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Accurate approximate equations for intensive sub-sonic evaporation

John W. Rose*

Department of Engineering, Queen Mary and Westfield College, University of London, London, UK

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Abstract

The paper describes an approximate solution of the problem of intensive evaporation of a monatomic substance at a plane surface and with condensation coefficient equal to unity. The result is in the form of a set of algebraic equations which may readily be solved and is in excellent agreement with recent numerical solutions. © 2000 Elsevier Science Ltd. All rights reserved.

1. Introduction

During evaporation or condensation of a pure substance, there are, in general, differences between the temperatures, pressures and specific Gibbs functions on either side of the liquid–vapour interface. More accurately, these differences occur across the so-called Knudsen layer which divides the liquid–vapour interface from the region in the vapour where the continuum equations hold. The study of this problem, by the methods of molecular kinetic theory, dates back more than 100 years. For monatomic molecules, a notable early contribution was made by Schrage [1] followed by related approaches such as those of Ytrehus [2] and Labuntsov and Kryukov [3]. These studies, which use assumptions for the form of the velocity distribution function of the molecules in the Knudsen layer, lead to algebraic results. Most recently, numerical solutions of the Boltzmann–Krook–Welander approximation of the Boltzmann equation have been obtained by Sone and co-workers [4]. Reviews have been given recently by Ytrehus [5] and Rose [6].

The problem of interphase matter transfer is complicated by uncertainty regarding the value of the so-called condensation coefficient, σ, defined as the fraction of those molecules incident on the liquid surface which remain in the liquid phase. Over the years there has been, and remains, controversy over this quantity. The term "reflection", when viewed in detail as is done in molecular dynamics approaches, is not clear — a vapour molecule entering the interface region (which is not in reality a simple plane surface) may return to the vapour phase after one or more interactions with "surface molecules". Experiments in the past have been interpreted, on the basis of various theories, as indicating values of σ ranging from 1 to 0.003. Measurements for condensation of metals, e.g. [7], suggest that values near unity are probably appropriate for use in molecular kinetic theory approaches but this remains an area of debate. Results of approximate solutions with $\sigma < 1$, which require additional assumptions, show strong effect of σ [8].

The present paper reports a modification of the early approach of Schrage for $\sigma = 1$ which gives algebraic results virtually identical to the numerical sol-

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* Tel.: +171-975-5275; fax: +181-983-1007.
E-mail address: j.w.rose@qmw.ac.uk (J.W. Rose).

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Nomenclature

B	disposable parameter, see Eqs. (9b), (13), (18)
c	molecule speed, see Eq. (4)
F	defined in Eq. (16)
f_s	velocity distribution function, see Eq. (5)
f_b	velocity distribution function for bulk vapour, see Eq. (7)
f_0	velocity distribution function for vapour adjacent to surface
G	defined in Eq. (17)
m	net interphase mass flux outward from surface
$\tilde{m}$	mass of molecule
n_b	molecule density of bulk vapour
n_s	molecule density for saturated vapour at temperature T_s
P_b	pressure of bulk vapour
P_s	saturation pressure at temperature T_s
R	specific ideal-gas constant
T_b	temperature of bulk vapour
T_s	temperature of surface
U_b	velocity of bulk vapour, directed away from surface
u	velocity component measured outward from surface
v	velocity component parallel to surface
w	velocity component parallel to surface
Γ_1	defined in Eq. (22)
Γ_2	defined in Eq. (23)
Γ_3	defined in Eq. (24)
Γ_4	defined in Eq. (25)
Γ_5	defined in Eq. (26)
β_b	parameter defined in Eq. (8)
β_s	parameter defined in Eq. (6)
ρ_b	density of bulk vapour
σ	condensation coefficient
ϕ_b	dimensionless bulk vapour velocity away from surface, see Eq. (12)

utions. This suggests that the assumed form of the velocity distribution function for molecules adjacent to the surface is very accurate or, at any rate, consistent with that found from solutions of the Boltzmann–Krook–Welander equation, and could prove useful in providing starting or limiting results in new approaches using values of σ less than unity and perhaps for the case of polyatomic molecules and mixtures.

