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Upper and Lower Bounds on Transport Coefficients Arising from a Linearized Boltzmann Equation*

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A systematic approach to the construction of upper and lower bounds for transport coefficients is presented for systems described by a linearized Boltzmann equation. The usefulness and efficacy of the bounds is tested by applying them to a particular Boltzmann equation whose solution is known. One easily calculable bound is found to differ from the exact result by less than 0.03%.

I. INTRODUCTION

The coefficients describing transport phenomena like viscosity, diffusion, and conduction of heat or electric charge are determined by a Boltzmann equation which is a linear inhomogeneous integral equation. Of course, such an equation can only be solved exactly in very special cases, and generally one has to rely on other methods in order to calculate transport coefficients from the Boltzmann equation.

It is a cherished[1] topic of transport theory that the Boltzmann equation is equivalent to a variational principle from which one can determine lower bounds on transport coefficients like electrical and thermal conductivity. That there also exist principles[2] which lead to upper bounds for the same transport coefficients is largely unknown. Recently, variational principles for a class of integral equations (which include the linearized Boltzmann equation) have been discussed by several authors.[3,4]

In this paper, we show how a variety of bounds arise from simple applications of the Schwarz inequality. By applying these bounds to a nontrivial Boltzmann equation, whose solution is known, we discuss their relative usefulness and efficacy. The particular Boltzmann equation is that of a Fermi liquid with particle-particle scattering as the relaxation mechanism. Recently,[5] the bounds have been applied to this Boltzmann equation with impurity scattering included in addition to particle-particle scattering.

In Sec. II we derive the variational principles for a class of integral equations. Section III contains the application to the calculation of transport coefficients in a Fermi liquid at very low temperature. The results are compared with exact expressions for the coefficients, which have recently[6] been obtained (Appendix C). In Appendix A, we sketch Synge's geometrically intuitive formalism of reciprocal variational principles.[7] We also discuss their significance in terms of an electrical network analogy for the Boltzmann equation. In Appendix B, it is shown how the Boltzmann equation for a Fermi liquid may be reduced to a one-dimensional integral equation. Appendix C contains the exact solution of this equation. Connection with Emery's treatment[8] of this equation is given in Appendix D. Further special points are treated in Appendixes E and F.

II. VARIATIONAL METHODS

In this section we discuss the variational methods in a general context, since they may in principle be applied to linear inhomogeneous integral equations other than the (linearized) Boltzmann equation. We shall, however, make frequent reference to the application to transport theory in order to prepare for the discussion of a specific example in Sec. III, namely, that of the linearized Boltzmann equation for a Fermi liquid.

We apply variational methods to the solution of linear inhomogeneous integral equations of the form

$$X(t)=f(t)Q(t)-\alpha\int_{-\infty}^{\infty}dt'F(t,t')\,Q(t')$$
$$=HQ(t). \qquad (2.1)$$

Here, the unknown function is $Q(t)$, whereas $X(t)$, $f(t)$, and the kernel $F(t,t')$ are all known (real) functions of the real variables t and t'. We restrict ourselves to considering symmetric kernels, i.e., $F(t,t')=F(t',t)$. The parameter α might have been included in the kernel, but we prefer to exhibit it to make the connection with Sec. III as direct as possible. The second line of (2.1) defines the (real) symmetric integral operator H. In the convention

$$(A,B)=\int_{-\infty}^{\infty}dt\,A(t)B(t)=(B,A),$$

the symmetry property of H implies

$$(A,HB)=(B,HA), \qquad (2.2)$$

for arbitrary A and B. Everywhere in the following we assume that H is either positive or negative semidefinite, which is equivalent to assuming that its eigenvalues are all positive (or zero) or all negative (or zero). The integrations always run from $-\infty$ to $+\infty$.

It is shown in Appendix B, that the Boltzmann equation for a Fermi liquid may be reduced to the form (2.1). In that case, t is an (reduced) energy variable, and $Q(t)$ is related to the deviation from local equilibrium of the distribution function. The inhomogeneous term $X(t)$ arises from the driving term of the Boltzmann equation (caused, for example, by a temperature gradient), whereas the whole of the right-hand side of (2.1) is the result of appropriate simplifications of the collision integral.

The thermal conductivity, viscosity, and spin-diffusion coefficients of a Fermi liquid can be shown (see Appendix B) to be proportional to a reduced transport coefficient T defined by

$$T=\int dt\,X(t)Q(t)\equiv(X,Q). \qquad (2.3)$$

Instead of attempting a direct solution of the integral equation, we shall derive various upper and lower bounds on the (reduced) transport coefficient T.

As mentioned in Sec. I, the lower bound on T (first used in transport theory by Kohler) has received a great deal of attention in the literature. This bound can be thought of as arising from a Schwarz inequality being applied to the basic integral equation $HQ=X$.[9] We shall therefore derive it by a traditional proof of the Schwarz inequality.

A. Upper and Lower Bounds

Let us assume that the integral operator H is positive semidefinite, so that all its eigenvalues are positive or zero. Then for an arbitrary function $U(t)$ and arbitrary parameter λ

$$((Q-\lambda U),H(Q-\lambda U))\geq 0. \qquad (2.4)$$

Using the symmetry property of H, we get

$$(Q,HQ)-2\lambda(U,HQ)+\lambda^2(U,HU)\geq 0. \qquad (2.5)$$

The left-hand side of (2.5) is a minimum, when $\lambda=(U,HQ)/(U,HU)$. With this value of λ, the inequality (2.5) becomes the Schwarz inequality

$$(Q,HQ)(U,HU)\geq(U,HQ)^2,$$

or, since $HQ=X$,

$$T=(Q,X)\geq(U,X)^2/(U,HU)\ . \qquad (2.6)$$

This lower bound on T is seen to be independent of the normalization of the trial function $U(t)$.[10]

When H is negative semidefinite, the inequality (2.6) becomes simply reversed, that is,

$$T=(Q,X)\leq(U,X)^2/(U,HU). \qquad (2.7)$$

Since the existence of a lower bound (2.6) only depends on H being positive semidefinite, one might hope to obtain other (lower and upper) bounds on T by rewriting the integral equation $HQ=X$ in a form $H'Q=X'$ such that H' differs from H but fulfills the requirement of symmetry and positive (or negative) semidefiniteness.

This may in fact be achieved in the case where H may be written as the sum of two symmetric positive semidefinite operators J and L, one of which (J, say) possesses an inverse J^{-1}

$$H=J+L\ . \qquad (2.8)$$

The operator H' is then defined by

$$H'=(HJ^{-1}-1)H=L+LJ^{-1}L, \qquad (2.9)$$

the second line showing that H' is positive semidefinite and symmetric. Applying the operation $(HJ^{-1}-1)$ to the integral equation $HQ=X$, leads directly to the desired form

$$H'Q=(HJ^{-1}-1)\,X\equiv X'. \qquad (2.10)$$

The Schwarz inequality (2.6) implies the existence of a lower bound on (Q,X') and hence an upper bound on (Q,X). In terms of the original H and X this bound is seen to be

$$T=(Q,X)\leq(X,J^{-1}X)-\frac{(U,(HJ^{-1}-1)X)^2}{(U,(HJ^{-1}-1)HU)}\ . \qquad (2.11)$$

If the positive semidefinite H can be written as a sum of a positive definite J (possessing an inverse) and a negative definite L, then H' becomes negative semidefinite (a proof of this is given in Appendix F). As a consequence, the inequality (2.11) becomes reversed.

We now list various ways of decomposing H in the sense of (2.8). As we discuss the resulting bounds, we shall point out their connection to previous work.

(1) $J=a$, $L=H-a$, where a is the smallest positive eigenvalue of H.[11] Clearly J and L are positive semidefinite and the inverse $J^{-1}=a^{-1}$ exists. From (2.11), we get, upon substitution, the upper bound

$$T=(Q,X)\leq\frac{1}{a}\left[(X,X)-\frac{(U,(H-a)X)^2}{(U,(H-a)HU)}\right]\ . \qquad (2.12)$$

Of course, a could be a number less than the smallest positive eigenvalue in cases where this was not immediately known. If H is negative definite, we subtract the largest (negative) eigenvalue and get just the reversed inequality of (2.12).

