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Asymptotic behaviour of rigid-rotor partition functions

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Abstract. The Euler–Maclaurin and Poisson summation formulae are used to derive an asymptotic expansion for the function

$$\Psi(a,\sigma) \equiv \sum_{n=0}^{\infty}(n+a)\exp[-(n+a)^2\sigma]$$

in powers of σ, where $0 \leqslant a < 1$. An exact formula for the remainder terms in this expansion is established. The theory of theta functions and the terminant method developed by Dingle are also applied to the problem. Finally, the results are used to investigate the high-temperature behaviour of the rigid-rotor partition functions which arise in statistical mechanics.

1. Introduction

It is well known (Fowler 1936, Mayer and Mayer 1977, Wilson 1960) that the canonical partition functions

$$Z(\sigma) = \sum_{n=0}^{\infty}(2n+1)\exp[-n(n+1)\sigma] \tag{1.1}$$

$$Z_+(\sigma) = \sum_{n=0}^{\infty}(4n+1)\exp[-2n(2n+1)\sigma] \tag{1.2}$$

$$Z_-(\sigma) = \sum_{n=0}^{\infty}(4n+3)\exp[-2(n+1)(2n+1)\sigma] \tag{1.3}$$

play a crucial rôle in the theoretical investigation of the rotational contribution to the thermodynamic properties of an ideal diatomic gas. In this application the parameter σ can be written in the form

$$\sigma = \Theta/T \tag{1.4}$$

where Θ is a characteristic temperature which is associated with the rotational motion of the molecule and T is the thermodynamic temperature. The partition functions $Z_+(\sigma)$ and $Z_-(\sigma)$ are obtained from (1.1) by performing the summation over even and odd values of n respectively. We see, therefore, that the partition functions satisfy the simple relation

$$Z(\sigma) = Z_+(\sigma) + Z_-(\sigma)\,. \tag{1.5}$$

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The series in (1.1)–(1.3) clearly converge very rapidly for $\sigma \geqslant 1$, and they provide one with accurate low-temperature representations for $Z(\sigma)$, $Z_+(\sigma)$ and $Z_-(\sigma)$. However, as σ approaches zero the series become more slowly convergent and alternative procedures must be used to analyse the high-temperature behaviour of the partition functions. Mulholland (1928) used a contour integral method to derive asymptotic expansions for $Z(\sigma)$, $Z_+(\sigma)$ and $Z_-(\sigma)$ in powers of σ. From these expansions it was found that the asymptotic equalities

$$Z_+(\sigma) \sim Z_-(\sigma) \sim \tfrac{1}{2}Z(\sigma) \tag{1.6}$$

are valid to *all* orders in σ. Mulholland made the following comment on this interesting result.

The partition functions as $\sigma \to 0$ no doubt actually differ by terms of the type $(1/\sigma)^\mu \exp(-\alpha/\sigma)$ (α, μ constant), but this the analysis does not suffice to show. These exponentially small differences between the odd and even terms are no doubt associated with the fact that the forms of these Z series are closely related to the ϑ-functions.

In the present paper we shall use the general Euler–Maclaurin summation formula to analyse the detailed structure of the remainder terms in the Mulholland asymptotic expansions for the rotational partition functions. The Poisson summation formula, the theory of theta functions and the asymptotic methods of Dingle (1973) will also be used to investigate the problem.

2. Application of the Euler–Maclaurin summation formula

We begin the analysis by defining the function

$$\Psi(a,\sigma) \equiv \sum_{n=0}^{\infty}(n+a)\exp[-(n+a)^2\sigma] \tag{2.1}$$

where $0 \leqslant a < 1$. It is possible to express the partition functions (1.1)–(1.3) in terms of $\Psi(a,\sigma)$ using the relations

$$Z(\sigma) = 2\exp(\tfrac{1}{4}\sigma)\Psi(\tfrac{1}{2},\sigma) \tag{2.2}$$

$$Z_+(\sigma) = 4\exp(\tfrac{1}{4}\sigma)\Psi(\tfrac{1}{4},4\sigma) \tag{2.3}$$

$$Z_-(\sigma) = 4\exp(\tfrac{1}{4}\sigma)\Psi(\tfrac{3}{4},4\sigma)\,. \tag{2.4}$$