2. Approximate solutions

As in [1], for monatomic molecules and with $\sigma = 1$, conservation of mass, momentum and energy across the Knudsen layer give

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{m}uf_0 \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{m}uf_b \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \rho_b U_b \tag{1}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{m}u^2 f_0 \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{m}u^2 f_b \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \frac{\rho_b}{2\beta_b^2}\left(1 + 2\phi_b^2\right) \tag{2}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\tilde{m}c^2/2\right)uf_0 \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \left(\tilde{m}c^2/2\right)uf_b \,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \frac{\rho_b\phi_b}{2\beta_b^3}\left(\frac{5}{2} + 2\phi_b^2\right) \tag{3}$$

where

$$c^2 = u^2 + v^2 + w^2 \tag{4}$$

The results given on the RHS of Eqs. (1)–(3) are readily obtained, as in [1], from the second integral in each case using Eq. (7) below.

In [1], and all other approaches, the distribution function for emitted molecules f_s is taken as the Maxwellian with the liquid (or solid) surface temperature and corresponding saturation vapour density, i.e.

$$f_s = n_s\left(\frac{\beta_s^3}{\pi^{3/2}}\right)\mathrm{e}^{-\beta_s^2\left(u^2+v^2+w^2\right)} \tag{5}$$

where n_s is the molecule density of the saturated vapour at the surface temperature T_s and

$$\beta_s = (2RT_s)^{-1/2} \tag{6}$$

For the bulk continuum vapour, f_b is taken as the Maxwellian modified to have a “drift” bulk velocity U_b, i.e.

$$f_b = n_b\left(\frac{\beta_b^3}{\pi^{3/2}}\right) e^{-\beta_b^2\left[(u-U_b)^2+v^2+w^2\right]} \tag{7}$$

where

$$\beta_b = (2RT_b)^{-1/2} \tag{8}$$

For the distribution function of vapour molecules adjacent to the liquid/solid surface f_0 Schrage, in his second theory, used

$$f_0 = f_s \quad u > 0 \tag{9a}$$

$$f_0 = (1 + Bu)f_s \quad u < 0 \tag{9b}$$

where B is an unknown. The form of Eq. (9b) was based on the work on diffusion in binary systems by Furry [9]. It is noted that the bulk vapour plays no part in the assumed distribution function for the gas at the interface.

Eqs. (1)–(3), when integrated using Eqs. (7), (9a) and (9b), lead to the simple results

$$\frac{P_s}{P_b} = 1 + 2\phi_b^2 + 4\phi_b\sqrt{\frac{1+(2/5)\phi_b^2}{\pi}} \tag{10}$$

$$\frac{T_s}{T_b} = 1 + \frac{2}{5}\phi_b^2 \tag{11}$$

where ϕ_b is a dimensionless vapour velocity or mass evaporation rate given by

$$\phi_b = (m/\rho_b)(2RT_b)^{-1/2} = U_b(2RT_b)^{-1/2} \tag{12}$$

As noted by Rose [6], Eqs. (10) and (11) differ significantly from the more recent solutions and give unsatisfactory results when applied to the case of condensation.

Ytrehus [2] and Labuntsov and Kryukov [3] independently gave solutions in which Eq. (9b) was replaced by

$$f_0 = Bf_b \quad u < 0 \tag{13}$$

The involvement of f_b in the distribution function for the vapour molecules adjacent to the surface somewhat complicates the analysis, but when the integrals in the conservation equations are evaluated, the resulting equations may be solved explicitly for the temperature and pressure ratios, giving

$$\left(\frac{T_b}{T_s}\right)^{1/2} = \frac{-\sqrt{\pi}}{8}\phi_b + \left(1 + \frac{\pi}{64}\phi_b^2\right)^{1/2} \tag{14}$$

$$\frac{P_s}{P_b} = 2\,e^{-\phi_b^2}\left[F + G\left(\frac{T_b}{T_s}\right)^{1/2}\right]^{-1} \tag{15}$$

where

$$F = e^{-\phi_b^2} - \phi_b\sqrt{\pi}\left[1 - \operatorname{erf}(\phi_b)\right] \tag{16}$$

and

$$G = \left(1 + 2\phi_b^2\right)\left[1 - \operatorname{erf}(\phi_b)\right] - \frac{2}{\sqrt{\pi}}\phi_b\,e^{-\phi_b^2} \tag{17}$$

Eqs. (14) and (15) are in much closer accord with the numerical solutions.