(2) $J = f$, $L = -\alpha F$, where f is the function $f(t)$, and the operator F is defined by

$$FU = \int dt' F(t, t')U(t').$$

Both f and F are assumed to be positive semidefinite. It follows that H' is positive semidefinite for $\alpha < 0$ and negative semidefinite for $\alpha > 0$. Inserting these choices in (2.11), we get

$$T \geqslant (X, f^{-1}X) + \frac{(f^{-1}X, FU)^2}{\alpha^{-1}(U, FU) - (f^{-1}FU, FU)}, \quad (2.13)$$

for $\alpha > 0$. If $\alpha < 0$, the inequality sign in (2.13) becomes reversed. When $\alpha = 0$, the bound (2.13) is simply the exact result since the exact solution of the integral equation (2.1) with $\alpha = 0$ is $Q(t) = f^{-1}(t)X(t)$.[12]

(3) $J = c$, $L = \alpha G$, where c is the function

$$c(t) = f(t) - \alpha \int dt' F(t, t'),$$

and the symmetric positive semidefinite operator G is defined by

$$GU = \int dt' F(t, t')(U(t) - U(t')).$$

[As in (2), f and F are assumed to be positive semidefinite.] Provided $c(t) > 0$ [which, since $\int dt F(t, t') > 0$, is certainly the case for negative α, but may also hold for some positive α], we obtain the bound

$$\begin{aligned} T = (X, Q) \leqslant & \int dt X^2(t)/c(t) \\ & - \left[\int dt \frac{X(t)}{c(t)} \int dt' F(t, t')(U(t) - U(t'))\right]^2 \\ & \times \left\{ \iint \frac{dt dt'}{2\alpha} F(t, t')(U(t) - U(t'))^2 \right. \\ & \left. + \int \frac{dt}{c(t)} \left[\int dt' F(t, t')(U(t) - U(t'))\right]^2 \right\}^{-1} \end{aligned} \quad (2.14)$$

for $\alpha > 0$. For $\alpha < 0$, the inequality sign in (2.14) is reversed, and for $\alpha = 0$, we recover the exact result as before. The bound (2.14) is a special case of the more general type of bound derived in Ref. 3, to which we shall direct our attention in the next paragraph. It is, however, a highly useful special case and in fact the only bound of this more general type we have had occasion to use in the application to the Boltzmann equation of a Fermi liquid.

The derivation of this more general bound due to Prager and Strieder[3] proceeds in a slightly different manner from the previous ones, but as we shall see the result is again simply a Schwarz inequality. The basic integral equation (2.1) may be written

$$X(t) = I(t) + \int dt' I(t, t'), \quad (2.15)$$

where $I(t) = c(t)Q(t)$, and the antisymmetric

$$I(t, t') = \alpha F(t, t')[Q(t) - Q(t')] .$$

As in the previous example (3), we have

$$c(t) = f(t) - \alpha \int dt' F(t, t') .$$

In terms of $(I(t);\ I(t, t'))$, the exact transport coefficient T is

$$T = \int dt \frac{I^2(t)}{c(t)} + \tfrac{1}{2} \int \int dt\, dt' \frac{I^2(t, t')}{\alpha F(t, t')} = ((I, I)). \quad (2.16)$$

We have here introduced the notation

$$((A, B)) \equiv \int dt A(t)B(t)/c(t) + \tfrac{1}{2} \int \int dt dt' [A(t, t')B(t, t')/\alpha F(t, t')]$$

for any two pairs of functions $(A(t);\ A(t, t'))$ and $(B(t);\ B(t, t'))$. Provided $c(t) > 0$ and $\alpha F(t, t') > 0$, we have for any pair of functions $(S(t); S(t, t'))$

$$((S, S)) > 0. \quad (2.17)$$

In particular,

$$((I - S, I - S)) \geqslant 0,$$

or $$((I, I)) - 2((I, S)) + ((S, S)) \geqslant 0 . \quad (2.18)$$

From the inequality (2.18), we observe that we can get an upper bound on $T = ((I, I))$ by choosing trial functions $(S(t);\ S(t, t'))$ such that $((I, S)) = ((I, I))$. This is achieved under the conditions that $S(t, t')$ is antisymmetric [like $I(t, t')$] and that

$$S(t) + \int S(t, t')dt' = X(t) \quad (2.19)$$

[*cf.* (2.15)]. The condition (2.19) and the antisymmetry of $S(t, t')$ together ensure that

$$((I, I)) = ((I, S)), \quad (2.20)$$

so that from (2.18) we get the upper bound

$$T = ((I, I)) \leqslant ((S, S)), \quad (2.21)$$

or $$T \leqslant \int dt \frac{S^2(t)}{c(t)} + \tfrac{1}{2} \int \int dt dt' \frac{S^2(t, t')}{\alpha F(t, t')}, \quad (2.22)$$

provided that the antisymmetry condition and (2.19) are satisfied. The trial function $S(t)$ may be eliminated by virtue of (2.19) so that the upper bound contains only one trial function $S(t,t')$. To ensure that the bound is as small as possible, we substitute everywhere in it $\mu S(t,t')$ for $S(t,t')$ and minimize with respect to the constant μ. The resulting minimum upper bound is

$$
\begin{aligned}
T \leq & \int dt X^2(t)/c(t) \\
& - \left\{ \int dt [X(t)/c(t)] \int S(t,t') dt' \right\}^2 \\
& \times \left\{ \tfrac{1}{2} \int \int dt\, dt' S^2(t,t')/\alpha F(t,t') \right. \\
& \left. + \int dt [c(t)]^{-1} \left[\int dt' S(t,t') \right]^2 \right\}^{-1} .
\end{aligned}
\qquad (2.23)
$$

Like the other bounds, (2.12)–(2.14), and (2.6), this expression is explicitly independent of a constant multiplying $S(t,t')$. Inequality (2.23) is due to Prager and Strieder.[3] With the special choice

$$S(t,t') = F(t,t')[U(t) - U(t')]$$

it reduces to (2.14).

If, as in many applications, $c(t)$ is identically zero, (2.19) and (2.22) still apply, provided the terms containing $I(t)$ and $S(t)$ are left out. The bound (2.23), however, has no meaning in this case.

Finally, the connection between (2.22) and the Schwarz inequality can be made. In the notation of Appendix A, we write $((I,S)) = \vec{I} \cdot \vec{S}$ and $((I,I)) = |\vec{I}|^2$. The condition (2.20) then becomes $|\vec{I}| = \vec{I} \cdot \vec{S}/|\vec{I}|$, and the inequality (2.21) may be written as the Schwarz inequality $|\vec{I} \cdot \vec{S}| \leq |\vec{I}|\, |\vec{S}|$.

III. BOLTZMANN EQUATION OF A FERMI LIQUID

We now proceed to apply the bounds of Sec. II to the Boltzmann equation of a Fermi liquid. In Appendix B, it is shown how this equation may be simplified to the following linear inhomogeneous integral equation of the form (2.1):

$$X(t) = f(t) Q(t) - \alpha \int dt' F(t-t') Q(t') . \qquad (3.1)$$

Here $Q(t)$ is related to the deviation from local equilibrium of the distribution function. The integration over the (reduced) energy variables t and t' always runs from $-\infty$ to $+\infty$. The inhomogeneous term $X(t)$ in (3.1) originates from the total time derivative of the distribution function (the driving term), whereas the right-hand side of (3.1) arises from the collision integral.

For the case of thermal conductivity $X(t)$ is $t/\cosh \frac{1}{2}t$ whereas it is $(\cosh \frac{1}{2}t)^{-1}$ in the case of viscosity and spin diffusion. The functions $f(t)$ and $F(t)$ are even and positive and in all three cases given by

$$f(t) = \pi^2 + t^2, \quad \text{and} \quad F(t) = \tfrac{1}{2} t / \sinh \tfrac{1}{2} t . \qquad (3.2)$$

Finally, α is a ratio of two angular averages of the collision probability w. Both the angular averaging and the collision probability itself, are in principle, different for each of the three transport processes considered. An actual calculation of α requires knowledge of the interaction between the quasiparticles in the Fermi liquid. In the following, we shall consider α to be a known parameter which reduces the problem of calculating transport coefficients to that of solving (3.1) and inserting the solution in

$$T = \int dt X(t) Q(t). \qquad (3.3)$$

The solution[6] of (3.1) can be determined as a function of α in terms of a rapidly converging expansion. For the sake of completeness this solution is included in Appendix C. In the present context we shall only state the result for the (reduced) thermal conductivity K

$$
\begin{aligned}
K = & \tfrac{1}{3}(12 - \pi^2) \\
& + 4\alpha \sum_{n=2,4,\ldots} \frac{2n+1}{n^2(n+1)^2} \, \frac{1}{n(n+1) - \alpha} .
\end{aligned}
\qquad (3.4)
$$

The convergence is so fast that it is sufficient for most purposes to include only the first term with $n = 2$. A simple approximate form for the (reduced) thermal resistance is

$$1/K = 1.41 [1 - \alpha/(7.7 - 0.3\alpha)] . \qquad (3.5)$$

The viscosity and spin-diffusion coefficients are given by a similar series involving odd n (Appendix C). The Boltzmann equation (3.1) has thus been solved exactly in the sense that for a given value of α the transport coefficients can be determined with any desired accuracy.

