Journal of Statistical Physics, Vol. 37, Nos. 5/6, 1984

The Density Profile for the Klein–Kramers Equation Near an Absorbing Wall

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Received March 6, 1984; revision received June 26, 1984

We derive asymptotic series for the expansion coefficients of a function in terms of the Pagani functions, which occur in the boundary layer solutions of the Klein–Kramers equation. The results enable us to determine the density profile in the stationary solution of this equation near an absorbing wall from the numerically determined velocity distribution at the wall, with an accuracy of about 2%. We also obtain information about the analytic behavior of the density profile: this profile increases near the wall with the square root of the distance to the wall. Finally, the asymptotic analysis leads to an understanding of the slow convergence of variational approximations to the solution of the absorbing-wall problem and of the exponents that occur when one studies the variational approximations to various quantities of interest as functions of the number of terms in the variational ansatz. This is used to obtain a better variational estimate for the density at the wall.

KEY WORDS: Boundary layer; Brownian motion; Milne problem; asymptotic expansions.

1. INTRODUCTION AND SURVEY

The kinetic boundary layer problem for the Klein–Kramers equation near a plane absorbing boundary, posed a long time ago by Wang and Uhlenbeck,[1] has received a considerable amount of attention in recent years. The history and background of the problem were reviewed extensively in a recent paper by Selinger and Titulaer,[2] so we shall restate it only briefly here. In dimensionless units the stationary Klein–Kramers equation[3]

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0022-4715/84/1200-0589$03.50/0

for the distribution function of velocity u and position x of a Brownian particle in one dimension reads

$$u \frac{\partial}{\partial x} P(u, x) = \left[\frac{\partial^2}{\partial u^2} + \frac{\partial}{\partial u} u \right] P(u, x) \tag{1.1}$$

The equation has two easily determined solutions of Chapman–Enskog type, the equilibrium solution

$$\psi_0(u, x) = \phi_0(u) = (2\pi)^{-1/2} \exp(-\tfrac{1}{2}u^2) \tag{1.2}$$

and a current-carrying solution

$$\psi_0'(u, x) = (xu^{-1} - 1)\, \phi_0'(u) \tag{1.3a}$$

with

$$\phi_0'(u) = u\phi_0(u) \tag{1.3b}$$

The problem posed by Wang and Uhlenbeck was to construct a solution $P^M(u, x)$ such that

$$P^M(u, x) \cong \psi_0'(u, x) + x_M \psi_0(u, x) \qquad \text{for } x \to \infty \tag{1.4a}$$

with the boundary condition for an absorbing wall

$$P^M(u, 0) = 0 \qquad \text{for } u > 0 \tag{1.4b}$$

and to determine the parameter x_M, the Milne extrapolation length. The solution (1.4) is called the Milne solution of (1.1).

Simple approximate Milne solutions were given by Harris[4] and by Razi Naqvi *et al.*[5] A more systematic approach[7] starts from the observation by Pagani[6] that (1.1) has the additional solutions

$$\psi_{\pm n}(u, x) = \phi_{\pm n}(u) \exp(\mp n^{1/2} x) \qquad (n = 1, 2, 3,...) \tag{1.5}$$

with known functions $\phi_{\pm n}(u)$ given explicitly in Section 2. Moreover, Pagani showed that the $\phi_{\pm n}(u)$ are orthogonal with respect to the indefinite scalar product

$$\langle f, g \rangle = \int_{-\infty}^{+\infty} du\, u \exp(\tfrac{1}{2}u^2) f(u)\, g(u) \tag{1.6}$$

and, together with $\phi_0(u)$ and $\phi_0'(u)$, complete on $-\infty < u < \infty$. It was then conjectured by Burschka and Titulaer[7] that the Wang–Uhlenbeck problem has a solution of the type

$$P^M(u, x) = \psi_0'(u, x) + d_0^M \psi(u, x) + \sum_{n=1}^{\infty} d_{+n}^M \psi_{+n}(u, x) \tag{1.7}$$

This conjecture was later proved by Beals and Protopopescu.[8] The coefficients d^M_{+n} are given by

$$d^M_{+n} = -\int_{-\infty}^{0} du\, u \exp(\tfrac{1}{2}u^2)\, P^M(u, 0)\, \psi_{+n}(u, x) \tag{1.8}$$

Since this expression contains the unknown function $P^M(u, 0)$, it cannot be used to determine the d^M_{+n} directly. This was done in Ref. 7 by means of a variational procedure starting with a finite approximation to the infinite sum in (1.7). However, this scheme exhibited very slow convergence, and it was found necessary to combine it with an empirical extrapolation procedure in order to find reliable results for x_M and other quantities of interest. For some quantities, such as the density profile

$$n^M(x) = \int_{-\infty}^{+\infty} du\, P^M(u, x) \tag{1.9}$$

a reliable extrapolation was not feasible.

To circumvent some of these difficulties, the function $P^M(u, 0)$ was determined numerically in Ref. 2. This allows a direct determination of x_M; moreover, the d^M_{+n}, and with them the full solution (1.7), can be determined in principle via (1.8). However, the series in (1.7) turns out to be slowly converging and the numerical accuracy in $P^M(u, 0)$ does not suffice to evaluate (1.8) reliably for high n, as is argued more fully in Section 3.

In the present paper we treat this remaining difficulty with the solution procedure of Ref. 2, further denoted by I, by providing an asymptotic expansion of d^M_{+n} for large n. Such an expansion was provided before by Mayya and Sahni.[9a] (For a criticism of Ref. 9a, see a work by Protopopescu *et al.*[9b]) These authors used the expansion in combination with an *ad hoc* ansatz for $P^M(u, 0)$; hence their results do not yield a qualitative improvement over those of Refs. 4 and 5. However their work yields one new prediction: the density profile $n^M(x)$ is found to have an infinite derivative at $x = 0$; for small x it has the form $a + bx^{1/3}$.