Here, rather than Eq. (13), we use a modified form of Eq. (9b) for the distribution function for the interface gas molecules moving towards the surface

$$f_0 = (1 + Bu)f_b \quad u < 0 \tag{18}$$

that is, we replace f_s in Schrage's expression by f_b. This complicates the analysis considerably but leads (see Appendix A) to the algebraic results

$$\frac{P_s}{P_b}\left(\frac{T_b}{T_s}\right)^{1/2} = 2\sqrt{\pi}\phi_b + \Gamma_1 - \frac{1}{2}B\sqrt{2RT_b}\Gamma_2 \tag{19}$$

$$\frac{P_s}{P_b} = 2\left(1 + 2\phi_b^2\right) - \frac{\Gamma_2}{\sqrt{\pi}} + 2B\sqrt{2RT_b}\Gamma_3 \tag{20}$$

$$\frac{P_s}{P_b}\left(\frac{T_s}{T_b}\right)^{1/2} = \sqrt{\pi}\phi_b\left(\frac{5}{2} + \phi_b^2\right) + \Gamma_4 - \frac{1}{4}B\sqrt{2RT_b}\Gamma_5 \tag{21}$$

where Γ_1, Γ_2, Γ_3, Γ_4, Γ_5 are all functions of ϕ_b only, given by

$$\Gamma_1 = e^{-\phi_b^2} - \phi_b\sqrt{\pi}\left[1 - \operatorname{erf}(\phi_b)\right] \tag{22}$$

$$\Gamma_2 = \sqrt{\pi}\left(1 + 2\phi_b^2\right)\left[1 - \operatorname{erf}(\phi_b)\right] - 2\phi_b\,e^{-\phi_b^2} \tag{23}$$

$$\Gamma_3 = \frac{\phi_b^2\,e^{-\phi_b^2}}{\sqrt{\pi}} + \frac{e^{-\phi_b^2}}{\sqrt{\pi}} - \phi_b\left(\frac{3}{2} + \phi_b^2\right)\left[1 - \operatorname{erf}(\phi_b)\right] \tag{24}$$

$$\Gamma_4 = e^{-\phi_b^2} + \frac{\phi_b^2\,e^{-\phi_b^2}}{2} - \frac{\sqrt{\pi}\phi_b}{2}\left(\frac{5}{2} + \phi_b^2\right)\left[1 - \operatorname{erf}(\phi_b)\right] \tag{25}$$

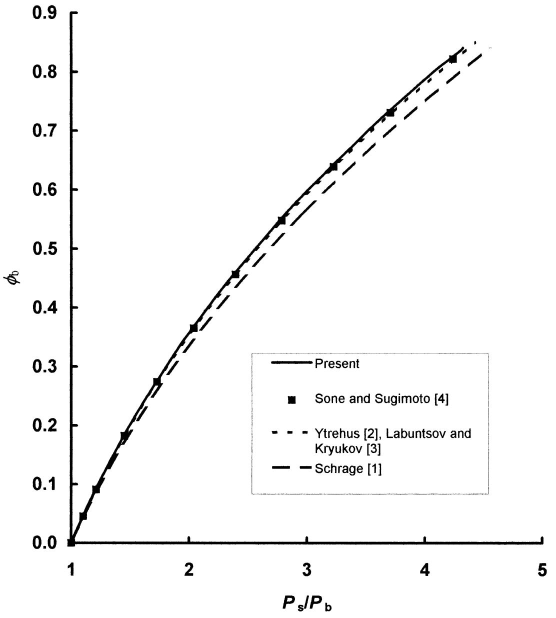

Fig. 1. Comparison of solutions: ϕ_b vs. P_s/P_b.