Prior to our discovery of the exact result (3.4), we applied variational methods to the integral equation (3.1) in order to decide whether previous attempts to get an approximate solution were reliable. Abrikosov and Khalatnikov[13] (AK) estimated the thermal conductivity K by neglecting t^2 with respect to π^2 in $f(t)$. By virtue of the approximation $f(t) \simeq f(0) = \pi^2$ the solution of (3.1) with $X = t/(\cosh \frac{1}{2}t)$ is readily found to be

$$Q(t) = \pi^{-2} (1 - \tfrac{1}{6}\alpha)^{-1} t / \cosh \tfrac{1}{2} t . \qquad (3.6)$$

The corresponding (reduced) thermal conductivity, found by AK, is from (3.3)

$$K_{\mathrm{AK}} = \tfrac{4}{3} (1 - \tfrac{1}{6}\alpha)^{-1} . \qquad (3.7)$$

Using variational methods, we were able to rule out (3.7) over the whole range of α from 0 to 6. By consideration of the integral equation (3.1) alone, one would not expect the approximation $t \ll \pi$ to be a good one, since $X(t)$ is an odd function, which peaks at $t \simeq 2.5$.

It was possible to find upper and lower bounds so close together that the resulting uncertainty in the determination of the transport coefficients was satisfactory for practical purposes. After the discovery of the exact result (3.4), the interest in these particular bounds was, of course, diminished. We think, however, that they serve to illustrate the power of variational methods and also throw some light upon the best choices of trial functions to be used in the bounds. Before we indicate some of these results, we shall examine the specific conditions for the various bounds to exist.

A. Existence of Bounds

In Sec. II the bounds were derived on the assumption that H was positive semidefinite. To investigate the validity of this assumption in our particular case, we Fourier transform the integral equation (3.1) with respect to the variable t/π (see Appendix C for details). The integral equation then becomes a differential equation

$$\tilde{H}\tilde{Q} = \tilde{X} \tag{3.8}$$

or

$$\left(-\frac{d^2}{dq^2} + 1 - \frac{\alpha}{\cosh^2 q}\right)\tilde{Q}(q) = 2\,\frac{\sinh q}{\cosh^2 q}\ . \tag{3.9}$$

If $\alpha < 0$, the operator $\tilde{H}$ has only positive eigenvalues. When $\alpha > 0$, we set $\alpha = n(n+1)$, where n is positive but not necessarily an integer. The lowest eigenvalue of $\tilde{H}$ is then $-n^2+1$. The corresponding eigenfunction is an even function of $q(\propto (\cosh q)^{-n})$. The integral operator H is therefore positive semidefinite provided $-n^2+1 \geqslant 0$ or

$$\alpha \leqslant 2. \tag{3.10}$$

Since the spin-diffusion coefficient and viscosity coefficient both involve only even functions $Q(t)$, (3.10) is the necessary condition for the bounds to exist. The thermal conductivity, however, involves only odd $Q(t)$, which allows us to consider only those eigenvalues that correspond to odd eigenfunctions. The lowest such eigenvalue for $n > 1$, is $1-(n-1)^2$, [with corresponding eigenfunction $\propto \sinh q(\cosh q)^{-n}$]. The condition that this eigenvalue be non-negative implies

$$\alpha \leqslant 6. \tag{3.11}$$

The condition (3.10) for spin diffusion and viscosity or (3.11) for thermal conductivity is sufficient for (2.12), (2.13), and (2.6) to exist with the provision that the equality sign does not apply in the case of (2.12).

On the other hand, as we noted in Sec. II, existence of the bound (2.14) requires that

$$c(t) = f(t) - \alpha \int dt' F(t, t')$$

be positive definite. For the explicit choices (3.2) for $f(t)$ and $F(t, t')$, $c(t) = \pi^2(1-\alpha) + t^2$. Thus, the bound (2.14) exists under the stricter condition $\alpha < 1$.

B Some Exact Results

For the case of thermal conductivity, i.e., with $X(t) = t(\cosh\frac{1}{2}t)^{-1}$, it is possible to find an explicit solution of (3.1) for two special values $\alpha = 0$ and $\alpha = 2$. By setting $\alpha = 0$ in (3.1), we obtain immediately

$$Q(t) = X(t)/f(t),$$

with the corresponding thermal conductivity

$$K = \tfrac{1}{3}(12 - \pi^2)\ . \tag{3.12}$$

The solution for $\alpha = 2$ can be determined from our knowledge of a solution to the homogeneous equation obtained from (3.8) by setting $\tilde{X}(q) = 0$. Such a solution is easily seen to be $\tilde{Q} = (\cosh q)^{-1}$ (it may also be obtained in the manner of Appendix C). By standard methods of differential equations we arrive at the complete solution for $\alpha = 2$:

$$\tilde{Q}_2(q) = \frac{q}{\cosh q} + c_1\left(\sinh q + \frac{q}{\cosh q}\right) + c_2\frac{1}{\cosh q}\ ,$$

where c_1 and c_2 are arbitrary constants, to be determined by the boundary conditions. Since K must be finite we set $c_1 = 0$. The value of c_2 is immaterial. Since only the odd part of $\tilde{Q}_2$ contributes to K, we may set it also to zero. The resulting solution $\tilde{Q}_2(q) = q(\cosh q)^{-1}$ has the Fourier transform

$$Q_2(t) = \tfrac{1}{4}(\sinh\tfrac{1}{2}t/\cosh^2\tfrac{1}{2}t)\ , \tag{3.13}$$

which gives a (reduced) thermal conductivity that is simply

$$K = 1. \tag{3.14}$$

For the case of spin diffusion and viscosity, the only simple solution is the $\alpha = 0$ solution.

C Lower Bounds on K

In the following, we discuss bounds on the thermal conductivity obtained with various trial functions in (2.12)–(2.14) and (2.6). We first consider the lower bound (2.6). An obvious choice of the (odd) trial function $U(t)$ is to take it to be equal to $X(t)$, which results in

$$K \geqslant \tfrac{5}{9}(1-\tfrac{1}{6}\alpha)^{-1}. \qquad (3.15)$$

This lower bound[14] is just $\frac{5}{12}$ times the estimate (3.7) of AK, whose approximate solution was proportional to $X(t)$ [see (3.6)].

A significant improvement over (3.15) is achieved by using a trial function containing a variational parameter. We choose $U(t) = te^{-a|t|}$ and vary a to get the highest lower bound. Both these lower bounds are shown on Fig. 1 in which K^{-1} is plotted against α. The difference between this variational lower bound and the exact K is at most 1%. In Table I we have summarized our numerical results for both upper and lower bounds for $\alpha = 0$, 1, and 2, the region $0 < \alpha < 2$ being that of main physical interest.

Since we have an exact solution for $\alpha = 2$, we can can use it as a trial function, i.e.,

$$U_1(t) = \sinh \tfrac{1}{2}t / \cosh^2 \tfrac{1}{2}t\ . \qquad (3.16)$$

Using this in the lower bound (2.6), we can get an analytical expression by virtue of the identity

$$HU_1(t) = (\pi^2 + t^2)(1 - \tfrac{1}{2}\alpha)\, U_1(t) + 2\alpha X(t), \qquad (3.17)$$

which follows from the fact that $Q(t) = \frac{1}{4} U_1(t)$ is a solution of (3.1) when $\alpha = 2$. The lower bound on K is conveniently written as an upper bound on K^{-1} as follows:

$$K^{-1} \leqslant (\tfrac{1}{9}\pi^2 + \tfrac{1}{3}) - \alpha(\tfrac{1}{18}\pi^2 - \tfrac{1}{3}).$$

On Fig. 1, this bound would be a straight line tangential to the exact K^{-1} curve at $\alpha = 2$.

