi_0(u) \tag{13}$$

where the relation

$$q(0; u) = \phi_0(u) + \int_0^\infty \mathrm{d}u' \,\phi_0(u')h(0, -u'; u) \tag{14}$$

from (5) at $x = 0$ has been used.

When equation (13) is introduced into (14), there results

$$h(0, -u; u_0) = \phi_0(u_0)\frac{u_0}{u + u_0} H(u_0)H(u) \tag{15}$$

where H is given by the following nonlinear integral equation:

$$H(u) = 1 + uH(u)\int_0^\infty \mathrm{d}u' \,\phi_0(u')\frac{H(u')}{u + u'} \tag{16a}$$

with

$$q(0; u_0) \equiv \phi_0(u_0)H(u_0)\,. \tag{16b}$$

Interior solutions. If u is extended to the complex s plane by formally replacing u by $1/s$, equation (6) becomes

$$h(0, -1/s; u_0)/s = L[q(x'; u_0)] \tag{17a}$$

where L is the Laplace transform operator

$$L \equiv \int_0^\infty \mathrm{d}x'\, \mathrm{e}^{-sx'}(\cdot)\,. \tag{17b}$$

Thus, by inversion, the net flow velocity of the perturbation is given by (from (15))

$$q(x; u_0) = u_0\phi_0(u_0)H(u_0)L_x^{-1}\left\{\frac{H(1/s)}{1+su_0}\right\}. \tag{18}$$

There are several ways of performing the Laplace transform inversion. Once the singularities of $H(1/s)$ have been identified, the Bromwich contour of the inversion operator

$$L_x^{-1} \equiv \frac{1}{2\pi\mathrm{i}}\int_{\gamma-\mathrm{i}\infty}^{\gamma+\mathrm{i}\infty} \mathrm{d}s\, \mathrm{e}^{sx}(\cdot) \tag{19}$$

where γ is greater than the largest real part of any singularity, can be appropriately deformed around the singularities leading to an integral along the branch cut as in [6]. This approach will not be followed here since a numerical Laplace transform inversion algorithm has been previously developed by the author. Its implementation will be briefly discussed in section 3.

Similarly from a Laplace transform of (3), we obtain (using (15)), since the Laplace transform of $q(x; u_0)$ is

$$\bar{q}(s; u_0) = u_0\phi_0(u_0)H(u_0)\frac{H(1/s)}{1+su_0} \tag{20}$$

the following Laplace transforms of $h(x, u; u_0)$ for $u > 0$:

$$\bar{h}(s, u; u_0) = \frac{u_0}{1+su_0}\delta(u-u_0) + u_0\phi_0(u_0)H(u_0)\frac{H(1/s)}{(1+su)(1+su_0)} \tag{21a}$$

$$\bar{h}(s, -u; u_0) = u_0\phi_0(u_0)\frac{H(u_0)}{1-su}\left[\frac{H(1/s)}{(1+su_0)} - \frac{uH(u)}{u+u_0}\right] \tag{21b}$$

which also can be inverted numerically.

2.1.2. Solution for f. Since h is a Green function (in velocity u), one can immediately write for the original source (equation (3*b*))

$$h(x, u) = \int_0^\infty \mathrm{d}u'\, g(u')h(x, u; u')/\phi_0(u') \tag{22}$$

and therefore from (2) the desired velocity distribution is

$$f(x, u) = \phi_0(u)\int_0^\infty \mathrm{d}u'\, g(u')h(x, u; u')/\phi_0(u')\,. \tag{23}$$

Similarly for the net flow velocity

$$n(x) \equiv \int_{-\infty}^\infty \mathrm{d}u\, f(x, u) = \int_0^\infty \mathrm{d}u'\, g\,(u')q(x; u')/\phi_0(u')\,. \tag{24}$$

Thus, the transform of f is from (23) and (21) for $u > 0$

$$\bar{f}(s,u) = \frac{u}{1+su} g(u) + \phi_0(u) \int_0^\infty du'\, u' g(u') H(u') \frac{H(1/s)}{(1+su)(1+su')} \tag{25a}$$

$$\bar{f}(s,-u) = \phi_0(u) \int_0^\infty du'\, u' g(u') \frac{H(u')}{1-su} \left[\frac{H(1/s)}{(1+su')} - \frac{uH(u)}{u+u'} \right] \tag{25b}$$

with corresponding inversions

$$f(x,u) = g(u) e^{-x/u} + \phi_0(u) \int_0^\infty du'\, u' g(u') H(u') L_x^{-1} \left[\frac{H(1/s)}{(1+su)(1+su')} \right] \tag{26a}$$

$$f(x,-u) = \phi_0(u) \int_0^\infty du'\, u' g(u') H(u') L_x^{-1} \left\{ \frac{1}{1-su} \left[\frac{H(1/s)}{(1+su')} - \frac{uH(u)}{u+u'} \right] \right\}. \tag{26b}$$

From (24) and (18), the transform of net flow velocity is simply

$$\bar{n}(s) = \int_0^\infty du'\, u' g(u') H(u') \frac{H(1/s)}{1+su'} \tag{27}$$

implying

$$n(x) = \int_0^\infty du'\, u' g(u') H(u') L_x^{-1} \left[\frac{H(1/s)}{1+su'} \right]. \tag{28}$$

