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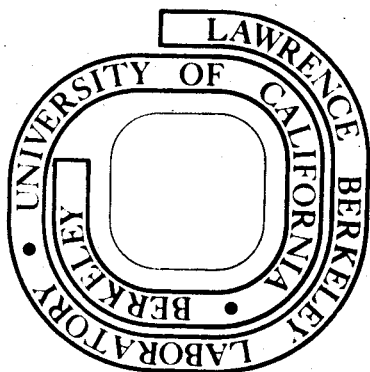
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ON THE DILUTE GAS TWO PARTICLE DENSITY
MATRICES OF p-H₂ AND He⁴

RUNNING TITLE: TWO PARTICLE DENSITY MATRICES

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ABSTRACT

In an earlier publication we demonstrated that the reduced two particle density matrix of simple quantum liquids could profitably be re-expressed in terms of a Taylor expansion of its logarithm about the diagonal. In the present publication we examine the Taylor coefficients which arise when the dilute gas two particle density matrix is expanded in this way. In particular, we evaluate the leading coefficients of p-H₂ and He⁴ exactly and extend the Wigner-Kirkwood approximation to provide approximate expressions for them. We demonstrate how these approximate expressions may be applied to yield results superior to those yielded by the ordinary Wigner-Kirkwood approximation. In an appendix we demonstrate how the Block equation for the dilute gas two particle density matrix may be reduced to an equivalent closed set of equations for the leading Taylor coefficients.

I. INTRODUCTION

In another publication¹ (henceforth referred to as I) we examined the functional form and symmetries of the reduced two particle density matrix in simple quantum liquids. In the limit of the dilute gas, this form is simplified by the fact that the density matrix clearly factors into center of mass and relative coordinate dependent portions. The center of mass factor is simply the density matrix of a free particle of mass $2m$. From the results of I we determine that the relative coordinate dependent portion may be written as

$$\begin{aligned} \rho(\tilde{\mathbf{r}}, \tilde{\mathbf{r}}'; \beta) &= \rho(\tilde{\mathbf{y}}, \tilde{\mathbf{z}}; \beta) & (1.1) \\ &= A \exp [f_0(\tilde{\mathbf{y}}; \beta) + {}^2\tilde{f}(\tilde{\mathbf{y}}; \beta) \textcircled{2} \tilde{z}^2 + {}^4\tilde{f}(\tilde{\mathbf{y}}; \beta) \textcircled{4} \tilde{z}^4 + \dots] \end{aligned}$$

where

$$\beta = (k_B T)^{-1}$$

$$\tilde{\mathbf{y}} \equiv \frac{1}{2}(\tilde{\mathbf{r}} + \tilde{\mathbf{r}}')$$

$$\tilde{\mathbf{z}} \equiv \frac{1}{2}(\tilde{\mathbf{r}} - \tilde{\mathbf{r}}')$$

and A is a normalization factor which is most conveniently chosen so that $f_0 \rightarrow 0$ as $|\tilde{\mathbf{y}}| \rightarrow \infty$. With this convention, f_0 is simply the logarithm of the ordinary radial distribution function g . ${}^2\tilde{f}$ and ${}^4\tilde{f}$ are cartesian tensors of second and fourth rank which are composed of the Taylor coefficients of second and fourth order of the expansion of $\log g$ about $\tilde{\mathbf{z}}=0$. The physical significance of these tensors has been discussed in I. ${}^2\tilde{f}$ has two independent elements and ${}^4\tilde{f}$, three. Setting $\tilde{\mathbf{y}} = \tilde{y}\hat{\mathbf{y}}$, we find these elements to be

$$k_{||} = \frac{1}{2} \frac{\partial^2}{\partial z_1^2} \log \rho$$

$$k_{\perp} = \frac{1}{2} \frac{\partial^2}{\partial z_2^2} \log \rho = \frac{1}{2} \frac{\partial^2}{\partial z_3^2} \log \rho$$

$$h_1 = \frac{1}{24} \frac{\partial^4}{\partial z_1^4} \log \rho$$

$$h_2 = \frac{1}{24} \frac{\partial^4}{\partial z_2^4} \log \rho = \frac{1}{24} \frac{\partial^4}{\partial z_3^4} \log \rho = \frac{1}{8} \frac{\partial^4}{\partial z_2^2 \partial z_3^2} \log \rho$$

$$h_3 = \frac{1}{24} \frac{\partial^4}{\partial z_1^2 \partial z_2^2} \log \rho = \frac{1}{24} \frac{\partial^4}{\partial z_1^2 \partial z_3^2} \log \rho$$

where z_1 , z_2 and z_3 are the components of \tilde{z} .