$$\Gamma_5 = -2\phi_b^3 e^{-\phi_b^2} - 7\phi_b e^{-\phi_b^2} + \sqrt{\pi}\left(\frac{5}{2} + 8\phi_b^2 + 2\phi_b^4\right)\left[1 - \mathrm{erf}(\phi_b)\right] \qquad (26)$$

Eqs. (19)–(21), which result from the conservation equations when the integrals are evaluated, involve four unknowns (ϕ_b, P_s/P_b, T_s/T_b, $B(2RT_b)^{1/2}$) so that any one of these can, in principle, be expressed in terms of any other. For example, explicit (albeit lengthy) algebraic expressions may be obtained for the temperature and pressure ratios in terms of ϕ_b by eliminating $B(2RT_b)^{1/2}$ from two pairs of the equations and eliminating either temperature or pressure ratio from the two resulting equations.

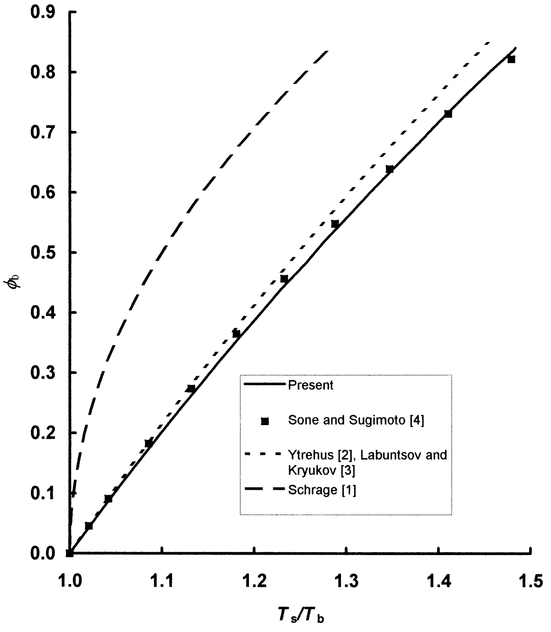

Fig. 2. Comparison of solutions: ϕ_b vs. T_s/T_b.

Figs. 1 and 2 compare the results found using this procedure with the approximate solutions of Schrage [1], Ytrehus [2] and Labuntsov and Kryukov [3] and with the numerical solutions of Sone and Sugimoto [4]. In Fig. 1, showing the dependence of ϕ_b on pressure ratio, it may be seen that the Schrage [1] values differ somewhat from the numerical solutions, while the later results are in close agreement. For the dependence of ϕ_b on temperature ratio (Fig. 2), the Schrage [1] values differ quite widely from the numerical results, while those of Ytyrehus [2] and Labuntsov and Kryukov [3] differ slightly. The values obtained from Eqs. (19)–(21) are again very close to the numerical solutions.

3. Concluding remarks

The approximate results reported here are virtually co-incident with numerical solutions of the Boltzmann–Krook–Welander equation for evaporation of a monatomic substance and with condensation coefficient equal to unity. This suggests that Eq. (18) gives a very close approximation to the velocity distribution function for inward moving vapour molecules adjacent to the surface. Such an approximation could prove useful in studies of polyatomic substances, mixtures or with condensation coefficient less than unity. It is also interesting to note that different, somewhat simpler, assumed distribution functions [1,2,3] do not give widely different results.

Previous investigators have noted that the theories show that the bulk vapour is generally supersaturated (metastable). It has also been pointed out that the approximate methods give (invalid) results for bulk gas Mach numbers exceeding unity ($\phi_b > 0.913$).

Condensation results may be obtained, as in [1], by using negative values of ϕ_b in the approximate solutions. On physical as well as theoretical grounds, one would expect that for condensation, the bulk vapour pressure and temperature might be specified independently for a given value of the surface temperature. Modified approximate approaches for condensation have been given by Labuntsov and Kryukov [3] and Ytrehus and Alvestad [10]. These, and numerical solutions of Aoki and Sone [11], show that for condensation, ϕ_b depends on both pressure and temperature ratios. The results of Aoki