Next we consider the general Euler–Maclaurin summation formula (Steffensen 1950)

$$\sum_{n=0}^{\infty} f(n+a) = \int_0^\infty f(x)\,\mathrm{d}x - \sum_{k=1}^{m}\frac{B_k(a)}{k!}f^{(k-1)}(0) + \mathcal{R}_m(a) \tag{2.5}$$

where $0 \leqslant a < 1$ and $B_k(a)$ denotes a Bernoulli polynomial of order k. The remainder term in (2.5) is given by

$$\mathcal{R}_m(a) = -\frac{1}{m!}\int_0^\infty \overline{B}_m(a-x)f^{(m)}(x)\,\mathrm{d}x \tag{2.6}$$

where

$$\overline{B}_m(x) = B_m(x - [x]) \tag{2.7}$$

is the periodic Bernoulli function of order m, and $[x]$ is the largest integer which is less than or equal to x.

We now apply (2.5) to the summation (2.1) with

$$f(x) = x \exp(-\sigma x^2) = -(2\sigma)^{-1} \mathrm{D}[\exp(-\sigma x^2)] \tag{2.8}$$

where $\mathrm{D} \equiv \mathrm{d}/\mathrm{d}x$. For this particular case we find that

$$f^{(m)}(x) = \tfrac{1}{2}(-1)^m \sigma^{(m-1)/2} \exp(-\sigma x^2) H_{m+1}(\sigma^{1/2} x) \tag{2.9}$$

$$f^{(2r-1)}(0) = \tfrac{1}{2}[(2r)!/r!](-\sigma)^{r-1} \tag{2.10}$$

$$f^{(2r-2)}(0) = 0 \tag{2.11}$$

where $H_n(z)$ denotes the Hermite polynomial of order n and $r = 1, 2, \ldots$. Hence we obtain

$$\Psi(a, \sigma) = \frac{1}{2\sigma}\left(1 + \sum_{r=1}^{p} \frac{B_{2r}(a)}{r!}(-\sigma)^r + \mathcal{E}_p(a, \sigma)\right) \tag{2.12}$$

where

$$\mathcal{E}_p(a, \sigma) = -\frac{\sigma^{(2p+1)/2}}{(2p)!} \int_0^\infty \overline{B}_{2p}(a - x) \exp(-\sigma x^2)\, H_{2p+1}(\sigma^{1/2} x)\, \mathrm{d}x \tag{2.13}$$

and $p = 1, 2, \ldots$.

The structure of the remainder term $\mathcal{E}_p(a, \sigma)$ in (2.12) can be analysed by substituting the standard Fourier series (Rademacher 1973)

$$\overline{B}_{2p}(x) = (-1)^{p-1} 2(2p)! \sum_{k=1}^{\infty} \frac{\cos(2\pi k x)}{(2\pi k)^{2p}} \tag{2.14}$$

in (2.13). In this manner we find that

$$\mathcal{E}_p(a, \sigma) = 2(-\sigma)^p \left[\sum_{k=1}^{\infty} \frac{\cos(2\pi k a)}{(2\pi k)^{2p}} \mathrm{Jc}(p, \pi k \sigma^{-1/2}) + \sum_{k=1}^{\infty} \frac{\sin(2\pi k a)}{(2\pi k)^{2p}} \mathrm{Js}(p, \pi k \sigma^{-1/2})\right] \tag{2.15}$$

where

$$\mathrm{Jc}(p, \omega) = \int_0^\infty \cos(2\omega y) \exp(-y^2)\, H_{2p+1}(y)\, \mathrm{d}y \tag{2.16}$$

$$\mathrm{Js}(p, \omega) = \int_0^\infty \sin(2\omega y) \exp(-y^2)\, H_{2p+1}(y)\, \mathrm{d}y\,. \tag{2.17}$$