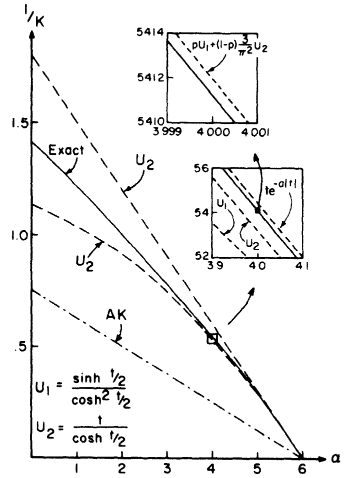

FIG. 1. Various bounds on the (inverse) reduced thermal conductivity K^{-1} plotted (dashed lines) as functions of the parameter α. The exact solution is shown by the full line, and the approximate solution of AK (3.7) as a dash-dotted line. All upper bounds on K^{-1} are calculated with (2.6) and lower bounds with (2.12) using the trial function indicated on the figure. To show how close some of the bounds lie to the exact solution we have blown up small regions around $\alpha = 4$ by factors of ten and a thousand.

The best easily calculable result is found using a trial function which is a variable linear combination of an exact solution at $\alpha = 2$, $U_1(t)$, and a function which mimics the behavior of $Q(t)$ for α near 6,

$$U_2(t) = X(t) = t/\cosh \tfrac{1}{2}t\ . \qquad (3.18)$$

The constant $3/\pi^2$ in this trial function

$$U(t) = pU_1(t) + (1-p)(3/\pi^2)\, U_2(t)$$

is chosen so that (U, X) is independent of the variational parameter p. Note that by allowing p to be greater than unity, $U(t)$ can even mimic $Q(t)$ for small α. The result is a lower bound on K

TABLE I. Bounds on the (reduced) thermal conductivity. The lower bounds are based on Eq. (2.6), except when otherwise noted. The exact result is listed in the bottom line.

Trial function	$\alpha = 0$		$\alpha = 1$		$\alpha = 2$	
	Lower	Upper	Lower	Upper	Lower	Upper
$U_2 = t/\cosh \frac{1}{2}t$	0.556 0.710^{c}	0.710^{a} 0.884^{b}	0.667 0.821^{c}	1.030^{a} 0.973^{b}	0.883 0.988^{c}	1.100^{b}
$te^{-a\|t\|}$	0.704		0.821		0.993	
$U_1 = \sinh \frac{1}{2}t/\cosh^2 \frac{1}{2}t$	0.699	0.710^{b} 0.730^{c}	0.823	0.829^{a} 0.834^{c}	1	1^{b}
$pU_1 + (1-p)(3/\pi^2)U_2$	0.710		0.827		1	
Exact result (3.4)	0.710		0.827		1	

[a] From (2.14). [b] From (2.12). [c] From (2.13).

which nowhere deviates more than 0.03% from the exact result (3.4)

$$K \geqslant \tfrac{5}{9}(1-\tfrac{1}{6}\alpha)^{-1} \times\left(1-\frac{1-\frac{1}{6}\alpha}{20[(\pi^2/9-\frac{13}{15})-\alpha(\pi^2/18-\frac{8}{15})]}\right)^{-1} \qquad (3.19)$$

The choice of trial function ensures that the lower bound (3.19) is equal to the exact $K=1$ at $\alpha=2$ and diverges at $\alpha=6$ just like the exact result (3.4).[15] The inequality (3.19) has been written so as to illustrate the corrections to the AK result (3.7) and the simple variational result (3.15).

D. Upper Bounds on K

It is evident that the bounds (2.12)–(2.14) are generally more complicated to evaluate than the lower bound (2.6). We shall first consider (2.14) which gives an upper bound on K for $0<\alpha<1$ and a lower one for $\alpha<0$. As before an obvious choice is $U(t)=t/\cosh\frac{1}{2}t$, which permits a simple evaluation of (2.14). The resulting upper bound has been calculated for $0\leqslant\alpha\leqslant 1$. The values for $\alpha=0$ and $\alpha=1$ are exhibited in Table I. One can calculate the point $\alpha=1$, since the integrals in (2.14) are well defined, even though $c(t)=0$ for $t=0$. The general variational principle used to derive (2.23) still holds for $\alpha=1$, since $c(t)$ never becomes negative. This upper bound by itself excludes the estimate of AK for $0\leqslant\alpha\leqslant 1$. At $\alpha=0$, it coincides with the exact solution, but deviates increasingly from the exact K as α increases from 0 to 1. We could improve on this situation by taking a trial function $U(t)$ with a variational parameter like $te^{-a|t|}$ and then minimize the upper bound with respect to a for a given value of α. We have not carried this through, since the result is rather obvious, when we consider the upper bound one gets by using

$$U(t)=U_1(t)=\sinh\tfrac{1}{2}t/\cosh^2\tfrac{1}{2}t$$

in (2.14). Since U_1 is proportional to the exact solution of the integral equation with $\alpha=2$, we can again reduce the two-dimensional integrals in (2.14) to one-dimensional ones and work out the bound rather easily. Numerical results are given in Table I. We see that at $\alpha=1$ the trial function U_1 gives an upper bound that lies even closer to the exact solution than the lower bound (2.6) with $U=U_1$. This substantiates our belief that we can do as well with a variational trial function like $te^{-a|t|}$ in the upper bound (2.14) as we previously were able to in the lower bound (2.6).

The bound (2.12) may be used to determine an upper bound on K over the whole range of α from 0 to 6. Since only odd functions $Q(t)$ are of interest for the thermal conductivity, we subtract from H the lowest eigenvalue belonging to an odd eigenfunction. In the region $0<\alpha<2$ the lowest eigenvalue (belonging to odd eigenfunctions) of the operator $\tilde{H}$ defined in (3.8) and (3.9) is 1; for $2<\alpha<6$ it is $[1-(n-1)^2]$ with $n(n+1)=\alpha$. The eigenvalues of H are equal to those of $\tilde{H}$ except for a factor π^2. We have calculated (2.12) with two different trial functions,

$$U=U_2=X \quad\text{and}\quad U=U_1=\sinh\tfrac{1}{2}t/\cosh^2\tfrac{1}{2}t\,.$$

The results are shown on Fig. 1 as lower bounds on K^{-1}. The bound with $U=X$ is shown in full. It lies rather close to the exact solution for $\alpha\gtrsim 3$, but deviates for smaller α. The bound with $U=U_1$ lies too close to the exact solution to be exhibited in full. It coincides with the exact solution at $\alpha=2$ (the values for $\alpha=0$ and 1 are listed in Table I) and has its largest deviation from the exact solution when α is between 3 and 4. Both these bounds are shown in the first blow-up of the region around $\alpha=4$.

Finally, we have calculated the bound (2.13) with the trial function $U(t)=X(t)$. We get

$$K\geqslant(12-\pi^2)/3+\tfrac{5}{9}[\alpha/(6-\alpha)] \qquad (3.20)$$

for $\alpha>0$. For $\alpha<0$, the inequality as usual becomes reversed. This result is a considerable improvement over (3.15) which was obtained using the same trial function in the bound (2.6). (The reasons for this improvement are discussed in Appendix E.) The bound (3.20) is a good approximation to the exact (reduced) thermal conductivity, since it is seen to equal the first two terms of the exact result (3.4). Emery[8] obtained (3.20) as an approximate result. The connection between his treatment and the variational method is discussed in Appendix D.

E. Spin Diffusion and Viscosity

The only difference involved in determining the (reduced) spin-diffusion and viscosity coefficients in terms of α is that $X(t)=(\cosh\frac{1}{2}t)^{-1}$ rather than $t(\cosh\frac{1}{2}t)^{-1}$. Now all trial functions are taken to be even and the range of α is $\alpha\leqslant 2$. The functional form of the bounds as well as the exact solution is similar to what we have found in the case of thermal conductivity. Whereas $t(\cosh\frac{1}{2}t)^{-1}$, which appears in the thermal conductivity, has its maximum at $t\simeq 2.5$, $(\cosh\frac{1}{2}t)^{-1}$ is centered about $t=0$. Accordingly, the approximation of AK, in which the t dependence of $f(t)=\pi^2+t^2$ is neglected, is more appropriate. For the same reason the upper and lower bounds with $U(t)=X(t)=(\cosh\frac{1}{2}t)^{-1}$ lie considerably closer to the exact solution than the corresponding bounds for the thermal conductivity. In Table II we illustrate this by comparing the values of these bounds for $\alpha = 0$ and $\alpha = 1$ with the exact result and the estimate of AK.