II. THE EXACT CALCULATION

We evaluate these functions exactly by simply differentiating the sum over states expression for the density matrix in respect to $\tilde{V}_{\tilde{z}} = \tilde{V}_{\tilde{r}} - \tilde{V}_{\tilde{r}'}$. Slightly modifying and extending the derivation of Pohl and Miller², we write the sum over states for the case of para-hydrogen as

$$\rho(\tilde{r}, \tilde{r}' ; \beta) = \frac{\lambda_T^3 \sqrt{2}}{\pi} \sum_{l=0}^{\infty} (2l+1) \int_0^{\infty} \psi_{\kappa l}(\mathbf{r}) \psi_{\kappa l}(\mathbf{r}') P_l(\alpha) \exp\left(-\frac{\kappa^2 \lambda_T^2}{2\pi}\right) d\kappa + \frac{\lambda_T^3}{\pi \sqrt{2}} \sum_{l=0}^{\infty} (2l+1) \psi_l^b(\mathbf{r}) \psi_l^b(\mathbf{r}') P_l(\alpha) \exp(-\beta E_l^b) \quad (2.1)$$

where $\mathbf{r} \equiv |\tilde{\mathbf{r}}|$, $\mathbf{r}' \equiv |\tilde{\mathbf{r}}'|$
 $\alpha \equiv \frac{\tilde{\mathbf{r}} \cdot \tilde{\mathbf{r}}'}{r r'}$

$$\lambda_T \equiv h(2\pi m k_B T)^{-\frac{1}{2}}$$

$$\beta \equiv (k_B T)^{-1}$$

and P_l is the Legendre polynomial of order l . The first term is a sum over continuum states. The continuum state radial wavefunctions ψ_{kl} are defined to be normalized in such a way that in the limit of large r

$$\psi_{kl}(r) = \kappa [j_l(\kappa r) \cos \eta_l(\kappa) + y_l(\kappa r) \sin \eta_l(\kappa)]$$

where j_l and y_l are the spherical Bessel functions of order l , and $\eta_l(\kappa)$ is the phase shift. The second term is the sum over bound states and is written in the form proper for p-H₂, which has only two bound states, one for $l=0$ and one for $l=1$. The bound state radial wavefunctions are normalized in such a way that

$$\int_0^{\infty} r^2 [\psi_l^b(r)]^2 dr = 1$$

The E_l^b are the bound state energy eigenvalues. He⁴ has no bound states, and the second term is to be ignored. (2.1) is correct for distinguishable particles. If the particles are indistinguishable, (2.1) must be multiplied by two, and the summation restricted to odd or even values of l , according to whether the particles obey Fermi or Bose statistics. Setting $\tilde{r}' = \tilde{r}$ in (2.1) makes the Legendre polynomials equal to one and yields an expression for the radial distribution function.

We employed the usual Lennard-Jones potential

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right]$$

The use of this spherically symmetrical potential for p-H₂ is justified by the fact that nearly all of the molecules are in the rigorously spherically symmetrical rotational ground state at the low temperatures with which we deal in this paper. The values of ϵ

and σ which we employed for the two gases are presented in Table 1.

We will not describe the calculation except for mentioning that we used the Taylor expansion algorithm³ and that in no case did our calculated values for the radial distribution function (rdf) differ from the published p-H₂ values of Poll and Miller² or the He⁴ values of Larsen, Witte and Kilpatrick⁴ by more than one percent. Calculating the rdf's from the values of the various tensor elements by means of certain equations which will be described further on indicated that the inconsistency between the various calculated functions is also no more than about 1%.

$$E_0^b = - 0.0990\epsilon$$

$$E_1^b = - 0.0387\epsilon$$

which differ by a few tenths of a percent from the values given by Poll and Miller.

A major reason for undertaking these calculations was to provide the necessary input data for the liquid state calculations in I.

III. THE APPROXIMATE EXPRESSIONS

We begin our derivation by following that of ter Haar and Boyd, Larsen and Kilpatrick⁵. First we formally expand the logarithm of the density matrix in powers of β :

$$\rho(\tilde{r}, \tilde{r}', \beta) \equiv \left(\frac{\mu}{2\pi\hbar^2\beta}\right)^{\frac{3}{2}} \exp\left[-\frac{\mu}{2\hbar^2\beta} |\tilde{r}-\tilde{r}'|^2 + \sum_{m=1}^{\infty} a_m(\tilde{r}, \tilde{r}')\beta^m\right] \quad (3.1)$$

where μ is the reduced mass and equal to $\frac{m}{2}$.

If all the a_m are set to zero, we obtain an exact expression for the corresponding ideal gas density matrix. Thus the power series in β is simply a formal expansion of the effect of a non-zero potential upon the logarithm of the density matrix.

Inserting (3.1) into the appropriate Bloch equation⁶ and separating powers of β yields a coupled hierarchy of equations which may be solved sequentially. We solve the first two equations to obtain a_1 and a_2 . Changing variables from \tilde{r}, \tilde{r}' to \tilde{y}, \tilde{z} we obtain

$$a_1(\tilde{y}, \tilde{z}) = \sum_{n=0}^{\infty} (-1)^{n+1} A_n \tilde{V}_y^n V(y) \textcircled{n} \tilde{z}^n \quad (3.2)$$

$$a_2(\tilde{y}, \tilde{z}) = \sum_{n=0}^{\infty} (-1)^{n+1} \frac{\hbar^2}{2\mu} B_n \tilde{V}_y^n L(y) \textcircled{n} \tilde{z}^n$$