In order to evaluate the integral (2.16) we expand the cosine factor as a Taylor series in powers of ω and then integrate term-by-term using the formula (Gradshteyn and Ryzhik 1980, p 838)

$$\int_0^\infty y^{2n}\exp(-y^2)\,H_{2p+1}(y)\,\mathrm{d}y = (-1)^p\,2^{2p}(\tfrac{3}{2})_p\,n!\,{}_2F_1(-p,n+1;\tfrac{3}{2};1) \tag{2.18}$$

where $(\frac{3}{2})_p$ denotes a Pochhammer symbol. After applying the result

$${}_2F_1(-p,n+1;\tfrac{3}{2};1) = (\tfrac{1}{2}-n)_p/(\tfrac{3}{2})_p \tag{2.19}$$

we obtain

$$\mathrm{Jc}(p,\omega) = (-1)^p\,2^{2p}\,(\tfrac{1}{2})_p\sum_{n=0}^{\infty}\frac{(-\omega^2)^n}{(-p+\frac{1}{2})_n} \tag{2.20}$$

where $|\omega| < \infty$. It is possible to express (2.20) in the confluent hypergeometric form

$$\mathrm{Jc}(p,\omega) = (-1)^p\,2^{2p}\,(\tfrac{1}{2})_p\;{}_1F_1(1;-p+\tfrac{1}{2};-\omega^2)\,. \tag{2.21}$$

We can also evaluate the integral (2.17) by following a similar procedure. The final result is (Gradshteyn and Ryzhik 1980, p 840)

$$\mathrm{Js}(p,\omega) = (-1)^p\,2^{2p}\,\pi^{1/2}\,\omega^{2p+1}\exp(-\omega^2)\,. \tag{2.22}$$

We now make the substitution $a = \frac{1}{2}$ in (2.12) and (2.15) and apply the relations (2.2) and (2.21). This procedure yields the basic formula

$$Z(\sigma) = \sigma^{-1}\exp(\tfrac{1}{4}\sigma)\left[1+\sum_{r=1}^{p}c_r\sigma^r+\mathcal{E}_p(\tfrac{1}{2},\sigma)\right] \tag{2.23}$$

where

$$c_r = (-1)^r(2^{1-2r}-1)\,B_{2r}/r! \tag{2.24}$$

$$\mathcal{E}_p(\tfrac{1}{2},\sigma) = 2\left(\frac{\sigma}{\pi^2}\right)^p(\tfrac{1}{2})_p\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{2p}}\;{}_1F_1(1;-p+\tfrac{1}{2};-\pi^2k^2/\sigma) \tag{2.25}$$

and B_{2r} denotes the Bernoulli number of order $2r$. The result (2.24) is in agreement with the work of Mulholland (1928), while the expression (2.25) gives a new *exact* representation for the remainder in the Mulholland asymptotic expansion for $Z(\sigma)$.

If we make the substitutions $a = \frac{1}{4}$ and $a = \frac{3}{4}$ in (2.12) and (2.15) and apply the relations (2.3), (2.4), (2.21) and (2.22) it is found that

$$Z_\pm(\sigma) = (2\sigma)^{-1}\exp(\tfrac{1}{4}\sigma)\left(1+\sum_{r=1}^{p}c_r\sigma^r+\mathcal{E}_p(\tfrac{1}{2},\sigma)\pm\mathcal{F}(\sigma)\right) \tag{2.26}$$

where

$$\mathcal{F}(\sigma) = (\pi^3/\sigma)^{1/2}\sum_{m=1}^{\infty}(-1)^{m-1}(2m-1)\exp[-\pi^2(2m-1)^2/(4\sigma)]\,. \tag{2.27}$$

We see from (2.26) that the asymptotic expansion for $Z_\pm(\sigma)$ has an additional remainder term $\pm\mathcal{F}(\sigma)$ which is *independent* of the value of p. It should also be noted that the structure of the formula (2.27) for $\mathcal{F}(\sigma)$ is consistent with the Mulholland conjecture quoted in the introduction of the present paper. A comparison of (2.23) with (2.26) yields the further relation

$$Z_\pm(\sigma) = \tfrac{1}{2}[Z(\sigma)\pm\sigma^{-1}\exp(\tfrac{1}{4}\sigma)\mathcal{F}(\sigma)]\,. \tag{2.28}$$

3. Alternative methods

In this section we shall describe several other methods which can be used to derive the basic results (2.23), (2.26) and (2.28).