In Section 2 of this paper we describe our technique for deriving an asymptotic series for d^M_{+n}, which is somewhat more general and easier to use than that of Ref. 9a. This technique is then used in Section 3 to determine the density profile $n^M(x)$ from the numerically determined $P^M(u, 0)$ found in I. The result depends critically on the behavior of $P^M(u, 0)$ near $u = 0$, which could not be determined unambiguously from the numerical results in I. In Section 4 we show that this ambiguity can be resolved by exploiting the requirement that the expansion coefficients

$$d^M_{-n} = \int du\, u \exp(\tfrac{1}{2}u^2)\, P^M(u, 0)\, \phi_{-n}(u) \tag{1.10}$$

vanish identically. We show that this can occur only when

$$P^M(u,0) \cong \text{cst}\, u^{1/2+3k} \qquad \text{for } u \to 0 \quad (k=0,1,2,\ldots) \tag{1.11}$$

A glance at the numerical results shows that only $k=0$ yields acceptable agreement. This is shown to lead to a density profile

$$n^M(x) \cong n^M(0) + \text{cst}\, x^{1/2} \qquad \text{for } x \to 0 \tag{1.12}$$

exhibiting the infinite tangent predicted Mayya and Sahni, but with a different power of x.

In Section 5 we exploit our asymptotic results to shed some light on the convergence properties of variational solutions of the type used in Ref. 7. We explain the inverse powers of N (the number of terms in the variational ansatz) with which various physical quantities of interest approach their correct value in the limit $N \to \infty$. We also indicate how the results of this paper can be used to improve and simplify calculations as performed in Ref. 7.

Our aim throughout this paper is to develop asymptotic techniques as a practical aid in the study of kinetic boundary layers. Some steps in our derivations are not fully rigorous; there we give plausibility arguments and use *a posteriori* consistency checks and comparisons with numerical data to support our method. Also, for clarity, we confine ourselves in the main part of the paper to a discussion of the Milne solution. Some remarks on the applicability of our techniques to other kinetic boundary layer problems are given in the concluding section.

2. ASYMPTOTIC SERIES FOR THE PAGANI EXPANSION COEFFICIENTS

The Pagani eigenfunctions introduced in (1.5) are given by[6]

$$\begin{aligned}\phi_{\pm n}(u) &= (n!)^{-1/2}(8\pi n)^{-1/4}(2e)^{-n/2}\exp[-\tfrac{1}{2}(u \mp n^{1/2})^2]\, H_n[2^{-1/2}(u \mp 2n^{1/2})] \\ &= (n!)^{-1/2}(8\pi n)^{-1/4} 2^{-n/2}\exp[-\tfrac{1}{4}u^2])\exp[-\tfrac{1}{4}(u \mp 2n^{1/2})^2] \\ &\quad \times H_n[2^{-1/2}(u \mp 2n^{1/2})]\end{aligned} \tag{2.1}$$

For large n and not too large u these functions can be approximated by an asymptotic expression due to Olver,[10] a variant of the Plancherel–Rotach formula (Ref. 11; this book uses differently defined Airy functions). If we define

$$\xi = \nu x, \qquad \nu = (2n+1)^{1/2} \tag{2.2}$$

then Olver's asymptotic formula reads

$$\exp(-\tfrac{1}{2}\xi^2)\, H_n(\xi) \cong (2\pi)^{1/2} e^{-(1/4)\nu^2} \nu^{(3\nu^2-1)/6} \left(\frac{\zeta}{x^2-1}\right)^{1/4} \{Ai(\nu^{4/3}\zeta) + \varepsilon(x)\} \quad (2.3a)$$

with $\mathrm{Ai}(z)$ the Airy function, ζ given by

$$\zeta = 2^{1/3}[(x-1) + \tfrac{1}{10}(x-1)^2 - \tfrac{2}{175}(x-1)^3 + \cdots] \quad (2.3b)$$

and $\varepsilon(x)$ of order n^{-1} times the amplitude of the Airy function. Using (2.3b) and $(1+n^{-1})^{\alpha n} \cong e^{\alpha}$ we find to leading order

$$\exp(-\tfrac{1}{2}\xi^2)\, H_n(\xi) \sim (2\pi)^{1/2} e^{-(1/2)n} (2n)^{(1/2)n+1/6}\, \mathrm{Ai}[\nu^{4/3} 2^{1/3}(x-1)] \quad (2.4)$$

Substitution in (2.1), use of Stirling's formula, replacement of $(2n+1)^{1/2} - (2n)^{1/2}$ by $2^{-3/2} n^{-1/2}$, and use of $H_n(-\xi) = (-1)^n H_n(\xi)$ yields

$$\phi_{\sigma n}(u) \sim (-\sigma)^n 2^{-1/2} n^{-1/3} \exp(-\tfrac{1}{4}u^2)\, \mathrm{Ai}(-\sigma n^{1/6} u - \tfrac{1}{2} n^{-1/3}) \quad (2.5)$$

with σ the sign of the index $\pm n$.