Since the transforms have been determined explicitly, the limiting values at $x = 0$ and ∞ can be obtained via the Tauberian theorem (assuming the necessary conditions are met)

$$Y(0) = \lim_{s\to\infty} [s\bar{Y}(s)] \qquad Y(\infty) = \lim_{s\to 0} [s\bar{Y}(s)]$$

which yields from (25) and (27)

$$f(0,-u) = \phi_0(u) H(u) \int_0^\infty du'\, u' g(u') \frac{H(u')}{u+u'} \tag{29a}$$

$$f(\infty,u) = \phi_0(u) \int_0^\infty du'\, u' g(u') H(u') \tag{29b}$$

and

$$n(0) = \int_0^\infty du'\, g(u') H(u') \tag{29c}$$

$$n(\infty) = \int_0^\infty du'\, u' g(u') H(u') \tag{29d}$$

where

$$H(1/s) = 1/s + O(1)$$

and from (16*a*)

$$H(0) = 1$$

have been used.

To compare to the results found in [4] let

$$g(u) = \delta(u - u_0)/u_0 \,. \tag{30}$$

Thus

$$n(0) = H(u_0)/u_0 \tag{31a}$$

$$n(\infty) = H(u_0) \,. \tag{31b}$$

This implies that $Q(u)$ in [4] is $H(u)$. Thus, H can actually be obtained analytically in terms of integrals as shown in [4]. A more convenient and less awkward evaluation can, however, be obtained from (16*a*). To complete this case (29*a*), (26) and (28) yield

$$f(0,-u) = \frac{\phi_0(u)}{u+u_0} H(u_0) H(u) \tag{32a}$$

$$f(x,u) = \delta(u-u_0)\frac{\mathrm{e}^{-x/u_0}}{u_0} + \phi_0(u) H(u_0) L_x^{-1}\left[\frac{H(1/s)}{(1+su)(1+su_0)}\right] \tag{32b}$$

$$f(x,-u) = \phi_0(u) H(u_0) L_x^{-1}\left\{\frac{1}{1-su}\left[\frac{H(1/s)}{(1+su_0)} - \frac{uH(u)}{u+u_0}\right]\right\} \tag{32c}$$

and

$$n(x) = H(u_0) L_x^{-1}\left[\frac{H(1/s)}{1+su_0}\right]. \tag{32d}$$

From the above analysis, it is apparent that the solution $h(0,-u;u_0)$ of the fundamental albedo problem serves as the basis for both the interior solutions $h(x,u;u_0)$ and $f(x,u)$. As will be shown in the following sections, $h(0,-u;u_0)$ will also provide the solution for the more general albedo problem with wall reflection as well as the Milne problem with reflection. Evidently, each solution builds upon the previous.

As the reader can readily see, the solution via the principle of invariance is based upon an H-function completely analogous to the one derived by Chandrasekhar [5]. From the analysis of [4], it is also apparent that the singular eigenfunction method is based on the H-function but involves singular integrals which have been avoided entirely in the formulation presented here, making the numerical evaluation more apparent. Also aiding in the evaluation is the numerical Laplace transform inversion which gives an efficient evaluation for a modest effort.

2.2. *Albedo problem with reflection*

In this section, the albedo problem with partial specular reflection,

$$\left[u\frac{\partial}{\partial x}+1\right] f(x,u) = \phi_0(u)\int_{-\infty}^{\infty} \mathrm{d}u'\, f(x,u') \tag{33a}$$

$$f(0,u) = g(u) + r(u) f(0,-u) \qquad u>0 \tag{33b}$$

$$\lim_{x\to\infty} f(x,u) < \infty \tag{33c}$$

is considered with

$$0 \leqslant r(u) < 1\,.$$

2.2.1. *Standard albedo problem.*

Let

$$g(u) = \delta(u-u_0)\,.$$

Thus, corresponding to section 2.1.1

$$\left[u\frac{\partial}{\partial x}+1\right] f(x,u;u_0) = \phi_0(u)\int_{-\infty}^{\infty} \mathrm{d}u'\, f(x,u';u_0) \tag{34a}$$

$$f(0,u;u_0) = \delta(u-u_0) + r(u) f(0,-u;u_0) \qquad u>0 \tag{34b}$$

$$\lim_{x\to\infty} f(x,u;u_0) < \infty \tag{34c}$$

is the standard albedo problem where as before explicit dependence on u_0 is indicated. From equation (23), the solution at $x = 0$ for the source specified as

$$g(u) = \delta(u - u_0) + r(u) f(0, -u; u_0) \tag{35}$$

can immediately be written as

$$f(0, -u; u_0) = \phi_0(u)\left[\frac{h(0, -u; u_0)}{\phi_0(u_0)} + \int_0^\infty du'\, \frac{r(u')}{\phi_0(u')} h(0, -u; u') f(0, -u'; u_0)\right] \tag{36}$$

or substituting (15) gives

$$f(0, -u; u_0) = \phi_0(u)\left[\frac{u_0}{u + u_0} H(u_0) H(u) + H(u)\int_0^\infty du'\, r(u') \frac{u'}{u + u'} H(u') f(0, -u'; u_0)\right]. \tag{37}$$