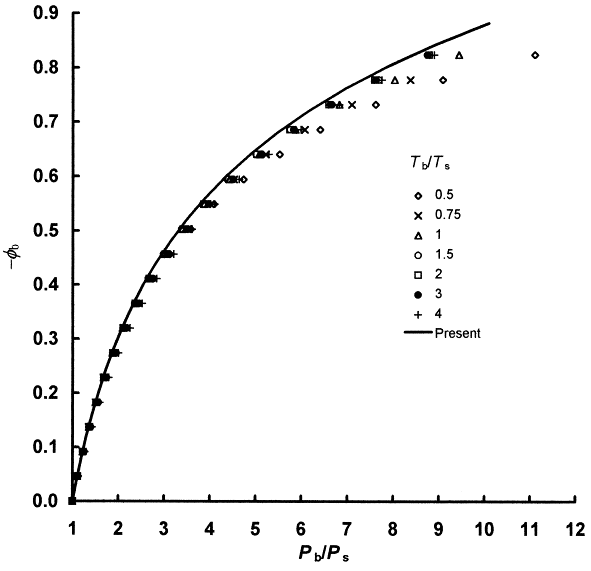

Fig. 3. Solutions of Aoki and Sone [11] for condensation.

and Sone [11] are shown in Fig. 3. It may be seen that the dependence on temperature ratio is weak except at high values of $-\phi_{\mathrm{b}}$ (approaching sonic bulk vapour velocity) and when $T_{\mathrm{b}}/T_{\mathrm{s}} \leq 1$, when the bulk vapour is supersaturated (metastable). The results are otherwise close to those given by Eqs. (19)–(21) where the corresponding values of $T_{\mathrm{b}}/T_{\mathrm{s}}$ (quoted in [6]) vary along the line from 1 at $-\phi_{\mathrm{b}} = 0$ to around 1.5 at $-\phi_{\mathrm{b}} = 0.9$.

Appendix A

A1. Conservation of mass

With Eqs. (9a) and (18), the LHS of Eq. (1) may be written as

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\tilde{m}u)f_{\mathrm{s}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}(\tilde{m}u) \times (1+Bu)f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A1)}$$

Now

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\tilde{m}uf_{\mathrm{s}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \frac{\rho_{\mathrm{s}}}{2\beta_{\mathrm{s}}\sqrt{\pi}} \qquad \text{(A2)}$$

and

$$\begin{aligned}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}(\tilde{m}u)(1+Bu)f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}(\tilde{m}u)f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \\ &\quad + B\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}(\tilde{m}u^2)f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A3)}\end{aligned}$$

Evaluating the terms of the RHS of Eq. (A3) separately

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\tilde{m}uf_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = -\frac{\rho_{\mathrm{b}}}{2\beta_{\mathrm{b}}\sqrt{\pi}}\Gamma_1 \qquad \text{(A4)}$$

where

$$\Gamma_1 = \mathrm{e}^{-\phi_{\mathrm{b}}^2} - \phi_{\mathrm{b}}\sqrt{\pi}\left[1 - \mathrm{erf}(\phi_{\mathrm{b}})\right] \qquad \text{(A5)}$$

$$B\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}\tilde{m}u^2f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \frac{B\rho_{\mathrm{b}}}{4\sqrt{\pi}\beta_{\mathrm{b}}^2}\Gamma_2 \qquad \text{(A6)}$$

where

$$\Gamma_2 = \sqrt{\pi}\left(1 + 2\phi_{\mathrm{b}}^2\right)\left[1 - \mathrm{erf}(\phi_{\mathrm{b}})\right] - 2\phi_{\mathrm{b}}\,\mathrm{e}^{-\phi_{\mathrm{b}}^2} \qquad \text{(A7)}$$

So

$$\rho_{\mathrm{b}}u_{\mathrm{b}} = \frac{\rho_{\mathrm{s}}}{2\sqrt{\pi}\beta_{\mathrm{s}}} - \frac{\rho_{\mathrm{b}}}{2\sqrt{\pi}\beta_{\mathrm{b}}}\Gamma_1 + \frac{B\rho_{\mathrm{b}}}{4\sqrt{\pi}\beta_{\mathrm{b}}^2}\Gamma_2 \qquad \text{(A8)}$$

Substitution of the definitions of β_{s} and β_{b} (Eqs. (6) and (8)) and using the ideal gas equation for ρ_{s} and ρ_{b} yields Eq. (19).