where

$$L \equiv \nabla^2 V$$

$$A_n \equiv \sum_{p=0}^n \frac{(-2)^p}{(n-p)! (p+1)!}$$

$$B_n \equiv \sum_{p=0}^n \frac{(-2)^p (p+1)}{(n-p)! (p+3)!}$$

These coefficients vanish for all odd values of n and, as anticipated, only even powers of \tilde{z} appear. Inserting the expressions (3.2) into (3.1) and replacing β wherever it appears by $(t-t')/i\hbar$ yields an expression for the corresponding quantum mechanical propagator which is correct up to and including terms in the square of the time difference $t-t'$.⁷ We wish to emphasize that our results up to this point are generally applicable to any system which does

not involve velocity dependent forces. One need only insert the proper variables and potential function.

We do not bother to solve for a_3 , as this function is non-linear in the potential and, thereby, rather difficult to work with.

At this point we change notation to so-called "reduced" or "dimensionless" variables. From now on we express all energies in units of ϵ , all lengths in units of σ and masses in units of m . In this system of units (which is specific to each gas individually) Planck's constant is replaced by

$$\Lambda = \frac{\hbar}{\sigma\sqrt{2\mu\epsilon}}$$

the so-called DeBoer wavelength. In these units the second order approximate expressions for the first three tensors are

$$f_0 = -tV - t^2 \frac{\Lambda^2}{6} L + o(t^3, \Lambda^2) \quad (3.3a)$$

$$2_{\tilde{f}}^{\approx} = -\frac{2_{\tilde{\delta}}^{\approx}}{\Lambda^2 t} - \frac{t}{6} \nabla^2 V - \frac{t^2 \Lambda^2}{60} \nabla^2 L + 2_{\tilde{o}}^{\approx}(t^3, \Lambda^2) \quad (3.3b)$$

$$4_{\tilde{f}}^{\approx} = -\frac{t}{120} \nabla^4 V - \frac{t^2 \Lambda^2}{1680} \nabla^4 L + 4_{\tilde{o}}^{\approx}(t^3, \Lambda^2) \quad (3.3c)$$

where $t \equiv \epsilon\beta$ and $2_{\tilde{\delta}}^{\approx}$ is the second rank tensor identity. We note that expressions good to t^2 for all higher $n_{\tilde{f}}$ tensors may also be extracted from (3.2). We also note that these expressions do not contain all terms proportional to Λ^2 . Traditionally, the derivation of the Wigner-Kirkwood approximation ends with a regrouping of terms by powers of Λ and a clean truncation with some power of Λ . This

strikes us as an arbitrary procedure and, therefore, we choose to accept (3.3) as the final form for our results. This decision saves us the trouble of deriving and dealing with terms which are non-linear in the potential. (More on this in Section 6.)

IV. THE RESULTS FOR p-H₂

We have calculated these results under the assumptions of both Bose and Fermi statistics. However, the magnitude of the statistical effects is insignificantly small for $T > 5^\circ\text{K}$ and, therefore, we present only the results (correctly) calculated under the assumption of Bose statistics.

Instead of presenting the actual values of the elements of $2 \approx f$, we converted them into functions with the dimension of temperature which are defined by

$$\Delta T_{\parallel \text{ or } \perp} = - \left(\frac{\epsilon}{k_B} \right) \Lambda^2 k_{\parallel \text{ or } \perp} - T$$

where T is the thermodynamic temperature. These functions vanish in the classical limit and are thus indicative of the magnitude of the quantum effects. We leave the elements of $4 \approx f$ in the natural unit σ^{-4} (i.e., in reduced form). They also vanish in the classical limit.

We present these results for 10 and 40°K in Tables 2 and 3. It is seen that only g is strongly temperature dependent. The various tensor elements, and especially ΔT_{\parallel} and h_1 , are seen to be only weakly temperature dependent.

In Table 3 we also present values of the various tensor

elements calculated from (3.3b and c). As it turned out, discarding the terms in t^2 from these expressions yielded significantly better results than including them, and, therefore, we present the tensor elements evaluated from (3.3b and c) with the quadratic terms struck out. The improvement resulting from striking out the t^2 terms underlines the dubious convergence of the Wigner-Kirkwood approximation. Such dubious convergence is only to be expected since, as we have seen, ΔT_{\parallel} , ΔT_{\perp} and the elements of $f^{\approx 4}$ are only weakly temperature dependent. This, of course, is excellent grounds for doubting the validity of any approximate expressions for them which are of the form of expansions in powers of β . Still, we see that the approximate values in Table 3 are quite good, although they rapidly worsen with decreasing temperature.

V. THE CALCULATED RESULTS FOR He⁴

We present these results for 1 and 2°K in Tables 4 and 5, calculated under both the assumption of Bose statistics and the assumption of Fermi statistics. At 2°K the effects of statistics are evident, but small. At and above 5°K they are insignificant. ΔT_{\parallel} and h_1 are only weakly influenced by the assumption of either sort of statistics. As in the case of p-H₂, only the rdf is strongly temperature dependent and ΔT_{\parallel} and h_1 are only very weakly temperature dependent.