Following the approach of Sobolev [7] for the equation of radiative transfer, the form

$$f(0, -u; u_0) = u_0 \phi_0(u) H(u) H(u_0)\left[\frac{A(u, u_0)}{u + u_0} + \frac{B(u, u_0)}{u - u_0}\right] \tag{38}$$

is suggested without loss of generality. When this expression is introduced into (37) there results after equating the coefficients of the terms $1/(u - u_0)$ and $1/(u + u_0)$

$$B(u, u_0) = \int_0^\infty du'\, K(u') A(u', u_0)\left[\frac{1}{u' + u_0} - \frac{1}{u + u'}\right] \tag{39a}$$

$$A(u, u_0) = 1 + \int_0^\infty du'\, K(u') B(u', u_0)\left[\frac{1}{u' - u_0} - \frac{1}{u + u'}\right] \tag{39b}$$

with

$$K(u) \equiv u r(u) [H(u)]^2 \phi_0(u)\,. \tag{39c}$$

As shown in [7], the specific dependence of A and B can be assumed to be separable of the form

$$A(u, u_0) = \alpha(u)\alpha(u_0) - \beta(u)\beta(u_0) \tag{40a}$$

$$B(u, u_0) = \alpha(u)\beta(u_0) - \alpha(u_0)\beta(u)\,. \tag{40b}$$

After some algebra, it can be shown that the following integral equations satisfy (39):

$$\alpha(u) = 1 + \int_0^\infty du'\, \frac{K(u')}{u + u'} \beta(u') \tag{41a}$$

$$\beta(u) = \int_0^\infty du'\, \frac{K(u')}{u + u'} \alpha(u')\,. \tag{41b}$$

Thus A and B have been specified and (38) provides the desired solution in a form never before presented.

The net flow velocity is obtained by noting, as in section 2.1.1 from integral transport theory,

$$f(0, -u; u_0) = \frac{\phi_0(u)}{u} \int_0^\infty dx'\, e^{-x'/u} n(x'; u_0) \tag{42}$$

which again is the Laplace transform of $n(x; u_0)$, and formally upon inversion gives

$$n(x; u_0) = u_0 H(u_0) L_x^{-1}\left\{H(1/s)\left[\frac{A(1/s, u_0)}{1 + s u_0} + \frac{B(1/s, u_0)}{1 - s u_0}\right]\right\} \tag{43a}$$

where

$$A(1/s, u_0) = \alpha(1/s)\alpha(u_0) - \beta(1/s)\beta(u_0) \tag{43b}$$

$$B(1/s, u_0) = \alpha(1/s)\beta(u_0) - \alpha(u_0)\beta(1/s) \tag{43c}$$

and

$$\alpha(1/s) = 1 + s\int_0^\infty \mathrm{d}u'\, \frac{K(u')}{1+su'}\beta(u') \tag{44a}$$

$$\beta(1/s) = s\int_0^\infty \mathrm{d}u'\, \frac{K(u')}{1+su'}\alpha(u')\,. \tag{44b}$$

These last two expressions are most easily evaluated once $\alpha(u)$ and $\beta(u)$ have been determined iteratively from (41). From equation (43), the asymptotic velocity in the free stream can be shown to be

$$n(\infty; u_0) = u_0\chi_+(u_0)H(u_0) \tag{45}$$

where

$$\chi_\pm(u) \equiv \alpha(u) \pm \beta(u)\,. \tag{46}$$

$\chi_\pm(u)$ satisfies the following integral equation:

$$\chi_\pm(u) = 1 \pm \int_0^\infty \mathrm{d}u'\, \frac{K(u')}{u+u'}\chi_\pm(u')\,. \tag{47}$$

2.3. *Milne problem with reflection*

The appropriate boundary conditions for the Milne problem with partial specular reflection are

$$f(0, u) = r(u)f(0, -u) \qquad u > 0 \tag{48a}$$

$$f(0, u) \to \phi_0(u)[A_0^r - (u - x)] \qquad \text{as} \quad x \to \infty\,. \tag{48b}$$

Equation (34*a*) is to be solved subject to these boundary conditions. A_0^r is an accommodation coefficient, or extrapolation distance, and is also to be determined in the process. To put the problem in terms of the albedo problem already solved, the following substitution is made:

$$\psi(x, u) = f(x, u) - [A_0^r - (u - x)]\phi_0(u) \tag{49}$$

which implies the following albedo problem is to be solved:

$$\left[u\frac{\partial}{\partial x} + 1\right]\psi(x, u) = \phi_0(u)\int_{-\infty}^\infty \mathrm{d}u'\, \psi(x, u') \tag{50a}$$

$$\psi(0, u) = \phi_0(u)[(1 + r(u))u - (1 - r(u))A_0^r] + r(u)\psi(0, -u) \tag{50b}$$