IV. CONCLUSION

The application of the variational methods to a particular Boltzmann equation demonstrates that the calculation of lower and upper bounds may provide a useful alternative to seeking exact solutions. It is evident that knowledge of one exact solution (i.e., the $\alpha = 2$ solution in the case of thermal conductivity) can be very helpful as a guide to choosing trial functions in both the lower and upper bounds. An advantage of the variational approach[5] is that (approximate) simple closed forms for the transport coefficients may be obtained.

The integrations necessary to calculate the bounds could in all but one case $[U(t) = te^{-\alpha|t|}$ in (2.6)] be performed analytically. Of the upper bounds (2.12) was the easiest to evaluate. The treatment of Sec. III also shows that the customary choice of trial function $U(t) = t/\cosh\frac{1}{2}t$ may give a rather poor approximation. The introduction of a variational parameter in the trial function makes it possible to obtain bounds that are very close to the exact result, the best and most easily calculable being the variable linear combination of two trial functions.

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APPENDIX A: CONNECTION WITH SYNGE'S FORMALISM

In this appendix we first show how the bounds (2.6) and (2.22) fit into the framework of Synge's general formulation of reciprocal variational principles.[7] Next, we mention a useful electrical network analogy to the Boltzmann equation.

TABLE II. Comparison of the exact result and the estimate of AK with bounds on the (reduced) spin-diffusion and viscosity coefficient. The upper bound is based on (2.14) and the lower bound on (2.6).

	$\alpha = 0$		$\alpha = 1$	
	Lower	Upper	Lower	Upper
Bound with the trial function $U = (\cosh\frac{1}{2}t)^{-1}$	0.304	0.333	0.608	0.676
Exact solution	0.333		0.639	
Estimate of AK	0.405		0.811	

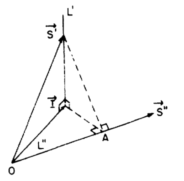

FIG. 2. Three-dimensional illustration of the significance of (A1). L'' is a plane through the origin; L' is a straight line perpendicular to this plane. Their intersection is I. It follows from the figure, that $\vec{S}' \cdot \vec{S}''/|\vec{S}''| \equiv OA \leq |\vec{I}| \leq |\vec{S}'|$.

In a vector space we define a scalar product $\vec{S}_1 \cdot \vec{S}_2$ and a positive definite norm $S^2 = \vec{S} \cdot \vec{S}$. Let L' and L'' be two linear mutually orthogonal subspaces. Linear means that if $\vec{S}_1'$ and $\vec{S}_2'$ belong to L', the same is true for $r\vec{S}_1' + (1-r)\vec{S}_2'$, where r is any real number. Orthogonal means that any vector $\vec{S}_1' - \vec{S}_2'$ connecting two vectors belonging to L' is orthogonal to any vector $\vec{S}_1'' - \vec{S}_2''$ connecting two vectors belonging to L''. We define L'' in such a way that it contains the origin $S'' = 0$.

Let us assume that the two subspaces have an intersection $\vec{I}$. Only one such intersection can exist owing to the orthogonality and the positive definite norm.

The norm of the intersection then has the following lower and upper bounds (compare Fig. 2)

$$(\vec{S}' \cdot \vec{S}'')^2/S''^2 \leq I^2 \leq S'^2 , \qquad \text{(A1)}$$

where $\vec{S}'$ and $\vec{S}''$ are arbitrary vectors belonging to L' and L'', respectively.

In order to apply (A1) to the integral equation (2.1) we rewrite it

$$X(t) = c(t)Q(t) + \alpha \int dt' F(t,t')[Q(t) - Q(t')] . \qquad \text{(A2)}$$

We then make the following identifications:

Vector: $\vec{S} = (S(t), S(t,t'))$;

$S(t)$ and $S(t,t')$ are real functions.

Scalar product:

$$\vec{S}_1 \circ \vec{S}_2 = \int dt\, S_1(t) S_2(t)/c(t) + \tfrac{1}{2}\int dt\,dt' \frac{S_1(t,t')S_2(t,t')}{\alpha F(t,t')} . \qquad \text{(A3)}$$

In the notation of Sec. II, see Eq. (2.16), this would be written $((S_1, S_2))$. In the subspace L' all vectors $\vec{S}'$ obey

$$S'(t) + \int dt' S'(t,t') = X(t),$$

where $$S'(t,t') = -S'(t',t). \qquad \text{(A4)}$$

In the subspace L'' all vectors $\vec{S}''$ obey

$$\frac{S''(t,t')}{\alpha F(t,t')} = \frac{S''(t)}{c(t)} - \frac{S''(t')}{c(t')} . \qquad \text{(A5)}$$

If $c(t) > 0$ and $\alpha F(t,t') > 0$ the norm is positive. L'' is seen to contain the origin, and it is easily verified that L' and L'' are linear and mutually orthogonal.

If, in (A4) and (A5), we put $\vec{S}' = \vec{S}'' = \vec{I} = (c(t)Q(t), I(t,t'))$ and eliminate $I(t,t')$ we obtain the integral equation (A2), the solution of which therefore is determined by the intersection between L' and L''. The norm of the intersection is seen to be $I^2 = (X, Q)$, i.e., equal to the transport coefficient T. Using (A1) we now obtain the bounds (2.6) and (2.22).

As all linear integral equations the Boltzmann equation has an electrical network analogy. In fact, the set of linear equations analogous to (A2), i.e.,

$$X_i = c_i Q_i + \textstyle\sum_k G_{ik}(Q_i - Q_k) \qquad \text{(A6)}$$

can be interpreted as Ohm's laws for a network of the type shown in Fig. 3, Q_i being potentials, G_{ik} and c_i are conductances, and X_i externally supplied currents. The analog of the transport coefficient, i.e., $\sum Q_i X_i$, is the total power dissipated in the resistors. The quantities S_i and S_{ik} corresponding to $S(t)$ and $S(t,t')$ in (A4) and (A5) are currents in the branches of the network. It is immediately seen that the two subspaces L' and L'' analogous to (A4) and (A5) are current distributions obeying Kirchhoff's first and second law, respectively.

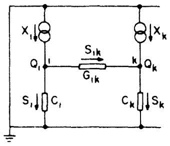

FIG. 3. Network analog of (A6) in the simplest case, corresponding to Fig. 2.

APPENDIX B: REDUCTION OF THE BOLTZMANN EQUATION

We here show how the Boltzmann equation for a Fermi liquid may be reduced to a one-dimensional integral equation. The notation of AK[13] is used as far as possible.

In the absence of any explicit time dependence the kinetic equation for the distribution function $n_1 = n(\vec{p}_1, \vec{x})$ of Landau quasiparticles with momentum $\vec{p}_1$ is

$$\frac{\partial \epsilon_1}{\partial \vec{p}_1} \cdot \frac{\partial n_1}{\partial \vec{x}} - \frac{\partial \epsilon_1}{\partial \vec{x}} \cdot \frac{\partial n_1}{\partial \vec{p}_1} = I(n_1) . \qquad \text{(B1)}$$

The collision integral $I(n_1)$ is

$$\begin{aligned} I(\vec{p}_1, \vec{x}) = {} & \int d\tau_{1'} \int d\tau_{2'} \int d\vec{p}_2 \, w(\vec{p}_1 \vec{p}_2; \vec{p}_{1'} \vec{p}_{2'}) [- n_1 n_2 (1 - n_{1'})(1 - n_{2'}) + n_{1'} n_{2'} (1 - n_1)(1 - n_2)] \\ & \times \delta(\vec{p}_1 + \vec{p}_2 - \vec{p}_{1'} - \vec{p}_{2'}) \delta(\epsilon_1 + \epsilon_2 - \epsilon_{1'} - \epsilon_{2'}) . \end{aligned} \qquad \text{(B2)}$$

In Eq. (B2) $w(\vec{p}_1 \vec{p}_2; \vec{p}_{1'} \vec{p}_{2'})$ is the collision probability for two quasiparticles of momenta $\vec{p}_1$ and $\vec{p}_2$ to scatter to $\vec{p}_{1'}$ and $\vec{p}_{2'}$. The bracket contains the usual occupancy factors for the process $(\vec{p}_1, \vec{p}_2) \rightarrow (\vec{p}_{1'}, \vec{p}_{2'})$ and the reverse process. The δ functions express conservation of the local equilibrium values of the total energy and of the total momentum involved in the collision. The integration over $\tau_{1'}$ and $\tau_{2'}$ are phase-space integrations $[d\tau = 2d\vec{p}/(2\pi\hbar)^3]$. We also integrate over all possible values of the momentum $\vec{p}_2$.