A2. Conservation of momentum

With Eqs. (9a) and (18), the LHS of Eq. (2) may be written as

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}(\tilde{m}u^2)f_{\mathrm{s}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}(\tilde{m}u^2)(1+Bu)f_{\mathrm{b}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A9)}$$

Evaluating the integrals separately

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\tilde{m}u^2f_{\mathrm{s}}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w = \frac{\rho_{\mathrm{s}}}{4\beta_{\mathrm{s}}^2} \qquad \text{(A10)}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}\tilde{m}u^2(1+Bu)f_\mathrm{b}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w$$

$$=\frac{\rho_\mathrm{b}}{4\sqrt{\pi}\beta_\mathrm{b}^2}\Gamma_2+\frac{B\rho_\mathrm{b}\beta_\mathrm{b}}{\sqrt{\pi}}\int_{-\infty}^{0}u^3\,\mathrm{e}^{-\beta_\mathrm{b}^2(u-U_\mathrm{b})^2}\,\mathrm{d}u \qquad \text{(A11)}$$

and

$$\frac{B\rho_\mathrm{b}\beta_\mathrm{b}}{\sqrt{\pi}}\int_{-\infty}^{0}u^3\,\mathrm{e}^{-\beta_\mathrm{b}^2(u-U_\mathrm{b})^2}\,\mathrm{d}u=-\frac{B\rho_\mathrm{b}}{2\beta_\mathrm{b}^3}\Gamma_3 \qquad \text{(A12)}$$

where

$$\Gamma_3=\frac{\phi_\mathrm{b}^2\,\mathrm{e}^{-\phi_\mathrm{b}^2}}{\sqrt{\pi}}+\frac{\mathrm{e}^{-\phi_\mathrm{b}^2}}{\sqrt{\pi}}-\phi_\mathrm{b}\left(\frac{3}{2}+\phi_\mathrm{b}^2\right)\left[1-\mathrm{erf}\left(\phi_\mathrm{b}\right)\right] \qquad \text{(A13)}$$

so

$$\frac{\rho_\mathrm{s}}{4\beta_\mathrm{s}^2}+\frac{\rho_\mathrm{b}}{4\sqrt{\pi}\beta_\mathrm{b}^2}\Gamma_2-\frac{B\rho_\mathrm{b}}{2\beta_\mathrm{b}^3}\Gamma_3=\frac{\rho_\mathrm{b}}{2\beta_\mathrm{b}^2}\left(1+2\phi_\mathrm{b}^2\right) \qquad \text{(A14)}$$

and substitution for β_s, β_b, ρ_s and ρ_b yields Eq. (20).

A3. Conservation of energy

With Eqs. (9a) and (18), the LHS of Eq. (3) may be written as

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\left(\frac{1}{2}\tilde{m}c^2\right)uf_\mathrm{s}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}\left(\frac{1}{2}\tilde{m}c^2\right)u(1+Bu)f_\mathrm{b}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A15)}$$

which may be expressed as

$$I_1+I_2+I_3 \qquad \text{(A16)}$$

where

$$I_1=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty}\frac{1}{2}\tilde{m}\left(u^2+v^2+w^2\right)uf_\mathrm{s}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w=\frac{\rho_\mathrm{s}}{2\sqrt{\pi}\beta_\mathrm{s}^3} \qquad \text{(A17)}$$

$$I_2=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}\left(\frac{1}{2}\tilde{m}c^2\right)uf_\mathrm{b}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A18)}$$

$$I_3=B\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}\left(\frac{1}{2}\tilde{m}c^2\right)u^2f_\mathrm{b}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A19)}$$