In I we noted that we have employed dilute gas He⁴ tensors

which were slightly in error. The results presented here have, however, been corrected.

VI. A POSSIBLE USE FOR THE APPROXIMATE EXPRESSIONS

In I we derived equations which relate f_0 , f_2 and f_4 of the reduced equilibrium two particle density matrix of a simple quantum liquid. Setting the density equal to zero in these equations gives an exact set of equations which relate f_0 and the independent elements of f_2 and f_4 of the dilute gas two particle density matrix. (We sketch an alternate derivation of these equations in the Appendix.) In terms of reduced variables these equations are

$$K_{||} + \frac{2}{y}(K_{||} - K_{\perp}) + f_0 K_{||} + \frac{1}{2}V = 0 \tag{6.1a}$$

$$\frac{1}{2}G_1 + f_0 h_1 - \frac{1}{24}V^2 + K_{||} K_{||} = 0 \tag{6.1b}$$

$$\begin{aligned} \frac{3}{2}G_2 + f_0 h_3 - \frac{1}{8}V^2 \left(\frac{V}{y} - \frac{V}{y^2} \right) + K_{||} K_{\perp} \\ + 2 \frac{K_{\perp}}{y} (K_{||} - K_{\perp}) = 0 \end{aligned} \tag{6.1c}$$

where

$$\begin{aligned} K_{||} &\equiv - \frac{\hbar^2}{4\mu\epsilon} k_{||} \\ K_{\perp} &\equiv - \frac{\hbar^2}{4\mu\epsilon} k_{\perp} \\ G_1 &\equiv h_1 + \frac{2h_1}{y} - \frac{6h_3}{y} \\ G_2 &\equiv h_3 - \frac{4}{3} \frac{h_2}{y} + \frac{4h_3}{y} \end{aligned}$$

In the classical limit and the limit $y \rightarrow \infty$

$$K_{\parallel} = K_{\perp} = \frac{1}{2t} = \frac{k_B T}{2\epsilon}$$

Using (3.3c) to provide approximate values of h_1 , h_2 and h_3 , we can integrate these equations to obtain f_0 (and, hence, g), K_{\parallel} and K_{\perp} . Alternatively, we can use (3.3b) to provide approximate values of K_{\parallel} and K_{\perp} , and integrate (6.1a) alone to obtain f_0 . These options are, respectively, analogous to the "three equation" and "one equation" approaches of I. We also have the option of employing (3.3b) and (3.3c) either with the t^2 terms excluded or included. We may label these options as "one term" and "two term", respectively. Therefore, we have a total of four possible options. The relative quality of the calculated rdf's yielded by each of these options when applied to p-H₂ is roughly

3 eq., 1 term > 3 eq., 2 term > 1 eq. 2 term > 1 eq., 1-term

In order to be consistent with the approximate values presented in Section 4, we present only the one-term results, both one equation and three equation. These calculated rdf's are presented for p-H₂ at 40°K in the Figure and compared with exactly calculated values. It is evident that the three equation approach gives quite good results except for the divergence at $y \approx 0.75$. This divergence is due to the fact that the Wigner-Kirkwood approximation is, after all, an expansion in the derivatives of the potential and, therefore, of dubious validity in the core region. Fortunately, this divergence is, in practice, easily dealt with by simply setting the rdf equal to zero in this region. For comparison, we also present the rdf calculated directly from the usual form of the Wigner-Kirkwood approximation:

$$\begin{aligned}
 f_0 = & -tV + \Lambda^2 \left\{ -\frac{1}{6}t^2 \left(\frac{2V^I}{y} + V^{II} \right) + \frac{t^3}{12}(V^I)^2 \right\} \\
 & + \Lambda^4 \left\{ -\frac{t^3}{60} \left[4\frac{V^{III}}{y} + V^{IV} \right] + \frac{t^4}{90} \left[(V^{II})^2 + 3V^I V^{III} + 6\frac{V^I V^{II}}{y} - 4\frac{(V^I)^2}{y^2} \right] \right. \\
 & \left. - \frac{t^5}{60}(V^I)^2 V^{II} \right\} + o(t^4, \Lambda^6) \tag{6.2}
 \end{aligned}$$

which we quote from Larsen, Witte, and Kilpatrick⁴. Although this expression is much more complicated than our expressions (3.3b and c), it yields clearly inferior results. (It may be objected that this expression is a correctly truncated expansion in powers of Λ rather than in powers of t as are (3.3b and c). However, converting it to an expansion correctly truncated in powers of t by discarding the terms in t^4 and t^5 has no significant effect on the results. This is another reason for doubting the validity of the final regrouping into powers of Λ .)

The moral of all this is that the number of terms in a Wigner-Kirkwood expansion which one chooses to employ matters much less than the level at which one chooses to approximate. Even the very simple first term of (3.3c) gives excellent results at 40°K when inserted into the three equation approach. This is because here the approximate expression (3.3c) enters the calculation of g so indirectly that its fundamental shortcomings are largely suppressed at this reasonably high temperature. (3.3b) inserted into the one equation approach effects the calculated values of g rather more directly and, therefore, the one equation approach yields noticeably worse results. Finally, (6.2) yields g completely directly and, thereby, produces the worst results.