$$\lim_{x\to\infty} \psi(x, u) = 0\,. \tag{50c}$$

From equation (23), the distribution exiting at the wall for a general incoming distribution is

$$\psi(0, -u) = \phi_0(u)\left[H(u)\int_0^\infty \mathrm{d}u'\, g(u')\frac{u'}{u+u'}H(u') + H(u)\int_0^\infty \mathrm{d}u'\, g(u')\frac{u'r(u')}{u+u'}H(u')\psi(0, -u')\right] \tag{51a}$$

where

$$g(u) \equiv [(1 + r(u)) - (1 - r(u))A_0^r]\phi_0(u)\,. \tag{51b}$$

Reintroducing the assumed form (equation (49)) and analytically evaluating the integrals where possible yields (using several well known H-function relations)

$$f(0,-u) = \phi_0(u)\left[H(u) - H(u)\int_0^\infty \mathrm{d}u'\, \frac{u' r(u')}{u+u'} H(u') f(0,-u')\right]. \tag{52}$$

The solution to (52) is obtained by noting that (37) can be reformulated as

$$f(0,-u;u_0) = H(u_0) W(u,u_0) \tag{53a}$$

where

$$W(u,u_0) = \phi_0(u)\left[\frac{u_0}{u+u_0} H(u) + H(u)\int_0^\infty \mathrm{d}u'\, \frac{u' r(u')}{u+u'} H(u') W(u',u_0)\right]. \tag{53b}$$

Thus, on comparing (52) and (53*b*) and assuming uniqueness, we have

$$f(0,-u) = W(u,\infty)\,. \tag{54}$$

From equation (38), however,

$$W(u,u_0) = \phi_0(u) H(u)\left[\frac{A(u,u_0)}{u+u_0} + \frac{B(u,u_0)}{u-u_0}\right] \tag{55a}$$

which in the limit implies

$$f(0,-u) = \phi_0(u) H(u) \chi_+(u)\,. \tag{55b}$$

Equation (55*b*) is a rather surprisingly simple expression and is independent of A_0^r. As before, the net flow velocity is the Laplace transform inversion

$$n(x) = L_x^{-1}\{H(1/s)\chi_+(1/s)/s\} \tag{56}$$

and the transform of the velocity distribution for $u > 0$ is obtained from a transform of (34*a*) as

$$f(s,-u) = \frac{\phi_0(u)}{1-su}[H(1/s)\chi_+(1/s)/s - uH(u)\chi_+(u)] \tag{57a}$$

$$f(s,u) = \frac{\phi_0(u)}{s(1+su)} H(1/s)\chi_+(1/s)\,. \tag{57b}$$

The net flow velocity at the wall can be obtained from a Tauberian limit of (56) as

$$n(0) = \chi_+(1/s)\,. \tag{58}$$

A_0^r is determined by first expressing $\psi(0,-u)$ (from (49) and (55*b*)) as

$$\psi(0,-u) = \phi_0(u)[H(u)\chi_+(u) - (A_0^r + u)]\,.$$

Then, the transform of the net flow velocity is

$$\bar{q}(s) = \frac{1}{s}[H(1/s)\chi_+(1/s) - A_0^r - 1/s]\,.$$

But $q(\infty)$ vanishes requiring

$$\lim_{s\to 0} s\bar{q}(s) = 0 = \lim_{s\to 0}[H(1/s)\chi_+(1/s) - A_0^r - 1/s]\,. \tag{59}$$

From an asymptotic analysis of the H-function, it can be shown that

$$\chi_+(1/s) = 1 + s\chi_{+0} + \mathrm{O}(s^2)$$

where

$$\chi_{+0} \equiv \int_0^\infty \mathrm{d}u'\, K(u')\chi_+(u')\,.$$

Equation (59) becomes

$$A_0^r = \alpha_2 + \chi_{+0}\,. \tag{60}$$

The important non-reflective case ($r = 0$) can be shown to give (using H-function relations)

$$f(0, -u) = \phi_0(u)H(u) \tag{61a}$$

$$n(x) = L_x^{-1}[H(1/s)/s] \tag{61b}$$

$$A_0^0 = \alpha_2\,. \tag{61c}$$

3. Numerical implementation and results

At the heart of the above theoretical treatment is the evaluation of the H-function given by (16*a*). Unlike the corresponding H-function for radiative transfer, the range of the independent variable u varies over the half-real line making the evaluation by quadrature rather delicate. Several standard quadratures were tried, such as the Gauss–Hermite shifted to $[0, \infty)$ and a Gauss–Laguerre quadrature as well as the Shizgal quadrature [8], especially constructed for the half-real line with weight e^{-u^2}. These all failed to give the desired accuracy. After some experimentation, it was found that several transformations to bring the integration interval to $[0, 1]$, so that a shifted Gauss–Legendre quadrature could be applied, were most effective. If, for integrals of the form

$$I \equiv \int_0^\infty \mathrm{d}u'\,\phi_0(u')f(u')$$

the following transformation is introduced:

$$u' = \tan\omega$$

there results

$$I \equiv \int_0^{\pi/2} \mathrm{d}\omega\;\sec^2\omega\,\phi_0(\tan\omega)f(\tan\omega)\,.$$

Then letting

$$\omega = \frac{\pi}{2}\omega'$$

results in

$$I = \frac{\pi}{2}\int_0^1 \mathrm{d}\omega'\;\sec^2\left(\frac{\pi}{2}\omega'\right)\phi_0\left(\tan\left(\frac{\pi}{2}\omega'\right)\right)f\left(\tan\left(\frac{\pi}{2}\omega'\right)\right) \tag{62}$$

which can be evaluated by a shifted Gauss–Legendre quadrature. Using this quadrature, most of the results contained in [4, 9] could be reproduced. Additional results, including interior distributions for reflective boundaries were also obtained.