After integration and some manipulation, I_2 may be written as

$$I_2=-\frac{\rho_\mathrm{b}}{2\sqrt{\pi}\beta_\mathrm{b}^3}\Gamma_4 \qquad \text{(A20)}$$

where

$$\Gamma_4=\mathrm{e}^{-\phi_\mathrm{b}^2}+\frac{\phi_\mathrm{b}^2\,\mathrm{e}^{-\phi_\mathrm{b}^2}}{2}-\frac{\sqrt{\pi}\phi_\mathrm{b}}{2}\left(\frac{5}{2}+\phi_\mathrm{b}^2\right)\left[1-\mathrm{erf}\left(\phi_\mathrm{b}\right)\right] \qquad \text{(A21)}$$

and

$$I_3=\frac{B\rho_\mathrm{b}}{2\pi^{3/2}}\beta_\mathrm{b}^3\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}u^2\left(u^2+v^2+w^2\right)\mathrm{e}^{-\beta_\mathrm{b}\left[(u-U_\mathrm{b})^2+v^2+w^2\right]}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w \qquad \text{(A22)}$$

and

$$\begin{aligned}&\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}u^2\left(u^2+v^2+w^2\right)\mathrm{e}^{-\beta_\mathrm{b}^2\left[(u-U_\mathrm{b})^2+v^2+w^2\right]}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\\&=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}u^4\,\mathrm{e}^{-\beta_\mathrm{b}^2\left[(u-U_\mathrm{b})^2+v^2+w^2\right]}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\\&\quad+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}u^2v^2\,\mathrm{e}^{-\beta_\mathrm{b}^2\left[(u-U_\mathrm{b})^2+v^2+w^2\right]}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\\&\quad+\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{0}u^2w^2\,\mathrm{e}^{-\beta_\mathrm{b}^2\left[(u-U_\mathrm{b})^2+v^2+w^2\right]}\,\mathrm{d}u\,\mathrm{d}v\,\mathrm{d}w\end{aligned} \qquad \text{(A23)}$$

Denoting the three integrals on the RHS of Eq. (A23) by $I_{3(1)}$, $I_{3(2)}$, and $I_{3(3)}$, respectively, it is found that after integration and some manipulation

$$I_{3(1)}=\frac{\pi}{4\beta_\mathrm{b}^2}\left\{-2\phi_\mathrm{b}^3\,\mathrm{e}^{-\phi_\mathrm{b}^2}-5\phi_\mathrm{b}\,\mathrm{e}^{-\phi_\mathrm{b}^2}+\sqrt{\pi}\left(\frac{3}{2}+6\phi_\mathrm{b}^2+2\phi_\mathrm{b}^4\right)\left[1-\mathrm{erf}\left(\phi_\mathrm{b}\right)\right]\right\} \qquad \text{(A24)}$$

$$I_{3(2)}=I_{3(3)}=\frac{\pi}{8\beta_\mathrm{b}^7}\left\{-2\phi_\mathrm{b}\,\mathrm{e}^{-\phi_\mathrm{b}^2}+5\sqrt{\pi}\left(1+2\phi_\mathrm{b}^2\right)\times\left[1-\mathrm{erf}\left(\phi_\mathrm{b}\right)\right]\right\} \qquad \text{(A25)}$$

So

$$I_3=\frac{B\rho_\mathrm{b}}{2\pi^{3/2}}\beta_\mathrm{b}^3\left(I_{3(1)}+I_{3(2)}+I_{3(3)}\right)=\frac{B\rho_\mathrm{b}}{8\sqrt{\pi}\beta_\mathrm{b}^4}\Gamma_5 \qquad \text{(A26)}$$

where

$$\Gamma_5 = -2\phi_b^3 \, e^{-\phi_b^2} - 7\phi_b \, e^{-\phi_b^2} + \sqrt{\pi}\left(\frac{5}{2} + 8\phi_b^2 + 2\phi_b^4\right)\left[1 - \operatorname{erf}(\phi_b)\right] \tag{A27}$$

Eq. (3) then becomes

$$\frac{\rho_s}{2\sqrt{\pi}\beta_s^3} - \frac{\rho_b \Gamma_4}{2\sqrt{\pi}\beta_b^3} + \frac{B\rho_b}{8\sqrt{\pi}\beta_b^4}\Gamma_5 = \frac{\rho_b\phi_b}{2\beta_b^3}\left(\frac{5}{2} + \phi_b^2\right) \tag{A28}$$

and substitution for β_s, β_b, ρ_s and ρ_b yields Eq. (21).

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