In reality, the rdf which we calculated approximately in this section can also be, and was, calculated exactly. However, the exact calculation requires that the wavefunctions of the system be calculable. This is usually simply not the case, and, very often, the Wigner-Kirkwood approximation is all that is available in the case of more complex systems. We hope that our extension of the Wigner-Kirkwood approximation and the new way which we have developed for applying it will prove useful in the study of such complex systems.

ACKNOWLEDGEMENTS

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In deepest sorrow, I dedicate this work to the memory of Rick Abramson, who did not live to see it completed. His persistent encouragement and interest helped me enormously.

APPENDIX: SOME ADDITIONAL RELATIONS

A derivation of the Eqns.(6.1) which is analogous to the arguments of I begins by inserting the two particle density matrix written in the form (1.1) into the equilibrium equation

$$[H_2, \rho] = 0 \quad (A1)$$

However, beginning with the Bloch equation

$$H_2 \rho = - \frac{\partial}{\partial \beta} \rho \quad (A2)$$

instead gives the Eqns. (6.1) and more. Inserting the proper form of the Hamiltonian

$$\begin{aligned} H_2 &= - \frac{\hbar^2}{2\mu} \nabla_{\vec{r}}^2 + V(\vec{r}) \\ &= - \frac{\hbar^2}{8\mu} [\nabla_{\vec{y}}^2 + 2\vec{\nabla}_{\vec{y}} \cdot \vec{\nabla}_{\vec{z}} + \nabla_{\vec{z}}^2] + V(\vec{y} + \vec{z}) \end{aligned}$$

and (1.1) into (A2) results in an equation both sides of which are power expansions in \vec{z} . Separating the powers of \vec{z} we obtain a heirarchy of tensor equations, the first four of which are

$$- \frac{\hbar^2}{8\mu} [\nabla_{\vec{y}}^2 f_0(\vec{y}; \beta) + |\vec{\nabla}_{\vec{y}} f_0(\vec{y}; \beta)|^2 + 2 \delta^{2\approx} \otimes 2\approx f(\vec{y}; \beta)] \quad (A3a)$$

$$+ V(\vec{y}) = - \frac{\partial}{\partial \beta} f_0(\vec{y}; \beta)$$

$$- \frac{\hbar^2}{2\mu} [\vec{\nabla}_{\vec{y}} \cdot 2\approx f(\vec{y}; \beta) + 2\approx f(\vec{y}; \beta) \cdot \vec{\nabla}_{\vec{y}} f_0(\vec{y}; \beta)] + \vec{\nabla} V(\vec{y}) = 0 \quad (A3b)$$

$$- \frac{\hbar^2}{8\mu} [\nabla_{\vec{y}}^2 (2\approx f(\vec{y}; \beta)) + 2\vec{\nabla}_{\vec{y}} f_0(\vec{y}; \beta) \cdot \vec{\nabla}_{\vec{y}} 2\approx f(\vec{y}; \beta) + 12 \delta^{2\approx} \otimes 4\approx f(\vec{y}, \beta)$$

$$+ 4 \delta^{2\approx} f(\vec{y}; \beta) \cdot 2\approx f(\vec{y}; \beta)] + \frac{1}{2} (\vec{\nabla}_{\vec{y}})^2 V(\vec{y}) = - \frac{\partial}{\partial \beta} 2\approx f(\vec{y}; \beta) \quad (A 3c)$$

$$\begin{aligned}
 & - \frac{\hbar^2}{2\mu} [2\tilde{\nabla}_y \cdot 4\tilde{f}(\tilde{y};\beta) + 2 \cdot 4\tilde{f}(\tilde{y};\beta) \cdot \tilde{\nabla}_y f_0(\tilde{y};\beta) + 2\tilde{f}(\tilde{y};\beta) \cdot \tilde{\nabla}_y 2\tilde{f}(\tilde{y};\beta)] \\
 & + \frac{1}{6} (\tilde{\nabla}_y)^3 V(\tilde{y}) = 0 \qquad (A3d)
 \end{aligned}$$

(As they stand, these equations are, again, not restricted to the dilute gas two particle density matrix.)

We recall that f_0 , $2\tilde{f}$ and $4\tilde{f}$ have a total of six independent elements between them. It is also possible to determine (cf. Section 3 of I) that the equations (A3) also have a total of six independent elements among them. Thus we come to the happy realization that Eqns. (A3) are equivalent to a closed set of six scalar equations for six scalar unknowns.

Inserting (1.1) into (A1), on the other hand, results in a heirarchy which consists of odd rank tensor equations only. These equations are, in fact, just the odd rank members of the heirarchy (A3). Eqns. (6.1) are simply the three independent elements of Eqns. (A3 b and d). They do not, of course, constitute a closed set and it is easy to determine that no finite subset of the odd rank heirarchy alone can be closed.