Let us now consider the expansion coefficients $d_{\sigma n}[f]$ in terms of the Pagani eigenfunctions of a function $f(u) = \tilde{f}(-u) \exp(-\tfrac{1}{2}u^2)$ that is nonzero only for negative u. Using the expansion formula (I.2.9) we find

$$d_{\sigma n}[f] = \sigma \int_{-\infty}^{0} du\, u \tilde{f}(-u)\, \phi_{\sigma n}(u) \quad (2.6)$$

To obtain an asymptotic series for these coefficients we make use of a formula due to Bleistein and Handelsman[12] for integral transforms of the type

$$H[g; \lambda] = \int_0^{\infty} dt\, h(\lambda t)\, g(t) \quad (2.7)$$

When $g(t)$ has an expansion near $t = 0$ of the type

$$g(t) = \sum_{m=1}^{\infty} g_m t^{a_m} \quad (2.8)$$

with a_m an increasing sequence of positive numbers, then asymptotically for large λ

$$H[g; \lambda] \sim \sum_{m=0}^{\infty} \lambda^{-1-a_m} g_m M[h; 1 + a_m] \quad (2.9)$$

with $M[h; z]$ the Mellin transform of $h(t)$, i.e., the analytic continuation of

$$\tilde{M}[h, z] = \int_0^\infty dt\, h(t) t^{z-1} \tag{2.10}$$

In view of the oscillating character of the $\phi_{\sigma n}(u)$ for large positive σu and the rapid decrease for large negative σu we may expect that the dominant contribution to the integrals (2.6) comes from the region where (2.5) is valid. When we substitute (2.5) in (2.6) and expand the Airy function in a Taylor series with respect to the argument shift $-\frac{1}{2}n^{-1/3}$, we have written (2.5) as a sum of contributions of type (2.7). The Mellin transforms of $\mathrm{Ai}(t)$ and $\overline{\mathrm{Ai}}(t) \equiv \mathrm{Ai}(-t)$ are given by[12]

$$M[\mathrm{Ai}; z] = (2\pi)^{-1}\, 3^{2z/3-7/6}\, \Gamma\left(\frac{z}{3}\right) \Gamma\left(\frac{z+1}{3}\right) \tag{2.11a}$$

and

$$M[\overline{\mathrm{Ai}}; a] = 2 \sin\left(\frac{\pi z}{3} + \frac{\pi}{6}\right) M(\mathrm{Ai}; z) \tag{2.11b}$$

and those of their derivatives follow from

$$M[h'; z] = -(z-1)\, M[h; z-1] \tag{2.12}$$

We note in passing that the derivatives of $\overline{\mathrm{Ai}}(t)$ beyond the second one do not have Mellin transforms in the usual sense; however, we shall not use such high terms in the asymptotic series anyhow, for reasons to be explained presently.

The asymptotic series we obtain in this way for the expansion coefficients (2.6) are

$$\begin{aligned} d_{+n}[f] \sim (-1)^{n+1} 2^{-1/2} \sum_{m=1}^{\infty} n^{-2/3-(1/6)a_m} g_m \{ &M[\mathrm{Ai}; 2 + a_m] \\ &- \tfrac{1}{2} n^{-1/3} (1 + a_m) M[Ai; 1 + a_m] + \cdots \} \end{aligned} \tag{2.13a}$$

and

$$\begin{aligned} d_{-n}[f] \sim 2^{-1/2} \sum_{m=1}^{\infty} n^{-2/3-(1/6)a_m} g_m \{ &M[\overline{\mathrm{Ai}}; 2 + a_m] \\ &- \tfrac{1}{2} n^{-1/3} (1 + a_m) M[\overline{\mathrm{Ai}}; 1 + a_m] + \cdots \} \end{aligned} \tag{2.13b}$$

where the g_m are the expansion coefficients according to (2.8) of

$$g(u) \equiv f(u) \exp(-\tfrac{1}{4} u^2) \tag{2.13c}$$

The terms in (2.13a, b) coresponding to second derivatives of the Airy function are of order $n^{-2/3}$ relative to the leading term, and thus of the same order as terms beyond the first one in (2.3b), that are neglected in passing from (2.3a) to (2.5). Thus only terms in (2.13) of order smaller than $n^{-2/3}$ relative to the leading one are meaningful; the next corrections can be worked out, however. Starting from the relative order n^{-1} we would need as yet unknown corrections to the asymptotic expression (2.3a), as well as third derivatives of the Airy function, for which (2.9) cannot be used without closer scrutiny. Generalizations to functions not confined to the negative half-axis are straightforward, but not needed for our analysis.

3. EXPANSION OF THE NUMERICALLY DETERMINED MILNE SOLUTION; DENSITY PROFILES

In I, we numerically determined the velocity distribution $P^M(u, 0)$ of particles at an absorbing wall for a system of Brownian particles that are supplied at a constant rate from the far interior, the so-called Milne solution of the Klein–Kramers equation discussed already in Section 1. To obtain the full solution $P^M(u, x)$ we must expand the boundary layer part of the function $P^M(u, 0)$ in terms of the Pagani eigenfunctions and provide each term in the expansion with a factor $\exp(-xn^{1/2})$.

The first few expansion coefficients $d_{+n}[P^M] \equiv d^M_{+n}$ can be determined from the numerically determined $P^M(u, 0)$, further denoted by $P^M(u)$, either via direct numerical integration or analytically via some parametrization. However, after the first few terms the numerical integration becomes unreliable, as the $\phi_{+n}(u)$ vary appreciably over the sampling intervals used in constructing the numerical $P^M(u)$. Similarly, the analytical calculations rapidly increase in complexity as n increases. In principle there are three possible ways out: (i) truncation of the Pagani series, (ii) empirical extrapolation of the coefficients, (iii) replacement of the higher coefficients by an asymptotic expression. The first two alternatives were tried in I, Section 4, and will be briefly reviewed here; then we shall explore the third alternative.