The second numerical method which is required for the evaluation of the desired distributions is the numerical Laplace transform inversion. The numerical inversion used was specifically developed for the evaluation of transport solutions. Central to the inversion is a change of variable reducing the Bromwich contour integration to a combination of sine and cosine integrals. These integrals are then transformed into an infinite series by decomposing the infinite integration interval into finite integrals over the period of the sine and cosine. The evaluation of the series is accelerated through the Euler–Knopp accelerator with each integral evaluated by a Romberg integration.

Table 1. Variation of x_m with quadrature order Lm and reflection coefficient r.

	r			
Lm	0.0	0.01	0.5	0.99
10	1.423 419 2E+00	1.450 573 5E+00	4.024 175 6E+00	2.541 314 2E+02
15	1.439 588 8E+00	1.466 912 7E+00	4.051 244 5E+00	2.500 171 8E+02
20	1.437 149 3E+00	1.464 445 0E+00	4.046 349 0E+00	2.497 407 3E+02
25	1.437 088 9E+00	1.464 384 0E+00	4.046 287 2E+00	2.498 000 1E+02
30	1.437 108 6E+00	1.464 404 0E+00	4.046 328 5E+00	2.498 047 0E+02
35	1.437 111 4E+00	1.464 406 8E+00	4.046 333 7E+00	2.498 047 1E+02
40	1.437 111 7E+00	1.464 407 1E+00	4.046 334 1E+00	2.498 046 7E+02
45	1.437 111 7E+00	1.464 407 1E+00	4.046 334 2E+00	2.498 046 6E+02
50	—	—	—	2.498 046 6E+02

Table 1. (Continued.) Variation of $n(0)$ with quadrature order Lm and reflection coefficient r.

	r			
Lm	0.0	0.01	0.5	0.99
10	1.000 000 0E+00	1.022 479 9E+00	3.354 313 3E+00	2.529 044 4E+02
15	1.000 000 0E+00	1.022 506 4E+00	3.358 446 5E+00	2.489 284 3E+02
20	—	1.022 503 4E+00	3.357 958 8E+00	2.487 877 8E+02
25	—	1.022 503 4E+00	3.357 953 6E+00	2.488 414 7E+02
30	—	—	3.357 957 9E+00	2.488 448 4E+02
35	—	—	3.357 958 3E+00	2.488 447 6E+02
40	—	—	3.357 958 4E+00	2.488 447 2E+02
45	—	—	3.357 958 4E+00	2.488 447 1E+02
50	—	—	—	2.488 447 1E+02

Table 1 indicates the high degree of accuracy to which the solution of the BGK equation can be obtained using the above methodology. The table displays the convergence of the Milne extrapolation distance and $n(0)$ with Gauss–Legendre quadrature order for several constant reflection coefficients as given by (60). No more than an order of 50 is required for seven place accuracy which is in agreement with the values in table 3 of [4]. The determination of α and β from (41) is accomplished through (46) and (47). In discrete form, (47) becomes

$$\sum_{k=1}^{Lm}\left[\delta_{kj} \pm \frac{\tilde{\omega}_k K_k}{u_j + u_k}\right]\chi_{\pm k} = 1 \qquad (63a)$$

where

$$\chi_{\pm k} \equiv \chi_{\pm}(u_k)$$

for a Gauss–Legendre quadrature rule of order Lm with weights ω_k and abscissas x_k giving from (62)

$$\tilde{\omega}_k = \sec^2\left(\frac{\pi}{2}x_k\right)\phi_0\left(\tan\left(\frac{\pi}{2}x_k\right)\right)\omega_k \qquad (63b)$$

$$u_k = \tan\left(\frac{\pi}{2}x_k\right). \qquad (63c)$$

Equation (63a) is solved by matrix inversion and α and β are recovered from

$$\alpha_k = \tfrac{1}{2}[\chi_{+k} + \chi_{-k}] \qquad \beta_k = \tfrac{1}{2}[\chi_{+k} - \chi_{-k}]. \qquad (64)$$