Unfortunately, simultaneously integrating the six scalar equations equivalent to Eqns. (A3) is quite impractical. However, the same situation occurs in the one dimensional case, except that here the closed set consists of merely two scalar equations:

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$$\begin{aligned}
 & -\frac{\hbar^2}{8m} \left\{ \frac{\partial^2}{\partial y^2} f_0(y;\beta) + \left[\frac{\partial}{\partial y} f_0(y;\beta) \right]^2 + 2 f_2(y;\beta) \right\} + V(y) \\
 & = -\frac{\partial}{\partial \beta} f_0(y;\beta)
 \end{aligned}$$

$$-\frac{\hbar^2}{2m} \left\{ \frac{\partial}{\partial y} f_2(y;\beta) + f_2(y;\beta) \frac{\partial}{\partial y} f_0(y;\beta) \right\} + V'(y) = 0$$

(All quantities in these equations are scalars)

Integrating just these two equations does seem easier than evaluating a sum over states, especially at high temperatures. If desired, higher order f functions may be calculated from the higher order odd "rank" equations, the first of which is

$$\begin{aligned}
 & -\frac{\hbar^2}{2m} \left[2 \frac{\partial}{\partial y} f_4(y;\beta) + f_2(y;\beta) \frac{\partial}{\partial y} f_2(y;\beta) + 2 f_4(y;\beta) \frac{\partial}{\partial y} f_0(y;\beta) \right] \\
 & + \frac{1}{6} V'''(y) = 0
 \end{aligned}$$

We note that these are ordinary first order differential equations which may easily be integrated in succession.

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TABLE 1

	σ (Å)	$\frac{\epsilon}{k_B}$ (°K)	μ (g $\times 10^{-24}$)	Λ
He ⁴	2.556	10.22	3.322	0.4259
p-H ₂	2.928	37.0	1.673	0.2753

TABLE 2

p-H₂, T=10°K

y	g	T	T _⊥	h ₁	h ₂	h ₃
0.82	0.01	4.88(2)*	-6.72(1)	-1.22(3)	-6.90(1)	1.99(2)
0.9	0.17	2.51(2)	-3.10(1)	-5.27(2)	-2.82(1)	8.51(1)
1.0	1.00	1.16(2)	-1.17(1)	-2.05(2)	-9.74	3.20(1)
1.1	2.31	5.55(1)	-3.87	-8.74(1)	-3.44	1.29(1)
1.2	3.29	2.65(1)	-0.71	-4.01(1)	-1.17	5.38
1.3	3.62	1.19(1)	0.51	-1.95(1)	-0.33	2.25
1.4	3.44	4.41	0.88	-9.76	-0.03	0.89
1.5	3.03	0.56	0.90	-4.91	0.06	0.29
1.6	2.57	-1.26	0.78	-2.34	0.08	0.04
2.0	1.41	-1.35	0.23	0.18	0.02	-0.05
2.5	1.08	-0.24	0.04	0.04	-0.00	-0.01

* (n) indicates the order of magnitude; i.e., 4.88(2) = 4.88 × 10².

TABLE 3

p-H₂, T=40°K

y	g	T	T (app)	T _⊥	T _⊥ (app)
0.82	0.01	4.62(2)	3.99(3)	-5.40(1)	-2.84(2)
0.9	0.11	2.27(2)	1.01(3)	-2.27(1)	-6.67(1)
1.0	0.61	9.51(1)	1.97(2)	-7.28	-1.04(1)
1.1	1.29	3.84(1)	3.72(1)	-1.80	-0.63
1.2	1.67	1.34(1)	4.13	-0.00	0.80
1.3	1.69	2.95	-2.06	0.45	0.75
1.4	1.54	-0.73	-2.50	0.45	0.52
1.5	1.38	-1.49	-1.91	0.34	0.33
1.6	1.26	-1.29	-1.32	0.22	0.21
2.0	1.06	-0.28	-0.27	0.05	0.04

y	h ₁	h ₁ (app)	h ₂	h ₂ (app)	h ₃	h ₃ (app)
0.82	-1.22(3)	-2.35(4)	-5.84(1)	-3.40(2)	1.89(2)	1.76(3)
0.9	-5.28(2)	-5.18(3)	-2.18(1)	-7.11(1)	7.74(1)	3.81(2)
1.0	-2.04(2)	-9.17(2)	-6.46	-1.11(1)	2.67(1)	6.44(1)
1.1	-8.39(1)	-1.84(2)	-1.81	-1.67	9.27	1.18(1)
1.2	-3.50(1)	-3.96(1)	-0.41	-0.12	3.02	2.05
1.3	-1.36(1)	-8.42	-0.02	0.09	0.82	0.20
1.4	-4.48	-1.41	0.06	0.08	0.12	-0.10
1.5	-1.02	0.08	0.06	0.05	-0.05	-0.11
1.6	0.01	0.30	0.04	0.03	-0.07	-0.08
2.0	0.08	0.08	0.01	0.00	-0.01	-0.01