To assess the validity of the various procedures we concentrate on the density profile

$$n^M(x) = \int_{-\infty}^{+\infty} du\, P^M(u, x)$$

$$= x + x_M + \sum_{n=1}^{\infty} \rho^M_n \exp(-xn^{1/2}) \qquad (3.1\text{a})$$

with

$$\rho^M_n = d^M_{+n} \int du\, \phi_{+n}(u) \qquad (3.1\text{b})$$

As we saw in I the integral in (3.1b) is given by

$$\int du\, \phi_{+n}(u) = (-1)^n (2n)^{-1/2}[1 - (24n)^{-1} + \cdots] \tag{3.2}$$

If we replace $\phi_{+n}(u)$ by its asymptotic form (2.5), which is already quite good for $n = 1$, we find after a straightforward rescaling

$$d^M_{+n} \cong (-1)^{n+1} 2^{-1/2} n^{-2/3} \int_0^\infty dt\, t\, \mathrm{Ai}[t - \tfrac{1}{2} n^{-1/3}] \times P^M(-n^{-1/6} t) \exp(+\tfrac{1}{4} n^{-1/3} t^2) \tag{3.3}$$

Since the integral is positive definite, all terms in the series in (3.1) are negative and any truncation yields an upper bound. Moreover, since both $P^M(u) \exp(\frac{1}{4}u^2)$ and $t\, \mathrm{Ai}(t)$ are functions with a single maximum, the integral also shows a single maximum as a function of n, situated roughly where the two maxima coincide. We found this maximum in $n^{2/3} d^M_{+n}$ at $n = 10$. Thus a lower bound for $n(x)$ can be found by replacing the integral in (3.3) for all $n > n_{\max}$ ($n_{\max} \geqslant 10$) by the corresponding quantity found from $d^M_{+n_{\max}}$. This was done in I for $n_{\max} = 12$. The density profile can then be calculated using a technique to be explained presently. We found that the upper and lower bound differ appreciably; moreover the values for $n^M(0)$ obtained from the approximations to (3.1) agree rather poorly with the value found directly by integrating $P^M(u)$.

To obtain better agreement we now attempt to exploit the asymptotic series expansions developed in Section 2. To apply them we must use a parametrization of $P^M(-u)$. If we use the analytic parametrization (I.4.1) we obtain for the function $g(u)$ in (2.13c)

$$g(u) = 0.1749 + 1.1286u - 0.5838u^2 - 0.1083u^3 + 0.1201u^4 + \cdots \tag{3.4}$$

This implies for the expansion coefficients in (3.1) the asymptotic expression $\tilde{\rho}^a_n$ given by

$$\tilde{\rho}^a_n \sim 0.0226n^{-7/6} + 0.2003n^{-8/6} - 0.1800n^{-9/6} + 0.0619n^{-10/6} + 0.0916n^{-11/6} + \cdots \tag{3.5}$$

where the last term includes a contribution -0.0088 from correction terms not included in (2.5) and (2.13a).

In Table I we give the expressions for $\tilde{\rho}^a_n$, $1 \leqslant n \leqslant 12$, obtained by truncating the series after the third and fourth term; we also give the exact ρ^M_n calculated analytically from the parametrization (I.4.1), which

Table I. The Expansion Coefficients ρ_n^M as Determined (a) from the Numerical Solution in I with the Parametrization (I.4.1); (b, c) from the Asymptotic Series (3.5) Truncated after Three and After Four Terms; (d) form (4.3) Truncated after the First Term

n	(a)	(b)	(c)	(d)
1	0.0980	0.0429	0.1048	0.1216
2	0.0461	0.0259	0.0454	0.0511
3	0.0293	0.0179	0.0278	0.0308
4	0.0211	0.0135	0.0197	0.0215
5	0.0163	0.0108	0.0150	0.0163
6	0.0133	0.0089	0.0120	0.0129
7	0.0111	0.0076	0.0100	0.0107
8	0.0095	0.0066	0.0085	0.0090
9	0.0083	0.0058	0.0074	0.0078
10	0.0073	0.0051	0.0065	0.0068
11	0.0066	0.0046	0.0058	0.0061
12	0.0059	0.0042	0.0052	0.0054

corresponds to (3.4). The series truncated after the fourth term is closest to the exact values; inclusion of the fifth term (not shown) leads to a much worse approximation for small n and a slightly better one for the last few ρ_n^M considered. This is a general feature of asymptotic series: the best approximation is usually obtained by truncation after the smallest term.

The density profile corresponding to the coefficients

$$\tilde{\rho}_{n,p} = \sum_{i=1}^{p} r_i n^{-\alpha_i} \tag{3.6a}$$

is given by

$$\tilde{n}_p^M(x) = x + x_M + \sum_{i=1}^{p} r_i Z(a_i; x) \tag{3.6b}$$

with

$$Z(\alpha, x) = \sum_{n=1}^{\infty} n^{-\alpha} \exp(-xn^{1/2}) \qquad (\alpha > 1) \tag{3.6c}$$

The function $Z(\alpha, x)$ for large x is readily calculated from the series (3.6c); it can then be continued to smaller x using the generalization of (I.4.7)

$$Z(\alpha, x) = \sum_{n=1}^{\infty} (-1)^{n+1} n^{-\alpha} \exp(-xn^{1/2}) + 2^{1-\alpha} Z(\alpha, 2^{1/2}x) \tag{3.7}$$

For small x, $Z(\alpha, x)$ approaches the Riemann ζ function $\zeta(\alpha)$. It is clear from (3.7) that the first correction term must be proportional to $x^{2(\alpha-1)}$, since the alternating series can be bounded by $\alpha Z(\alpha+1, x)$. Using the techniques of Mayya and Sahni[9] and the series expansion of the incomplete Γ function[13] we find

$$Z(\alpha, x) = \zeta(\alpha) - (\alpha-1)^{-1} x^{2(\alpha-1)} \Gamma(3-2\alpha) + O(x) \quad \text{for } 1 < \alpha < 1.5 \tag{3.8}$$

For $\alpha > 1.5$, $Z(\alpha, x)$ decreases no faster than linearly, as one sees from the relation

$$\frac{d}{dx} Z(\alpha, x) = -Z\left(\alpha - \frac{1}{2}, x\right) \tag{3.9}$$

The possibly anomalous case $\alpha = 1.5$ is not needed in this section or in the remainder of the paper.