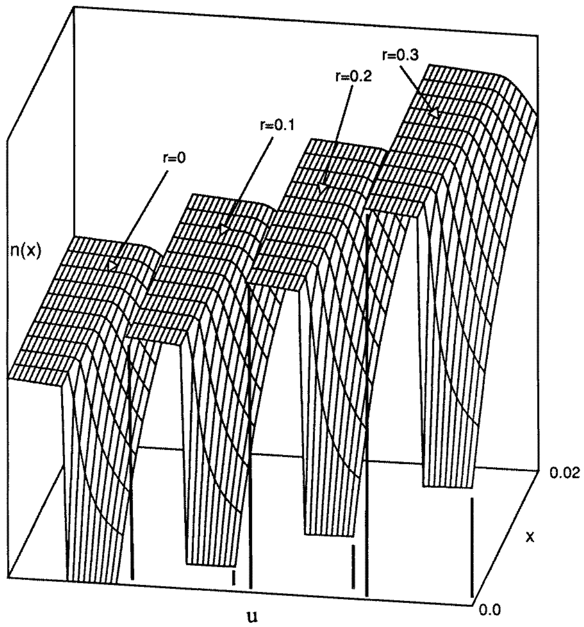

Figure 1. Milne solution near singularity at $u = x = 0$.

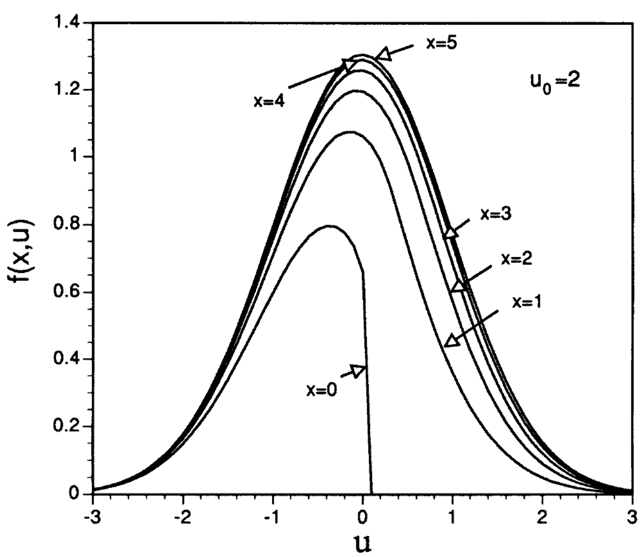

Figure 2. Velocity distribution for albedo problem for no reflection.

In the Milne solution, a natural discontinuity arises because of the non-reentrant condition imposed at the surface. The singularity manifests itself as a discontinuity in the velocity distribution at $u = x = 0$. A region near the singularity is shown in figure 1 for $r = 0$ (0.1) 0.3. Note the increase in the velocity distribution as more of the perturbation is reflected back into the medium. The nature of the singularity, however, remains unchanged.

Figures 2 and 3 are included to demonstrate the nature of the solution with and without wall reflection. In figure 2, the velocity distribution at several positions without wall

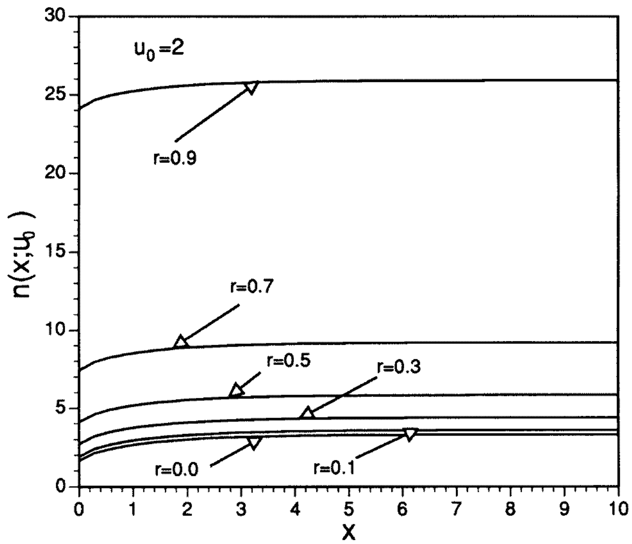

Figure 3. Approach of net flow velocity to the asymptotic value for the albedo problem.

reflection is shown. As expected, with increasing x the net flow velocity approaches an asymptotic value. Figure 3 displays the asymptotic approach for various constant reflection coefficients. The asymptotic value is apparently reached within a shorter distance from the surface with decreasing r.

While the above calculations were performed using α and β from (41), an alternative evaluation exists in (36). If

$$f(0,-u;u_0) = u_0\phi_0(u)H(u_0)H(u)Y(u,u_0) \tag{65a}$$

then

$$Y(u,u_0) = \frac{1}{u+u_0} + \int_0^\infty \mathrm{d}u'\,\frac{K(u')}{u+u'}Y(u',u_0) \tag{65b}$$

which can be numerically evaluated in the same way as for $\chi_\pm(u)$. In addition, when $u = 1/s$

$$Y(1/s,u_0) = \frac{s}{1+su_0} + s\int_0^\infty \mathrm{d}u'\,\frac{K(u')}{1+su'}Y(u',u_0) \tag{66}$$

for use in the Laplace transform inversion. Where applicable, the above calculations were repeated with Y as determined from (65*b*) with no apparent change in the results.