It is convenient to expand the distribution function about its local equilibrium value in order to discuss the linearized version of Eq. (B1)

$$n(\vec{p}_1) = n_0(\epsilon_1) + \frac{\partial n_0}{\partial \epsilon_1} \psi_{\vec{p}_1}(\epsilon_1). \qquad \text{(B3)}$$

The equilibrium distribution function is given by $n_0(\epsilon_1) = \{\exp[(\epsilon_1 - u)/kT] + 1\}^{-1}$. The expansion about local equilibrium ensures that the collision integral is zero when $\psi = 0$, consistent with the assumption of local equilibrium.

In the following we specialize to the case of thermal conductivity. In the presence of a thermal gradient the left-hand side of (B1) becomes (to linear order in $\vec{\nabla}_{\vec{x}} T$)

$$\frac{\partial \epsilon_1}{\partial \vec{p}_1} \circ \frac{\partial n_0}{\partial \vec{x}} = \frac{t}{4\cosh^2 \frac{1}{2} t} \frac{1}{kT} \vec{\nabla}_{\vec{x}}(kT) \circ \frac{\partial \epsilon_1}{\partial \vec{p}_1} . \qquad \text{(B4)}$$

Here we have introduced $t=(\epsilon_1-\mu)/kT$ as a reduced energy variable. When linearized with respect to ψ the collision integral becomes

$$I(n_1) = (kT)^{-1} \iiint d\tau_{1'}\, d\tau_{2'}\, d\vec{p}_2 [\psi_1+\psi_2-\psi_{1'}-\psi_{2'}]\, w(\vec{p}_1\vec{p}_2;\vec{p}_{1'}\vec{p}_{2'}) \times \delta(\vec{p}_1+\vec{p}_2-\vec{p}_{1'}-\vec{p}_{2'})\delta(\epsilon_1+\epsilon_2-\epsilon_{1'}-\epsilon_{2'}) n_{01}n_{02}(1-n_{01'})(1-n_{02'}) , \tag{B5}$$

since $n_{\vec{p}_1}(\epsilon_1)=n_{01}-(kT)^{-1}n_{01}(1-n_{01})\psi_1$, with $n_{01}\equiv n_0(\epsilon_1)$. We note that $I(n_1)$ according to (B5) is an integral over nine variables. The momentum and energy conserving δ functions reduce this number to five. By performing two more integrations we can obtain an expression for $I(n_1)$ in terms of an integral over two angular variables and one energy variable.

Following Ref. 13 we choose the two angular variables to be the angle θ between $\vec{p}_1$ and $\vec{p}_2$ and the angle φ between the plane of $\vec{p}_1$ and $\vec{p}_2$ and that of $\vec{p}_{1'}$ and $\vec{p}_{2'}$. The differential element $d\tau_{1'}$ may be expressed in terms of $dp_{1'}$, $dp_{2'}$, and $d\varphi$ as described in Ref. 13. Using $dp_{1'}=(m^*/p_F)\,d\epsilon_1'$ and $dp_{2'}=(m^*/p_F)d\epsilon_{2'}$ together with the definitions $x=(\epsilon_{1'}-\mu)/kT$ and $y=(\epsilon_{2'}-\mu)/kT$ we then get

$$d\tau_{1'} = (2\pi\hbar)^{-3}p_F^{-1}(m^*/\cos\tfrac{1}{2}\theta)(kT)^2\,dx\,dy\,d\varphi . \tag{B6}$$

The integration over $\vec{p}_{2'}$ just removes the (momentum) δ function. We also write $d\vec{p}_2=p_2{}^2dp_2\sin\theta\,d\theta\,d\varphi_2$ $=p_F m^* kT dz\sin\theta\,d\theta\,d\varphi_2$ where $z=(\epsilon_2-\mu)/kT$ and the polar axis is $\vec{p}_1$. Then $I(n_1)$ may be written as a six-dimensional integral (the energy integrations run from $-\infty$ to $+\infty$)

$$I(n_1) = (8\pi^4\hbar^6)^{-1}(m^*)^3kT\,\pi^{-1}\int_0^\pi d\varphi \int_{-1}^{1} \tfrac{1}{2}d(\cos\theta)\,[w(\theta,\varphi)/\cos\tfrac{1}{2}\theta]\,(2\pi)^{-1}\int_0^{2\pi} d\varphi_2 \iiint dx\,dy\,dz \times [\psi_1(t)+\psi_2(z)-\psi_{1'}(x)-\psi_{2'}(y)]\,\delta(t+z-x-y)n(t)n(z)[1-n(y)][1-n(x)] , \tag{B7}$$

where $n(t)=(e^t+1)^{-1}$. The angular variation of ψ_1 is set by the left-hand side of the Boltzmann equation

$$\psi_1=\psi(t)[(\partial\epsilon_1/\partial\vec{p}_1)\cdot(\partial T/\partial\vec{x})]\propto\cos\theta_1 ,$$

where θ_1 is the angle between $\partial\epsilon_1/\partial\vec{p}_1$ and $\vec{\nabla}_{\vec{x}}T$. Similarly $\psi_2\propto\cos\theta_2$, where θ_2 is angle between $\partial\epsilon_2/\partial\vec{p}_2$ and $\vec{\nabla}_{\vec{x}}T$. By virtue of the addition formula for spherical harmonics we observe that $(1/2\pi)\int_0^{2\pi}d\varphi_2\cos\theta_2$ $=\cos\theta\,\cos\theta_1$ with similar results for $\psi_{1'}$ and $\psi_{2'}$.

A characteristic time τ_0 is introduced through

$$1/\tau_0=[m^{*3}(kT)^2/8\pi^4\hbar^6]\langle w(\theta,\varphi)/\cos\tfrac{1}{2}\theta\rangle , \tag{B8}$$

where $\langle\cdots\rangle$ denotes angular averaging $(1/2\pi)\int_0^\pi d\varphi\int_{-1}^1 d(\cos\theta)$. [$2\tau_0/\pi^2$ is the relaxation time for a quasiparticle[16] at the Fermi surface ($t=0$).] $Q(t)$ is defined by

$$\psi_{\vec{p}}(t)=2\tau_0(\cosh\tfrac{1}{2}t)Q(t)[(\partial\epsilon/\partial\vec{p})\cdot\vec{\nabla}_{\vec{x}}(kT)] . \tag{B9}$$

The Boltzmann equation (B1) then assumes the form

$$\frac{t}{4\cosh^2\frac{1}{2}t}=\frac{m^{*3}(kT)^2}{8\pi^4\hbar^6}\int_0^\pi\frac{d\varphi}{\pi}\int_{-1}^1\frac{d(\cos\theta)}{2}\,\frac{w(\theta,\varphi)}{\cos\frac{1}{2}\theta}\,2\tau_0\iiint dx\,dy\,dz \times\delta(t+z-x-y)n(t)n(z)[1-n(x)][1-n(y)][Q(t)\cosh\tfrac{1}{2}t-Q(x)(\cos\theta+\cos\theta_{1'}+\cos\theta_{2'})\cosh\tfrac{1}{2}x] . \tag{B10}$$

Using the identities

$$\iiint dx\,dy\,dz\,\delta(t+z-x-y)n(t)n(z)[1-n(x)][1-n(y)]=\tfrac{1}{2}n(t)[1-n(t)](\pi^2+t^2) \tag{B11}$$

and $$\iint dy\,dz\,\delta(t+z-x-y)n(t)n(z)[1-n(x)][1-n(y)]=n(t)[1-n(t)]\,\frac{\cosh\frac{1}{2}t}{\cosh\frac{1}{2}x}\,\frac{\frac{1}{2}(x-t)}{\sinh\frac{1}{2}(x-t)} , \tag{B12}$$

we can perform two of the three energy integrals. This reduces the Boltzmann equation to the desired simple form [Eq. (3.1)]

$$t/\cosh\tfrac{1}{2}t=(\pi^2+t^2)Q(t)-\alpha\int dx F(t-x)Q(x) \tag{B13}$$

with $F(t)=\frac{1}{2}t/\sinh\frac{1}{2}t$ and α given by

$$\alpha = 2\langle[w(\theta,\varphi)/\cos\tfrac{1}{2}\theta](\cos\theta+\cos\theta_{1'}+\cos\theta_{2'})\rangle/\langle w(\theta,\varphi)/\cos\tfrac{1}{2}\theta\rangle\ . \tag{B14}$$