3.1. Poisson summation formula

We begin by applying the Poisson summation formula (Bellman 1961, Apostol 1974)

$$\sum_{n=-\infty}^{\infty} f(n+a) = \sum_{k=-\infty}^{\infty} \exp(2\pi i k a) \int_{-\infty}^{\infty} f(x) \exp(-2\pi i k x)\,dx \tag{3.1}$$

to the continuous function

$$f(x) = \begin{cases} x\exp(-\sigma x^2) & \text{for } x \geqslant 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{3.2}$$

where $0 \leqslant a < 1$. In this manner we find that

$$\Psi(a,\sigma) = (2\sigma)^{-1}\Bigg[1 + 2\sum_{k=1}^{\infty} \cos(2\pi k a) \int_0^{\infty} \cos(2\omega y) \exp(-y^2) H_1(y)\,dy \\ + 2\sum_{k=1}^{\infty} \sin(2\pi k a) \int_0^{\infty} \sin(2\omega y) \exp(-y^2) H_1(y)\,dy\Bigg] \tag{3.3}$$

where $\omega = \pi k \sigma^{-1/2}$. Next the integrals in (3.3) are evaluated using (2.16), (2.17), (2.21) and (2.22). Hence we obtain

$$\Psi(a,\sigma) = (2\sigma)^{-1}\Bigg[1 + 2\sum_{k=1}^{\infty} \cos(2\pi k a)\, {}_1F_1(1; \tfrac{1}{2}; -\pi^2 k^2/\sigma) \\ + 2(\pi^3/\sigma)^{1/2} \sum_{k=1}^{\infty} k \sin(2\pi k a) \exp(-\pi^2 k^2/\sigma)\Bigg]. \tag{3.4}$$

The confluent hypergeometric function in (3.4) can be expressed in the alternative form

$${}_1F_1(1; \tfrac{1}{2}; -\omega^2) = 1 - 2\omega \mathcal{D}(\omega) \tag{3.5}$$

where

$$\mathcal{D}(\omega) = \exp(-\omega^2) \int_0^{\omega} \exp(x^2)\,dx \tag{3.6}$$

is the Dawson integral (Gautschi 1965).

We now use the hypergeometric identity

$${}_1F_1(1; -m + \tfrac{3}{2}; -\omega^2) = (m - \tfrac{1}{2})\,\omega^{-2}\left[-1 + {}_1F_1(1; -m + \tfrac{1}{2}; -\omega^2)\right] \tag{3.7}$$

with $m = 1, 2, \ldots, p$ to establish the relation

$$ {}_1F_1(1; \tfrac{1}{2}; -\omega^2) = -\sum_{r=1}^{p} (\tfrac{1}{2})_r \, \omega^{-2r} + (\tfrac{1}{2})_p \, \omega^{-2p} \, {}_1F_1(1; -p + \tfrac{1}{2}; -\omega^2) . \tag{3.8} $$

The substitution of this result in (3.4), with $a = \frac{1}{2}$ and $\omega^2 = \pi^2 k^2/\sigma$, yields

$$ Z(\sigma) = \sigma^{-1} \exp(\tfrac{1}{4}\sigma) \left(1 + 2 \sum_{r=1}^{p} (\tfrac{1}{2})_r \, \eta(2r)(\sigma/\pi^2)^r + \mathcal{E}_p(\tfrac{1}{2}, \sigma) \right) \tag{3.9} $$

where

$$ \eta(2r) = \sum_{k=1}^{\infty} (-1)^{k-1} k^{-2r} \tag{3.10} $$

and $\mathcal{E}_p(\frac{1}{2}, \sigma)$ is defined in (2.25). If the standard formula

$$ \eta(2r) = (-1)^r (2^{1-2r} - 1)\,(2\pi)^{2r} B_{2r} / [2(2r)!] \tag{3.11} $$

is applied to (3.9) we obtain the expected asymptotic expansion (2.23) for $Z(\sigma)$. In a similar manner we can also derive the basic expansion (2.26) by substituting $a = \frac{1}{4}$ and $a = \frac{3}{4}$ in (3.4).

3.2. Connection with theta functions

We follow the theta function notation of Whittaker and Watson (1927) and write

$$ \vartheta_1(z|\tau) = 2q^{1/4} \sum_{n=0}^{\infty} (-1)^n q^{n(n+1)} \sin(2n+1)z \tag{3.12} $$

where

$$ q = \exp(\pi i \tau) \tag{3.13} $$

and $\mathrm{Im}(\tau) > 0$. From this definition we see that

$$ \vartheta_1'(0|\tau) = 2q^{1/4} \sum_{n=0}^{\infty} (-1)^n (2n+1) q^{n(n+1)} \tag{3.14} $$

where $\vartheta_1'(z|\tau)$ denotes the derivative of $\vartheta_1(z|\tau)$ with respect to the variable z.