The final demonstration involves the albedo problem for an incoming perturbation source distribution of a 'Maxwellian' form

$$g(u) = \frac{\nu^\alpha}{j^+(\alpha,\beta)}\mathrm{e}^{-\beta u^2/2} \tag{67a}$$

normalized to unit entering current:

$$j^+(\alpha,\beta) = \Gamma(1+\alpha/2)\beta^{-1}(\beta/2)^{-\alpha/2}\,. \tag{67b}$$

The treatment of a general source is particularly straightforward. Since equation (37) represents a Green's function, by integration of (65*a*) the exiting distribution is

$$f(0,-u) = \phi_0(u)H(u)Y(u) \tag{68}$$

where $Y(u)$ satisfies the following integral equation:

$$Y(u) = \int_0^\infty \mathrm{d}u' \, \frac{u'}{u+u'} H(u')g(u') + \int_0^\infty \mathrm{d}u' \, \frac{K(u')}{u+u'} Y(u') \,. \tag{69}$$

The interior net flow velocity is again obtained from the relation given by (43) resulting in

$$n(x) = L_x^{-1}\{H(1/s)Y(1/s)/s\} \tag{70a}$$

with

$$Y(1/s)/s = \int_0^\infty \mathrm{d}u' \, \frac{u'}{1+su'} H(u')g(u') + \int_0^\infty \mathrm{d}u' \, \frac{K(u')}{1+su'} Y(u') \,. \tag{70b}$$

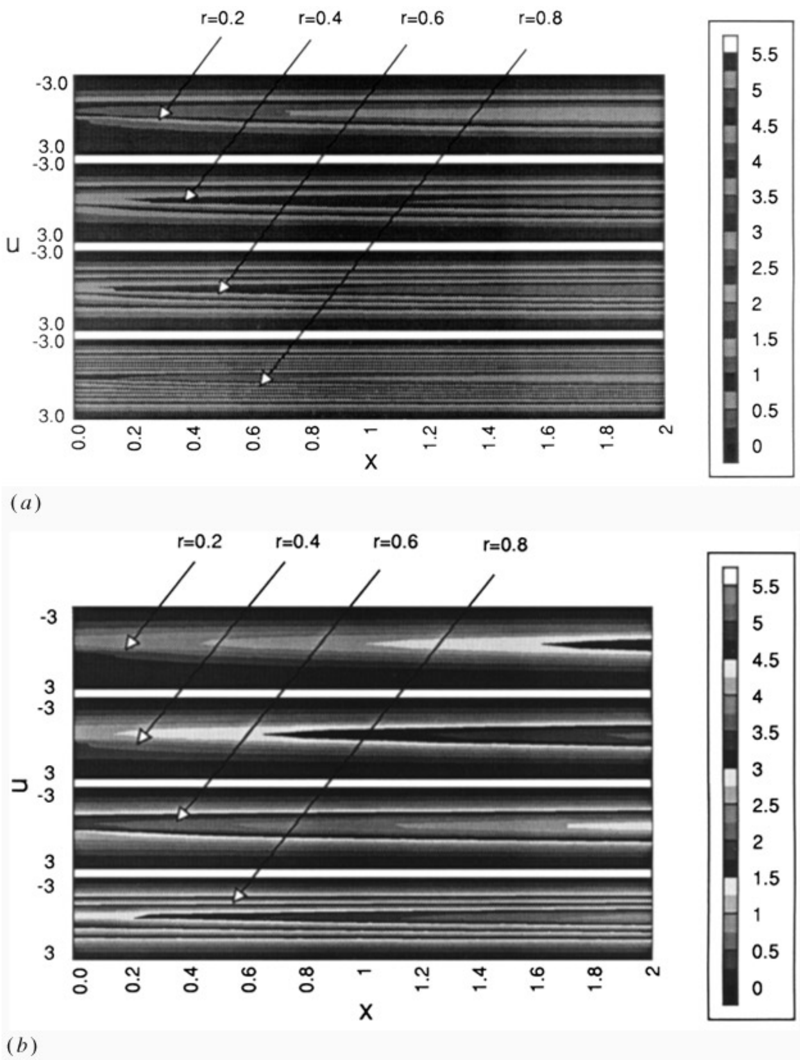

Figure 4. Variation of velocity distribution, (a) with r for $u_0 = 2$ for albedo problem, (b) for Milne problem.

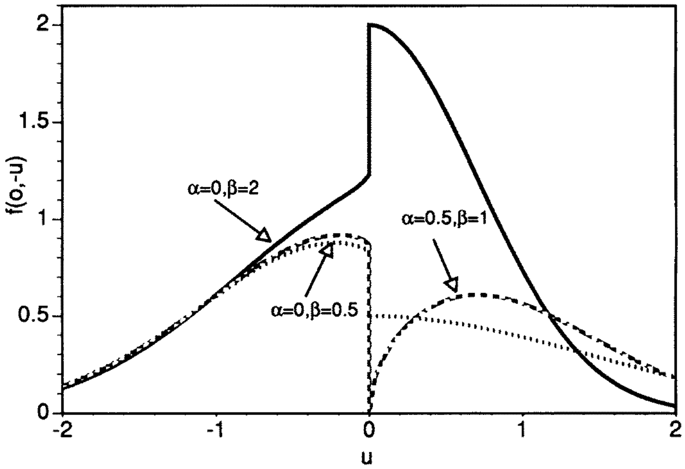

Figure 5. Wall distribution for three Maxwellian sources.