Finally, we use $\cos\theta_{1'}=\cos^2\frac{1}{2}\theta+\sin^2\frac{1}{2}\theta\cos\varphi$ and $\cos\theta_{2'}=\cos^2\frac{1}{2}\theta-\sin^2\frac{1}{2}\theta\cos\varphi$ both of which are consequences of the addition theorem of spherical harmonics and the fact that all momenta are at the Fermi surface. The parameter α occurring in (B14) is then simply

$$\alpha = 2\langle[w(\theta,\varphi)/\cos\tfrac{1}{2}\theta](1+2\cos\theta)\rangle/\langle w(\theta,\varphi)/\cos\tfrac{1}{2}\theta\rangle\ . \tag{B15}$$

When the transition probability $w(\theta,\varphi)$ is known as a function of θ and φ, α may be determined from (B15) and inserted in (B13), which is solved for $Q(t)$.[17]

We have only to relate $Q(t)$ to the thermal conductivity κ, defined by

$$\vec{J}=-\kappa\vec{\nabla}T\ . \tag{B16}$$

Under the condition of zero mass current the heat current $\vec{J}$ is

$$\vec{J}=\sum_{\vec{p},\sigma}(\epsilon_{\vec{p}}-\mu)\frac{\partial\epsilon}{\partial\vec{p}}n(\vec{p},\vec{x})\ .$$

Since $n=n_0-(kT)^{-1}n_0(1-n_0)\,\psi$ and ψ is given in terms of Q from (B9), we get under the assumption that the density of states and the Fermi velocity are constants at the Fermi surface

$$\vec{J}=(m^*k_F/\pi^2\hbar^2)(kT)^2\int dt\ t\,\tfrac{1}{3}V_F^{\,2}\,\vec{\nabla}_{\vec{x}}(kT)2\tau_0\cosh\tfrac{1}{2}t\,Q(t)(-1/4kT\cosh^2\tfrac{1}{2}t)=-\kappa\vec{\nabla}T\ ,$$

where V_F is the Fermi velocity. Then

$$\kappa=\tfrac{1}{3}C_V V_F^{\,2}\tau_0(3/2\pi^2)K\ . \tag{B17}$$

Here we have introduced the specific heat $C_V=k^2Tm^*k_F/(3\hbar^2)$ and defined

$$K=\int dt\ (t/\cosh\tfrac{1}{2}t)Q(t)\ . \tag{B18}$$

Once $Q(t)$ is obtained as a solution of (B13) we insert it in (B18) and get κ from (B17).

The coefficient of spin diffusion D and viscosity η are obtained by substituting $(\cosh\frac{1}{2}t)^{-1}$ for $t/\cosh\frac{1}{2}t$ as the inhomogeneous part of (B13) and otherwise leaving the equation unaltered. The meaning of α is, however, different. For the case of viscosity it is obtained from (B15) by replacing $(1+2\cos\theta)$ with $(1-3\sin^2\varphi\sin^4\frac{1}{2}\theta)$ and using the appropriate w_η. For spin diffusion α similarly involves $\cos\theta(1-\cos\varphi)+\cos\varphi$ and w_D (see Wheatley[18] for a discussion of the difference between w_κ and w_D). The characteristic time τ_0 is given by Eq. (B8) with w_η and w_D, respectively, instead of w.

The transport coefficients η and D are then given by

$$\eta=\tfrac{1}{5}nm^*V_F^{\,2}\tau_0\tfrac{1}{2}Y,\qquad D=\tfrac{1}{3}(\chi_0/\chi)V_F^{\,2}\tau_0 d,\quad\text{where}\quad Y,d=\int(\cosh\tfrac{1}{2}t)^{-1}Q(t)\,dt\ .$$

Here n is the number density and χ_0/χ the ratio of the Pauli susceptibility for the noninteracting system to that of the interacting one.

APPENDIX C: EXACT SOLUTION OF (3.1)

We here derive the exact result[6] (3.4) for the reduced thermal conductivity $K=\int dt\,X(t)Q(t)=(X,Q)$.[19] Consider the homogeneous equation obtained by setting $X=0$ in (3.1). We may write this as an eigenvalue equation

$$f(t)\varphi_n(t)=\lambda_n\int dt'F(t-t')\varphi_n(t') \tag{C1}$$

and seek to determine the eigenvalues λ_n and eigenfunctions $\varphi_n(t)$, which we shall normalize according to

$$\int dt\,f(t)\varphi_n(t)\varphi_m(t)=\delta_{n,m}\ . \tag{C2}$$

A complete set of eigenfunctions φ_n, if known, may be used to expand the unknown solution $Q(t)$ of the inhomogeneous equation (3.1) or for more rapid convergence $Q(t)-X(t)/f(t)$

$$Q(t)=X(t)/f(t)+\textstyle\sum_n a_n\varphi_n(t)\,. \qquad \text{(C3)}$$

By inserting (C3) in (3.1), using (C1) and (C2) we determine

$$a_n=[\alpha/(\lambda_n-\alpha)]\,(X,\varphi_n)\,, \qquad \text{(C4)}$$

and hence

$$K=(X,X/f)+\alpha\textstyle\sum_n (X,\varphi_n)^2/(\lambda_n-\alpha)\,. \qquad \text{(C5)}$$

We Fourier transform the Eq. (C1) according to

$$\varphi_n(t)=(2\pi)^{-1}\int dq\,\tilde{\varphi}_n(q)\,e^{iqt/\pi}\,. \qquad \text{(C6)}$$

The Fourier transforms of $f(t)$, $F(t-t')$, and $X(t)$ are $\pi^2(1-\partial^2/\partial y^2)$, $\pi/(\cosh y)^2$, and $-2\pi i\,\sinh y/(\cosh y)^2$, respectively. The integral equation (C1) then becomes the differential equation

$$\left(-\frac{d^2}{dq^2}+1-\frac{\lambda_n}{\cosh^2 q}\right)\tilde{\varphi}_n(q)=0\,. \qquad \text{(C7)}$$

Provided $\lambda_n=n(n+1)$, with n a positive integer, (C7) is just the equation for the associated spherical harmonics $P_n^{\,1}(\tanh q)$, which form a complete set. By virtue of the normalization condition (C2) the eigenfunctions of (C7) are now determined to be

$$\tilde{\varphi}_n=c_nP_n^{\,1}(\tanh q)$$

with $c_n^{\,2}=[(-1)^{n+1}/\pi^2]\,(2n+1)/n^2(n+1)^2\,.$ (C8)

The integrals in (C5) may be transformed into integrals over the transformed functions to yield[20]

$$K=\tfrac{1}{3}(12-\pi^2)+4\alpha\sum_{n=2,4,\ldots}\frac{2n+1}{n^2(n+1)^2}\,\frac{1}{n(n+1)-\alpha} \qquad \text{(C9)}$$

which is Eq. (3.4).

For the spin-diffusion and viscosity coefficients we get (cf. Appendix B)[20]

$$Y,d=\tfrac{1}{3}+\frac{4\alpha}{\pi^2}\sum_{n=1,3,\ldots}\frac{2n+1}{n^2(n+1)^2}\,\frac{1}{n(n+1)-\alpha}\,. \qquad \text{(C10)}$$

The results (C9) and (C10) are special cases of the general solution of an integral equation like (3.1) with $f(t)=\pi^2+t^2$ replaced by $\pi^2(1+\beta)+t^2$ (β positive). We have elsewhere[5] considered such an equation which arises when scattering against impurities is included in the collision integral of the Boltzmann equation in addition to the particle-particle scattering. Here $\beta=(2/\pi^2)\tau_0/\tau_{\text{imp}}$, where τ_{imp} is the relaxation time characterizing the elastic impurity scattering.