TABLE 4

He⁴, T=1°K

Bose (B) and Fermi (F) Statistics

y	g(B)	g(F)	ΔT_{\parallel} (B)	ΔT_{\parallel} (F)	ΔT_{\perp} (B)	ΔT_{\perp} (F)
0.82	0.03	0.02	213.19	212.84	-34.94	-30.73
0.9	0.19	0.13	111.73	111.36	-18.02	-14.60
1.0	0.70	0.48	53.70	53.34	- 8.40	- 5.71
1.1	1.37	0.95	27.52	27.18	- 4.12	- 1.99
1.2	1.94	1.38	14.77	14.47	- 2.08	- 0.37
1.3	2.31	1.69	8.16	7.91	- 1.06	0.31
1.4	2.49	1.87	4.56	4.36	- 0.53	0.58
1.5	2.53	1.95	2.52	2.37	- 0.25	0.65
1.6	2.48	1.97	1.33	1.22	- 0.10	0.63
1.7	2.38	1.94	0.62	0.55	- 0.02	0.58
1.8	2.25	1.89	0.19	0.15	0.02	0.51
2.0	1.98	1.74	-0.20	-0.21	0.06	0.37
2.2	1.74	1.59	-0.32	-0.31	0.06	0.25
2.5	1.45	1.39	-0.29	-0.28	0.04	0.13
3.0	1.18	1.17	-0.15	-0.15	0.02	0.04
3.5	1.06	1.07	-0.05	-0.06	0.01	0.01
y	h_1 (B)	h_1 (F)	h_2 (B)	h_2 (F)	h_3 (B)	h_3 (F)
0.82	-7.87(2)	-7.87(2)	-4.83(1)	-4.98(1)	1.32(2)	1.31(2)
0.9	-3.41(2)	-3.41(2)	-2.06(1)	-2.16(1)	5.72(1)	5.65(1)
1.0	-1.33(2)	-1.33(2)	-7.73	-8.38	2.23(1)	2.18(1)
1.1	-5.68(1)	-5.68(1)	-3.10	-3.54	9.46	9.13
1.2	-2.62(1)	-2.63(1)	-1.29	-1.59	4.30	4.08
1.3	-1.29(1)	-1.29(1)	-0.53	-0.76	2.06	1.90
1.4	-6.71	-6.72	-0.21	-0.37	1.03	0.91
1.5	-3.65	-3.64	-0.06	-0.19	0.52	0.44
1.6	-2.06	-2.04	0.00	-0.10	0.27	0.21
1.7	-1.19	-1.17	0.03	-0.05	0.14	0.09
1.8	-0.70	-0.68	0.03	-0.03	0.07	0.03
2.0	-0.25	-0.23	0.03	-0.01	0.01	-0.01
2.2	-0.08	-0.07	0.02	-0.00	-0.01	-0.02
2.5	0.00	0.00	0.01	0.00	-0.01	-0.01
3.0	0.01	0.01	0.00	0.00	-0.00	-0.00
3.5	0.01	0.01	-0.00	0.00	-0.00	-0.00