Our best estimate for $n^M(x)$ using the asymptotic series (3.5) is given by

$$n_a^M(x) = \tilde{n}_a^M(x) + \sum_{n=1}^{12} \{\rho_n^M - \tilde{\rho}_n^a\} \exp(-xn^{1/2}) \tag{3.10}$$

This function is given for a few values of x in the first row of Table II. Its behavior for small x is given by

$$n_a^M(x) = 0.918 + 0.184x^{1/3} + 1.610x^{2/3} + O(x) \tag{3.11}$$

Since the second term in (3.10) is analytic in x, the second and third term in (3.11) come from the contribution $\tilde{n}_a^M(x)$. The value for $n^M(0)$ found directly in I is $n^M(0) = 0.942$. The remaining discrepancy is due to the intrinsic limitations of the asymptotic series (3.5), but also to possible deficiencies of the parametrization (I.4.1). The latter point will be discussed in the following section.

Table II. The Boundary Layer Part of the Density Profile $|n^M(x) - x - x_M|$, as Calculated (a) from (3.10) with a Four-Term Approximation to $\tilde{n}_a^M(x)$; (b) from (4.4). For $x = 0$ We Found in I 0.512 ± 0.009.

x	4	1	2^{-2}	2^{-4}	2^{-6}	2^{-8}	2^{-10}	0
(a)	0.002	0.061	0.207	0.342	0.430	0.479	0.505	0.536
(b)	0.002	0.061	0.206	0.341	0.427	0.476	0.502	0.528

4. A CONSISTENT PARAMETRIZATION OF THE MILNE SOLUTION

The parametrization (I.4.1) was obtained as a best fit to the numerically obtained $P^M(-u)$ over its entire range of values, assuming a form $\exp(-\frac{1}{2}u^2) f(u)$ with $f(u)$ a polynomial of degree four. As we already noted in I, the data for $P^M(-u)$ near $u = 0$ might also be fitted by an $f(u)$ going to zero as some fractional power of u. To decide between the various fits we now use the requirement that all expansion coefficients d^M_{-n} should vanish for the actual solution of the Milne problem. This implies in particular that in the asymptotic series (2.13b) the coefficient of each inverse power of n should vanish separately. For the leading term this implies, as is seen from (2.11b), that a_1 should equal $\frac{1}{2} + 3k$ with integer k, hence that $g(u)$ should behave like $u^{1/2+3k}$ for small u. A comparison with the numerical result shows that only $k = 0$ yields an acceptable fit. The next term with g_1 in curly brackets in (2.1b) is then nonzero, but it can be compensated for by the first term with g_2, provided $a_2 = \frac{5}{2}$ and $g_2 = -\frac{1}{5} g_1$, as one sees using (2.11b). In a similar fashion the coefficient of $u^{9/2}$ in $g(u)$ can be determined from the requirement that the coefficient of $n^{-17/12}$ in the asymptotic series for d^M_{-n} vanishes. However, the coefficient of $u^{7/2}$, and more generally of $u^{1/2+3k}$, cannot be determined in this way. Later in this section we shall briefly discuss a systematic fitting procedure for $P^M(-u)$ based on these observations. Unfortunately, this scheme turns out to be impracticable, for reasons to be discussed.

However, the leading terms in the asymptotic series for d^M_{+n} involve only the behavior of $P^M(-u)$ for small u. In this region we must have, as we just saw,

$$g(u) = a[u^{1/2} - \tfrac{1}{5}u^{5/2} + O(u^{7/2})] \tag{4.1a}$$

or

$$P^M(-u) = a[u^{1/2} - \tfrac{9}{20}u^{5/2} + O(u^{7/2})] \tag{4.1b}$$

A fit of the constant a to the numerical data at low u yields

$$a = 0.8425 \pm 0.0325 \tag{4.2}$$

The relatively low accuracy is caused by the rather high uncertainty of the data at low u.

The fit (4.1) with a given by (4.2) yields expansion coefficients analogous to (3.5) given by

$$\tilde{\rho}^c_n = 0.1216n^{-5/4} + O(n^{-7/4}) \tag{4.3}$$

the superscript c denotes the consistent parametrization (4.1). The first term in (4.3) is given in Table I; it yields quite good agreement with the directly dtermined ρ_n^M. If (4.3) is regarded as an expansion in $n^{-1/6}$, like (3.5), then we see that two terms beyond the leading one vanish identically. Inclusion of one further term, obtained from a moment fitting procedure to be described presently, would worsen the correspondence with the directly determined ρ_n^M; the asymptotic series (4.3) is evidently best truncated after the first term. We note further that the directly determined ρ_n^M were calculated using the analytic parametrization (I.4.1), which for low u lies slightly above (4.1b). Therefore only the first few directly determined ρ_n^M can be considered superior to the asymptotic ones; the best estimate for $n_c^M(x)$ based on (4.3) is therefore given by

$$n_c^M(x) = x + x_M + 0.1216 Z(\tfrac{5}{4}, x) + \sum_{n=1}^{6} \{\rho_n^M - \tilde{\rho}_n^c\} \exp(-xn^{1/2}) \tag{4.4}$$

The values of this function for some values of x are given in the second row of Table II. The differences with the values derived from (3.10) are quite small in spite of the quite different asymptotic behavior for small x:

$$n_c^M(x) = 0.926 + 0.862 x^{1/2} + O(x) \tag{4.5}$$

The slightly better agreement with $n^M(0) = 0.942$, compared to (3.10), should be considered fortuitous in view of the large uncertainty in the coefficient a in (4.1). Thus, use of the consistent parametrization (4.1) yields some improvement in the complexity of the calculations, but little advantage in the numerical results, compared to the analytic parametrization (I.4.1).