A comparison of (3.14) with (1.1)–(1.3) gives the relation

$$ Z_+(\sigma) - Z_-(\sigma) = \tfrac{1}{2} \exp(\tfrac{1}{4}\sigma) \vartheta_1'(0 \mid i\sigma/\pi) . \tag{3.15} $$

It is also clear from (1.5) that

$$ Z_\pm(\sigma) = \tfrac{1}{2}[Z(\sigma) \pm \tfrac{1}{2} \exp(\tfrac{1}{4}\sigma) \vartheta_1'(0 \mid i\sigma/\pi)] . \tag{3.16} $$

We can now use the Jacobi imaginary transformation (Whittaker and Watson 1927)

$$ + (-i\tau)^{1/2} \vartheta_1'(0 \mid \tau) = i\tau^{-1} \vartheta_1'(0 \mid -\tau^{-1}) \tag{3.17} $$

to express (3.16) in the alternative form

$$ Z_\pm(\sigma) = \tfrac{1}{2}[Z(\sigma) \pm \tfrac{1}{2}(\pi/\sigma)^{3/2} \exp(\tfrac{1}{4}\sigma)\, \vartheta_1'(0 \mid i\pi/\sigma)] . \tag{3.18} $$

If the series (3.14) is substituted in this result we obtain (2.28) with

$$ \mathcal{F}(\sigma) = \tfrac{1}{2}(\pi^3/\sigma)^{1/2} \vartheta_1'(0 \mid i\pi/\sigma) . \tag{3.19} $$

Finally, we note that the derivative (3.14) can be written in terms of theta functions using the Jacobi identity (Whittaker and Watson 1927)

$$ \vartheta_1'(0 \mid \tau) = \vartheta_2(0 \mid \tau)\, \vartheta_3(0 \mid \tau)\, \vartheta_4(0 \mid \tau) . \tag{3.20} $$

3.3. Application of Dingle terminants

Our aim in this Subsection is to show that the remainder term $\mathcal{E}_p(\frac{1}{2},\sigma)$ in the basic formula (2.23) for $Z(\sigma)$ can be constructed *directly* from the late coefficients $\{c_{p+j}; j = 1,2,\ldots\}$. In the first stage of the analysis we *formally* define the termination of the asymptotic series in (2.23) as

$$\mathcal{T}_p(\sigma) \equiv \sum_{r=p+1}^{\infty} c_r \sigma^r . \tag{3.21}$$

We now use (3.9) to write (3.21) in the expanded form

$$\mathcal{T}_p(\sigma) = 2\sum_{k=1}^{\infty}(-1)^{k-1} Q_{p+1}(\pi^2k^2/\sigma) \tag{3.22}$$

where

$$Q_n(x) = \sum_{r=n}^{\infty} (\tfrac{1}{2})_r x^{-r} . \tag{3.23}$$

Next we give a meaningful interpretation of the series (3.23) by following a general procedure developed by Dingle (1973). In this manner we find that

$$Q_n(x) = (\tfrac{1}{2})_n x^{-n} \bar{\Lambda}_{n-\frac{1}{2}}(-x) \tag{3.24}$$

where $\bar{\Lambda}_{n-\frac{1}{2}}(-x)$ denotes one of Dingle's basic terminants. The application of (3.24) to (3.22) yields

$$\mathcal{T}_p(\sigma) = (2p+1)(\tfrac{1}{2})_p(\sigma/\pi^2)^{p+1} \sum_{k=1}^{\infty}(-1)^{k-1} k^{-2p-2} \bar{\Lambda}_{p+\frac{1}{2}}(-\pi^2k^2/\sigma) . \tag{3.25}$$

It can also be shown from the work of Dingle (1973, p 416) that

$$\bar{\Lambda}_{p+\frac{1}{2}}(-x) = -2x(2p+1)^{-1} {}_1F_1(1; -p+\tfrac{1}{2}; -x) . \tag{3.26}$$

If this result is substituted in (3.25) we find that $\mathcal{T}_p(\sigma)$ is equal to the remainder term $\mathcal{E}_p(\frac{1}{2},\sigma)$ which is defined in (2.25). We see, therefore, that the Dingle interpretative procedure leads to the *exact* termination of the truncated asymptotic series for $Z(\sigma)$. For the case of the partition functions $Z_\pm(\sigma)$, it is clear from (2.26) that the Dingle analysis of the late terms will only give an improved asymptotic *approximation* because of the presence of the additional terms $\pm\mathcal{F}(\sigma)$.