TABLE 5

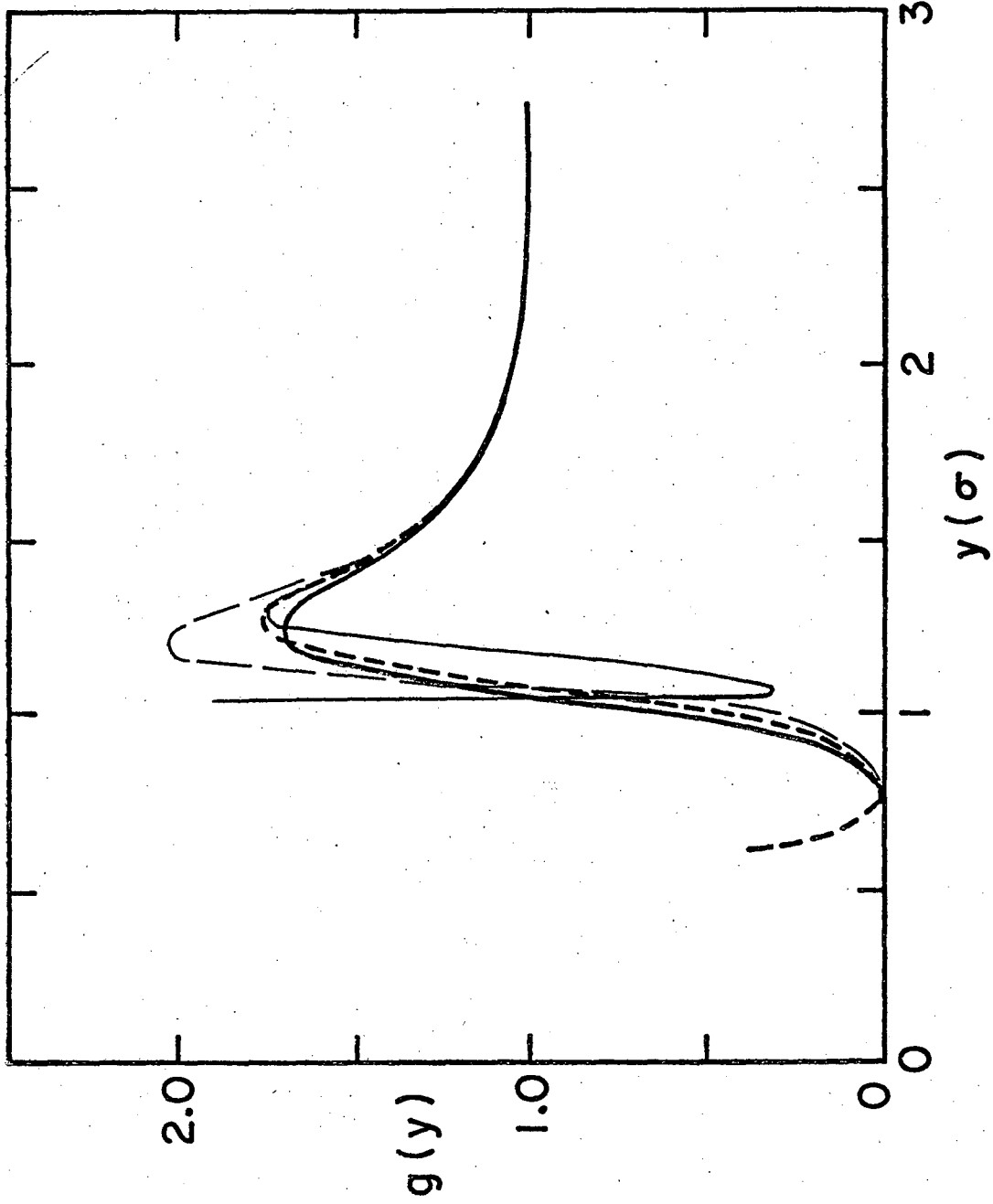
He⁴, T=2°K

Bose (B) and Fermi (F) Statistics

y	g(B)	g(F)	ΔT_{\parallel} (B)	ΔT_{\parallel} (F)	ΔT_{\perp} (B)	ΔT_{\perp} (F)
0.82	0.02	0.02	212.08	211.94	-32.85	-30.89
0.9	0.14	0.13	110.66	110.52	-16.40	-14.85
1.0	0.50	0.47	52.69	52.56	- 7.20	- 6.03
1.1	0.98	0.92	26.59	26.48	- 3.22	- 2.34
1.2	1.39	1.33	13.93	13.84	- 1.40	- 0.74
1.3	1.67	1.61	7.41	7.35	- 0.54	- 0.04
1.4	1.82	1.76	3.91	3.86	- 0.13	0.24
1.5	1.86	1.81	1.96	1.93	0.06	0.33
1.6	1.83	1.80	0.86	0.84	0.14	0.34
1.7	1.77	1.75	0.24	0.23	0.17	0.31
1.8	1.69	1.67	-0.11	-0.11	0.17	0.26
1.9	1.60	1.59	-0.29	-0.29	0.15	0.22
2.1	1.42	1.42	-0.38	-0.38	0.11	0.14
2.3	1.28	1.29	-0.33	-0.33	0.08	0.08
2.5	1.18	1.19	-0.23	-0.24	0.05	0.04
3.0	1.05	1.06	-0.07	-0.08	0.02	0.01
y	h_1 (B)	h_1 (F)	h_2 (B)	h_2 (F)	h_3 (B)	h_3 (F)
0.82	-7.87(2)	-7.87(2)	-4.58(1)	-4.87(1)	1.31(2)	1.30(2)
0.9	-3.41(2)	-3.41(2)	-1.90(1)	-2.09(1)	5.65(1)	5.62(1)
1.0	-1.33(2)	-1.33(2)	-6.74	-7.94	2.17(1)	2.16(1)
1.1	-5.68(1)	-5.68(1)	-2.49	-3.25	9.08	8.98
1.2	-2.62(1)	-2.62(1)	-0.90	-1.40	4.02	3.96
1.3	-1.28(1)	-1.28(1)	-0.29	-0.63	1.86	1.82
1.4	-6.62	-6.62	-0.06	-0.28	0.87	0.85
1.5	-3.54	-3.54	0.03	-0.12	0.41	0.39
1.6	-1.95	-1.94	0.05	-0.05	0.18	0.17
1.7	-1.08	-1.08	0.05	-0.02	0.07	0.06
1.8	-0.59	-0.59	0.04	-0.00	0.02	0.01
1.9	-0.32	-0.31	0.03	0.01	-0.00	-0.01
2.1	-0.06	-0.06	0.02	0.01	-0.02	-0.02
2.3	0.01	0.02	0.01	0.01	-0.02	-0.02
2.5	0.03	0.03	0.00	0.00	-0.01	-0.01
3.0	0.01	0.01	-0.00	0.00	-0.00	-0.00

FIGURE CAPTION

Calculated rdf's for p-H₂ at 40°K. Heavy solid line, exact. Light solid line, (6.2). Long dashes, 1 eq., 1-term. Short dashes, 3-eq., 1-term. (6.2) curve diverges explosively at $\tilde{y}=1.1$, 3-eq. curve diverges at $\tilde{y}=0.75$.



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Fig. 1

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