In principle, as we just saw, the requirement that all d_{-n}^M vanish could be used to provide an alternative parametrization of the form,

$$P^M(-u) = \sum_{k=0}^{\infty} a_k g_k(u) \exp(-\tfrac{1}{4}u^2) \tag{4.6a}$$

with

$$g_k(u) = u^{3k+1/2} - (5+6k)^{-1} u^{3k+5/2} + O(u^{3k+9/2}) \tag{4.6b}$$

where the functions are constructed recursively in such a way that the asymptotic series for $d_{-n}[g_k]$ vanish identically. The coefficients a_k could then be determined by fitting the known moments of $P^M(-u)$ using the formula

$$\int du\, u^\alpha \exp(-\gamma u^2) = \gamma^{-(1/2)\alpha + 1/2}\, \Gamma(\tfrac{1}{2}\alpha + \tfrac{1}{2}) \tag{4.7}$$

However, from the known asymptotic series only one term beyond the one shown in (4.6b) can be determined, whereas one further term may be put equal to zero arbitrarily. This means that only the first three a_k could be determined even from exact knowledge of $P^M(-u)$. In addition, the rapid increase of the coefficients (4.7) with α leads to a rather ill-conditioned fitting problem. The results depend very sensitively on whether two or three terms are used in (4.6a), where the $g_k(u)$ are truncated, and whether the factor $\exp(-\frac{1}{4}u^2)$ in (2.5) is expanded or retained, leading to $\gamma=\frac{1}{2}$ or $\gamma=\frac{1}{4}$ in (4.7). A common feature of all fits is that for a_0 compatible with (4.2), a_1 comes out negative, with values between -0.15 and -0.45 depending on the details of the fitting procedure. The sign of this first correction term was used to justify truncating the asymptotic series (4.3) after the first term.

Before concluding this section we note that the rather primitive approximate expression

$$P_0^M(-u)=a_0u^{1/2}\exp(-\tfrac{1}{2}u^2) \tag{4.8}$$

with $a_0=0.928$ to normalize to unit current, yields very good values for the moments, as is seen in Table III; note, however, that this value for a_0 is excluded by the low-u data (4.2). Clearly, the effect of the correction factor $(1-\frac{9}{20}u^2+\cdots)$ are to a large extent canceled again by terms with a_1 and a_2 in (4.6a), which partly explains the problems with the fitting procedure in the last paragraph.

5. CONVERGENCE RATES OF VARIATIONAL APROXIMATIONS

In Ref. 7 various moments of the Milne solution $P^M(u)$ were determined from an approximate expression

$$P_N^M(u)=\phi_0'(u)+\sum_{n=0}^{N-1} d_{+n}^N\phi_{+n}(u) \tag{5.1}$$

Table III. The Moments $\langle\langle u^\alpha\rangle\rangle=\langle u^{\alpha+1}\rangle/\langle u\rangle$ for the Approximation (4.8) to $P^M(-u)$, Compared to Those of the Numerically Determined $P^M(-u)$ Found in I; the Number in Parentheses Is the Error in Units of the Last Digit Given.

α	-1	1	2	3
App.	0.956	1.434	2.500	5.019
Num.	0.942(8)	1.454(5)	2.564(17)	5.200(50)

with the $d^N_{+n}(u)$ determined by minimizing the quantity

$$D_N^2 \equiv \int_0^\infty du\, u \exp(\tfrac{1}{2}u^2)\, |P_N^M(u)|^2 \tag{5.2}$$

The integral in (5.2 vanishes identically due to (1.4b) if $P_N^M(u)$ is replaced by the exact solution. It was found empirically that D_N^2 approaches a value D_∞^2 close to zero according to

$$D_N^2 = D_\infty^2 + aN^{-\gamma} \tag{5.3}$$

with $\gamma \cong 0.48$. This behavior can be understood if we consider the "trial function"

$$\tilde{P}_N^M(u) = \phi_0'(u) + \sum_{n=0}^{N-1} d^M_{+n} \phi_{+n}(u) \tag{5.4}$$

with d^M_{+n} the expansion coefficients of the *exact* P_N^M. When the d^M_{+n} behave asymptotically like $n^{-[2/3-(1/6)\alpha]}$ then in follows from the orthonormality of the $\phi_+(u)$ that

$$\begin{aligned}\tilde{\Delta}_N^2 &\equiv \int_{-\infty}^{+\infty} du\, u \exp(\tfrac{1}{2}u^2)\, |\tilde{P}_N^M(u) - P^M(u)|^2 \\ &= \sum_{n=N}^{\infty} (d^M_{+n})^2 = O(N^{-1/3-(1/3)\alpha})\end{aligned} \tag{5.5}$$