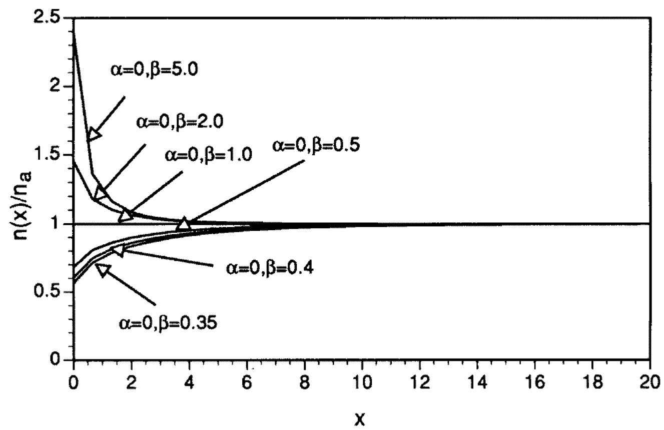

Figure 6. Normalized net flow velocity for Maxwellian sources (n_a is the asymptotic net flow velocity).

The asymptotic net flow velocity can be obtained from (29*d*). A special case arises when $\alpha = 0$ and $\beta = 1$ corresponding to injection at the background temperature $g(u) = \sqrt{2\pi}\phi_0(u)$. For this case with a constant reflection coefficient, the solution to (69) is

$$Y(u) = \sqrt{2\pi}[(1-r)H(u)]^{-1}$$

implying

$$f(0,-u) = \sqrt{2\pi}\phi_0(u)/(1-r) \qquad (71a)$$

and

$$n(x) = \sqrt{2\pi}/(1-r)\,. \qquad (71b)$$

Thus $n(x)$ is independent of x for this case.

Figure 4 displays the wall distributions for the Maxwellian sources indicated. These are the same sources considered in [9] and are in 'graphical' agreement with those presented

Table 2. Asymptotic net flow velocity for Maxwellian sources.

α	β	$n(\infty)$
0	0.5	3.413 423 8E+00
0	0.4	3.271 501 0E+00
0	0.5	3.053 621 0E+00
0	1.0	2.507 883 7E+00
0	2.0	2.110 975 6E+00
0	0.5	1.747 919 7E+00
0.5	1.0	2.701 557 6E+00
1.0	1.0	2.874 223 4E+00

there. The method in [9], misnamed the 'two stream approximation', should more properly be referred to as a half-range expansion and also does not involve numerical evaluation of principle value integrals. The method generally provides highly accurate asymptotic results. However, the expansion does not accurately reproduce discontinuities of the velocity distribution function at the wall. In figure 5, the approach of the net flow velocity with x to its asymptotic or equilibrium value is shown for $\alpha = 0$. It should be noted that the position when equilibrium is reached is relatively insensitive to the injection temperature. Finally, the asymptotic values for eight sources are given in table 2 to seven places. The maximum quadrature order required in table 2 was 55.

All evaluations were coded in FORTRAN and performed on an SGI workstation with the most comprehensive calculations taking no longer than 10 minutes.

4. Concluding remarks

An alternative approach to the determination of a highly accurate numerical solution to the linearized BGK equation of kinetic theory has been presented. The solution employs the principles of invariance approach which completely avoids the necessity to evaluate principal value integrals. The method features simplicity of solution with solutions to the albedo and Milne problems for wall reflection obtained from the solution to the fundamental albedo problem. The resulting explicit expressions can be evaluated to a high degree of accuracy using a shifted Gauss–Legendre quadrature and numerical Laplace transform inversion. The results found here are in complete agreement with those of [4, 8]. The numerical evaluations have been implemented in a fast running FORTRAN code available from the author (for information, please send e-mail to ganapol@cowboy.nee.arizona.edu).

The approach presented here has a wider application, for example, for more complicated scattering kernels, with no reflection. Another possible application is for a localized point perturbation propagating into a gas filling a half-space resulting in a two-dimensional problem. Additional applications include determination of the Green's function with application to finite media. Some of these considerations will be the subject of future efforts.

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References

[1] Case K and Zweifel P 1967 *Linear Transport Theory* (London: Addison-Wesley)
[2] van Kampen N G 1955 *Physica* **21** 949
[3] Cercignani C 1988 *The Boltzmann Equation and its Application* (Berlin: Springer)
[4] Kainz A J and Titulaer U M 1992 *J. Phys. A: Math. Gen.* **25** 3189
[5] Chandrasekhar S 1960 *Radiative Transfer* (New York: Dover)
[6] Busbridge I 1960 *The Mathematics of Radiative Transfer* (Cambridge: Cambridge University Press)
[7] Sobolev V 1963 *A Treatise on Radiative Transfer* (New York: Van Nostrand)
[8] Shizgal B 1981 *J. Comput. Phys.* **41** 309
[9] Kainz A J and Titulaer U M 1992 *J. Phys. A: Math. Gen.* **25** 1855