4. Application and concluding remarks

If we have a gas consisting of N molecules of parahydrogen then it can be shown (Fowler 1936) that the rotational contribution to the heat capacity of the gas is

$$C_+ = Nk_B\sigma^2 \frac{d^2}{d\sigma^2} \ln Z_+(\sigma) \tag{4.1}$$

while for a similar gas of orthohydrogen we have the rotational heat capacity

$$C_- = Nk_B\sigma^2 \frac{d^2}{d\sigma^2} \ln Z_-(\sigma) \tag{4.2}$$

where k_B is the Boltzmann constant. Normal hydrogen gas is a 3:1 metastable mixture of orthohydrogen and parahydrogen respectively and has, therefore, a rotational heat capacity

$$C_n = \tfrac{1}{4}C_+ + \tfrac{3}{4}C_- . \tag{4.3}$$

The application of the formula (2.26), *without* the remainder terms, to (4.1) and (4.2) leads to the asymptotic expansion

$$C_\pm/(Nk_B) \sim C_n/(Nk_B) \sim 1 + (\tfrac{1}{45})\sigma^2 + (\tfrac{16}{945})\sigma^3 + (\tfrac{59}{4\,725})\sigma^4 + (\tfrac{928}{93\,555})\sigma^5 + (\tfrac{1\,101\,578}{127\,702\,575})\sigma^6 + O(\sigma^7) \tag{4.4}$$

as $\sigma \to 0$. We can investigate the asymptotic behaviour of the *differences* between C_+, C_- and C_n by using the complete relation (2.28). In this manner, we obtain the new result

$$\begin{aligned}(C_+ - C_-)/(Nk_B) = 4(C_n - C_-)/(Nk_B) \sim \tfrac{1}{8}(\pi^{11}/\sigma^5)^{1/2} \exp[-\pi^2/(4\sigma)] \\ \times [1 - (\pi^{-2}/12)(144 + \pi^2)\sigma + (\pi^{-4}/1\,440)(17\,280 + 480\pi^2 - 11\pi^4)\sigma^2 \\ + (\pi^{-4}/120\,960)(40\,320 - 3\,696\pi^2 - 241\pi^4)\sigma^3 \\ - (\pi^{-4}/29\,030\,400)(2\,661\,120 + 694\,080\pi^2 + 22\,651\pi^4)\sigma^4 + O(\sigma^5)]\end{aligned} \tag{4.5}$$

as $\sigma \to 0$. The formula (4.5) also has, *to leading order*, a remainder term of the type $\gamma\sigma^{-7/2} \exp[-3\pi^2/(4\sigma)]$, where γ is a constant.

Finally, we substitute $a = 0$ in (2.12) in order to obtain the further asymptotic expansion

$$\sum_{n=0}^{\infty} n \exp(-n^2\sigma) = \frac{1}{2\sigma}\left(1 + \sum_{r=1}^{p} \frac{B_{2r}}{r!}(-\sigma)^r + \mathcal{E}_p(0,\sigma)\right) \tag{4.6}$$

where

$$\mathcal{E}_p(0,\sigma) = 2\left(\frac{\sigma}{\pi^2}\right)^p (\tfrac{1}{2})_p \sum_{k=1}^{\infty} \frac{1}{k^{2p}}\, {}_1F_1(1; -p + \tfrac{1}{2}; -\pi^2k^2/\sigma) . \tag{4.7}$$

The result (4.6), without the remainder term $\mathcal{E}_p(0,\sigma)$, has also been obtained by Sutherland (1930) and Cahn and Wolf (1976). It should be noted, however, that in *both* these papers the signs of the coefficients in the asymptotic expansion (4.6) are given incorrectly.

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