Thus we find an upper bound for D_N^2 given by

$$D_N^2 \leqslant \sum_{n=N}^{\infty} (d^M_{+n})^2 + \sum_{n=N}^{\infty} \sum_{m=N}^{\infty} d^M_{+n} d^M_{+m} G_{nm} \tag{5.6a}$$

with

$$G_{nm} = \int_{-\infty}^{0} |u| \exp(\tfrac{1}{2}u^2)\, \phi_{+n}(u)\, \phi_{+m}(u) \tag{5.6b}$$

Now, if one substitutes (2.5), replaces one of the Airy functions by its value at $u = 0$ and rescales the argument in the other one, one obtains the uniform order of magnitude estimate

$$|G_{nm}| < \text{cst}\, n^{-1/3} m^{-2/3} \tag{5.6c}$$

Substitution in (5.6a) then leads to the result that the second term is at most of the same order as the first one, hence

$$D_N^2 = O(N^{-1/3-(1/3)\alpha}) \tag{5.7}$$

The empirically found exponent 0.48 in (5.3) agrees well with the value 0.5 found from (5.7) with the value $\alpha = \frac{1}{2}$ that was also found in Section 4. Note, however, that (5.7) yields merely a lower bound for the exponent. Hence, the data in Ref. 7 exclude $\alpha > \frac{1}{2}$, when we assume that D_N^2 has already reached its asymptotic region, but not lower values of α, since the actual minimum of the variational procedure might converge faster than the trial function (5.4).

Next we consider the error made in a variational estimate of a quantity $A[P^M(u)]$ that is a linear functional of $P^M(u)$:

$$A[P_N^M(u)] - A[P^M(u)] = \sum_{n=0}^{N-1} (d_{+n}^N - d_{+n}^M) A[\phi_{+n}(u)] - \sum_{n=N}^{\infty} d_{+n}^M A[\phi_{+n}(u)] \tag{5.8}$$

When an order of magnitude estimate for $A[\phi_{+n}(u)]$ is available, the second term in (5.8) can be evaluated straightforwardly. To estimate the first term we consider

$$\begin{aligned}\sum_{n=0}^{N-1} |d_{+n}^N - d_{+n}^N|^2 &= \int_{-\infty}^{+\infty} u \exp[\tfrac{1}{2}u^2) \, |P_N^M(u) - \tilde{P}_N^M(u)|^2 \\ &\leqslant \int_0^{\infty} u \exp(\tfrac{1}{2}u^2) \, |P_N^M(u) - \tilde{P}_N^M(u)|^2 \\ &\leqslant \int_0^{\infty} u \exp(\tfrac{1}{2}u^2) \{|P_N^M(u)|^2 + |\tilde{P}_N^M(u)|^2\} \\ &= O(N^{-1/3-(1/3)\alpha})\end{aligned} \tag{5.9}$$

where we used the Schwartz inequality and the estimate (5.7), which holds for $\tilde{P}_N^M$ and *a fortiori* for P_N^M, which minimizes the integral (5.2). The result (5.9) may be used to estimate the first term in (5.8) via the Schwartz inequality for N-dimensional vectors. Thus we find for the case

$$A[\phi_{+n}(u)] = O(n^{-\beta}) \tag{5.10a}$$

the result

$$A[P_N^M(u)] - A[P^M(u)] = O(N^{-(1/6)\alpha - \beta + 1/3}) \tag{5.10b}$$

where both terms in (5.8) give contributions of the same order. The case $\beta = \frac{1}{2}$ may yield a logarithmic correction from the first term, but we shall see presently that the occurrence of such a correction can be probably be excluded.

Since $\phi_{+n}(0) = O(n^{-1/3})$ we conclude from (5.10):

$$P_N^M(0) - P^M(0) = O(N^{-(1/6)\alpha}) \tag{5.11}$$

Since, moreover, the logarithmic derivative of ϕ_{+n} is of order $n^{1/6}$ we expect that the range in u of the function $P_N^M(u) - P^M(u)$ should be of order $N^{-1/6}$. This scaling relation is, e.g., fulfilled by the first positive zero's of the functions $P_N^M(u)$ in Fig. 2 of Ref. 7. For

$$d_{+n}^N - d_{+n}^M = \int du\, u \exp(\tfrac{1}{2}u^2)\, \phi_{+n}(u)[P_N^M(u) - P^M(u)] \tag{5.12}$$

this leads, with (5.11) and (2.5), to the estimate

$$d_{+n}^N - d_{+n}^M = O(n^{-1/3} N^{-(1/6)\alpha - 1/3}) \tag{5.13}$$

This estimate leads again to (5.9) for the sum of the squares, but in addition it leads directly to the estimate (5.10b), without logarithmic terms for $\beta = \frac{1}{2}$. For the error in the Milne length x_M, which is proportional to d_0^M, (5.13) predicts

$$x_M^N - x_M = O(N^{-1/3-(1/6)\alpha}) \tag{5.14}$$

The exponent in (5.14) yields $\frac{5}{12} = 0.417$ for $\alpha = \frac{1}{2}$, in excellent agreement with the value 0.42 found empirically in Ref. 7. In (5.14) we treated the quantity $\exp(\frac{1}{4}u^2)\,\phi_0'(u)$, which occurs in (5.12) for $n = 0$, cf. (I.2.9c), as a quantity of order unity. For very high $N^{1/6}$ this function should be treated as of order u, and there will be crossover to an exponent $-\frac{1}{2} - \frac{1}{6}\alpha = \frac{7}{12}$ for $\alpha = \frac{1}{2}$.

For the density at the wall $n^M(0)$ we obtain from (3.2) and (5.10b) for $\alpha = \frac{1}{2}$

$$n_N^M(0) - n^M(0) = O(N^{-1/4}) \tag{5.15}$$

The agreement with the empirical exponent 0.18 is not as good as in the other cases. This may be due to the fact that the range of N values in Ref. 7 is not large enough to determine small exponents with sufficient precision. This guess is supported by the observation that an extrapolation of the data of Ref. 7 with the exponent 1/4 yields a value $n^M(0) = 0.951$, which is much closer to the value $n^M(0) = 0.942 \pm 0.008$ found in I than the value 0.914 found in Ref. 7 from a fit with freely varying exponent.[3]

[3] Also, this value, together with the value $\langle u^2\rangle(0) = 1.535$ found by extrapolation with exponent $-1/4$, fulfills the consistency relation $n(0)\langle u^2\rangle(0) = x_M$ better than the extapolations with freely varying exponent, yielding a value 1.460 rather than 1.453 for the left-hand side (the value for x_M found in Ref. 7 is 1.461).

To conclude this section we observe that the asymptotic analysis given in this paper may be used in two ways to improve and simplify variational calculations of the type performed in Ref. 7 and generalizations of them.[14,15] First one may replace integral expressions such as (3.4a) and (3.4b) in Ref. 7 by their asymptotic expressions for large values of their indices, and thereby increase the number of terms in trial functions such as (5.1) at a much lower cost in calculational effort. Secondly one may perform the extrapolations to $N = \infty$ using analytically determined exponents, as we just did for $n^M(0)$, thus reducing the number of parameters in the fitting procedure. Alternatively, one might determine the exponent of the leading corrections to expressions of type (5.3) and thus try and fit to a more accurate asymptotic expression.

6. CONCLUDING REMARKS

The asymptotic analysis of the Pagani coefficients as presented in this paper yields a good approximation for the density profile $n^M(x)$ for the Milne solution. Moreover it allows one to determine the analytic character of $P^M(-u)$ near $u = 0$ and of $n^M(x)$ near $x = 0$. Finally it explains the extrapolation exponents of the variationally determined quantities in Ref. 7, and it resolves the discrepancy in the values on $n^M(0)$ between I and Ref. 7.

The infinite derivative of $n^M(x)$ at $x = 0$ predicted in Ref. 9a is also found in our work; the convergence rate of D_N^2 found in Ref. 7 can be used as an additional argument to exclude the possibility $P^M(-u) \sim a_0 u^{1/2+3k}$ with $k \neq 0$, left open in Section 4. The derivative of $n^M(x)$ diverges like $x^{-1/2}$, rather than $x^{-2/3}$ as suggested in Ref. 9a. We note in this connection that the exact solution of the Milne problem for the one-speed neutron transport equation also shows an infinite derivative. However, in that case the divergence is only logarithmic.[16]

In principle the same techniques can be used for the Milne problem in the presence of an external field and for the Laplace transform of the time-dependent Milne problem, both discussed in Ref. 15. With straightforward modifications they can be used to supplement the analysis of the albedo problem, treated in I, and of the Milne problem for an incompletely absorbing wall, discussed in Ref. 14 and in Section 6 of I. In particular the analytic properties of the velocity distribution at the wall $P^f(u, 0)$ and the density profile $n^f(x)$ for the albedo problem are of the same type as for the Milne problem when the prescribed distribution of injected particles $P(u, 0)\,\Theta(u) = f(u)$ vanishes in an interval including $u = 0$, or increases at most linearly for small u. However, asymptotic series do not provide arbitrarily close approximations of the exact results; whether or not they provide useful information must be checked for each case separately.

To avoid misunderstanding we should perhaps emphasize once more that the techniques developed in this paper do not yield a new method to solve the Milne problem. Rather, they yield constraints on the form of the solution $P^M(-u)$ for small u and, moreover, provide a practical way to determine the full solution $P^M(u, x)$ and its integral, the density profile $n^M(x)$, from a given $P^M(u, 0)$. The latter may be an *ad hoc* ansatz or a numerical or variational solution. If the input is a numerical solution, the analytical details of the density profile will depend on the particular parametrization chosen to represent the numerical data. However, as is clear from Table II, the overall shape of $n^M(x)$ turns out to be surprisingly insensitive to the choice of parametrization.

From a theoretical point of view the parametrization (4.6) is clearly the peferable one. However, as long as we have only a few terms in the asymptotic series for $d_{\sigma n}[f]$ available, this method of parametrization remains impracticable, since the $g_k(u)$ cannot be determined to arbitrary order. Once the full asymptotic series for $d_{\sigma n}[f]$ is available, which would require a full asymptotic series to replace the asymptotic approximation (2.3a), the expansion (4.6a) would provide the starting point for a new way to solve the Milne problem: the parametrization assures that $P^M(-u)$ is orthogonal to the $\phi_{-n}(u)$ asymptotically for high n, and the coefficients a_k could be determined by requiring orthogonality to $\phi_{-n}(u)$ for a few low values of n (and normalization to unit current). The basic soundness of this approach is assured by the results of Beals and Protopopescu[(8)]; whether it is quicker in practice than the methods used in Refs. 2 and 7 remains to be seen.

After the submission of the present paper I received a preprint from Dr. Y. S. Mayya, in which he develops asymptotic techniques similar to those in the present paper, and obtains the same result for the shape of $n(x)$ near the boundary. Dr. Mayya further pointed out to me that a complete asymptotic expansion for the $d_{\sigma n}[f]$ could be constructed using the formula in Exercise 11.7.2 of Ref. 10.

ACKNOWLEDGMENT

It is a pleasure to thank Professor Eberhard Stark for a helpful discussion and for guidance through the mathematical literature, and Jonathan Selinger for computing the expansion coefficients given in Table I(a). I am also grateful to Dr. Y. S. Mayya for a helpful correspondence and for pointing out a calculational error in an earlier version of this paper.

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