If $\beta=m^2-1$ (m an integer) the solutions may be expanded in terms of a complete set consisting of the associated spherical harmonics $P_n^{\,m}(\tanh q)$ with $n=m,m+1,\ldots$. The resulting transport coefficients are then given by

$$T(\alpha,\beta)=c(m)+\sum_{n\geqslant m}\frac{\alpha}{n(n+1)-\alpha}\,\frac{2n+1}{\pi^2n(n+1)}\,\frac{(n-m)!}{(n+m)!}\,A_{nm}^{\;2}\,,$$

$$m=(1+\beta)^{1/2}\,. \qquad \text{(C11)}$$

We have listed expressions for $c(m)$ and A_{nm} in Table III for the cases $m=1$, 2, and 3.

In the more general case, where $1+\beta=\nu^2$ and is not necessarily an integer, one may use the set $(1-x^2)^{\nu/2}\,C_n^{\,\nu+1/2}(x)$ where $x=\tanh q$ and $n=0$, 1, 2 $\cdots$. The function $C_n^{\,\nu+1/2}(x)$ is a Gegenbauer polynomial.[21] When ν is an integer the set series with the same structure as (C11).[22] The nth term in the series belonging to a fixed ν (or β) is a lengthy expression involving Γ functions of various combinations of ν and n and we shall therefore not quote it here.

Simple approximate (but quite accurate) expressions for the transport coefficients $T(\alpha,\beta)$ are given in Ref. 5 as the result of applying the variational methods discussed in the present paper to the appropriate integral equation.

APPENDIX D: CONNECTION WITH EMERY'S APPROACH

To show the connection to the variational method we briefly review the method used by Emery (Ref. 8) to obtain an approximate solution of (3.1). We discuss only the case of thermal conductivity since the treatment of viscosity and spin diffusion is identical in form.

Emery noted that the homogeneous part of (3.1) at $\alpha=6$ has the solution $Q(t)=t(\cosh\frac{1}{2}t)^{-1}=X(t)$, which is not orthogonal to the inhomogeneous term. He then approximated for all values of α the kernel $F(t-t')$ in (3.1) with the separable kernel $\hat{F}(t,t')$ given by

$$\hat{F}=\frac{1}{6}\,\frac{f(t)X(t)f(t')X(t')}{\int du\,X^2(u)f(u)}\,. \qquad \text{(D1)}$$

This choice ensures that

$$\int dt'\,\hat{F}(t,t')X(t')=\int dt'\,F(t-t')X(t')$$

TABLE III. The values of $c(m)$ and A_{nm} in (C11) for $m=1, 2,$ and 3. The coefficients A_{nm} vanish when n is not even or odd as specified in the last column.

Transport coefficient	m	$c(m)$	A_{nm}	n
Thermal conductivity	1	$4-\pi^2/3$	2π	even
	2	$20-2\pi^2$	$\pi^2\,(n+2)!!\,(n-2)!!/(n+1)!!\,(n-3)!!$	odd
	3	$10-\pi^2$	$2\pi\,(n+3)\,(n-2)$	even
Spin diffusion and viscosity	1	$\frac{1}{3}$	2	odd
	2	$\frac{1}{2}-4/\pi^2$	$\pi(n+1)!!\,(n-1)!!/n!!\,(n-2)!!$	even
	3	$\frac{1}{9}-2/3\pi^2$	$2(n+2)\,(n-1)$	odd

$$=\tfrac{1}{6}f(t)X(t)\,.$$

With the replacement of F by $\hat{F}$ the integral equation (3.1) becomes

$$X=fQ-\tfrac{1}{6}\alpha fX\left[\int du\,X^2(u)f(u)\right]^{-1}\times\int dt' f(t')X(t')Q(t')\,. \qquad \text{(D2)}$$

To find Q from this equation we need to determine the constant $\int dt\,f(t)Q(t)X(t)$. This is done by multiplying (D2) with $X(t)$ and integrating over t. Then

$$\int dt\,f(t)X(t)Q(t)=\tfrac{4}{3}\pi^2(1-\tfrac{1}{6}\alpha)^{-1}\,, \qquad \text{(D3)}$$

which shows that $\hat{F}$ is positive definite for $\alpha<6$. We can now solve (D2) for $Q(t)$ with the result

$$Q(t)=X(t)/f(t)+(5/12\pi^2)[\alpha/(6-\alpha)]\,X(t)\,, \qquad \text{(D4)}$$

which corresponds to Eq. (3.10) of Ref. 8.

The value of the (reduced) thermal conductivity corresponding to the solution (D4) is

$$K=\tfrac{1}{3}(12-\pi^2)+\tfrac{5}{9}[\alpha/(6-\alpha)]\,. \qquad \text{(D5)}$$

We observe that (D5) is just the bound (3.20) or equivalently the first two terms of the exact solution (3.4). By his method, Emery therefore obtained a lower bound on K for $\alpha>0$ and an upper bound for $\alpha<0$.

Instead of solving the approximated integral equation directly, we could, of course, apply the variational methods to it since $\hat{F}$ is symmetric and positive definite for $\alpha<6$. With F replaced by $\hat{F}$ in (2.13) this bound becomes independent of the choice of trial function $U(t)$ and hence equal to the (exact) solution (D5) of the (approximated) integral quation (D2).

APPENDIX E: BETTER BOUNDS

Although lower bounds of the type (2.11), i.e., when H' is negative definite, are in general more difficult to work with than the simple (2.6), they have the appealing property of always being larger (i.e., better) than the lower bound (2.6), provided the trial functions are the same. This was demonstrated by Arthurs and Robinson[4] using their rather different approach for the special case $J=1$.

We shall consider the more general case, where the positive definite H can be written as a sum of a positive definite J and a negative definite L. Since H' then is negative definite (see Appendix F for proof of this), we obtain the inequality [compare Eq. (2.4)]

$$(Q,X')\leq 2(U,X')-(U,H'U)\,. \qquad \text{(E1)}$$

With $H'=HJ^{-1}H-H$ and $X'=HJ^{-1}X-X$ this inequality becomes upon rearrangement

$$(Q,X)\geq([Q-U),HJ^{-1}H(Q-U)]\;.+[2(U,X)-(U,HU)]\,. \qquad \text{(E2)}$$

The quantity in square brackets is the lower bound one obtains from (2.4) by setting $\lambda=1$. If the normalization of U is chosen such that $(U,X)=(U,HU)$, this bound becomes identical to (2.6). Since the first term on the right-hand side of (E2) is always positive, the bound (E2) with the chosen normalization of U is always better (i.e., larger) than (2.6). The best lower bound (E2) is of the form (2.11), in which the normalization of U does not appear explicitly. Therefore, a lower bound of type (2.11) is always better than (2.6), provided we use the same trial functions.

On the other hand, one does not in general know whether an upper bound of the type (2.11), i.e., when H' is positive definite, is closer to the exact result than the lower bound (2.6), for the same trial function.

APPENDIX F: CONDITIONS FOR H BEING NEGATIVE SEMIDEFINITE

In this Appendix, we prove that $H'=HJ^{-1}H-H$ is negative semidefinite for H and J positive definite and $L=H-J$ negative definite. We specify these conditions precisely (note that H is positive semidefinite) by the equations

$$(\varphi, H\varphi) \geq 0, \tag{F1a}$$

$$(\varphi, J\varphi) > 0, \tag{F1b}$$

$$(\varphi, L\varphi) < 0, \tag{F1c}$$

for arbitrary φ. We expand φ in terms of a complete orthonormal set of eigenfunctions φ_n obtained from

$$J\varphi_n = -\lambda_n L\varphi_n \tag{F2}$$

and orthonormalized according to

$$(\varphi_m, J\varphi_n) = \delta_{n,m}\ , \tag{F3}$$

which is compatible with (F2) in the sense that it follows from (F2) for $\lambda_n \neq \lambda_m (n \neq m)$.

With $\varphi = \sum_n a_n \varphi_n$ we have

$$\begin{aligned}(\varphi, H'\varphi) &= (\varphi, (L + LJ^{-1}L)\varphi) \\ &= \sum_{mn} a_m a_n \left\{ \left(\varphi_m, -\frac{1}{\lambda_n} J\varphi_n\right) + \left(\varphi_m, -\frac{1}{\lambda_n}\left[-\frac{1}{\lambda_n}\right] J\varphi_n\right)\right\} \\ &= \sum_n a_n^2 \left[-\frac{1}{\lambda_n}\right]\left(1 - \frac{1}{\lambda_n}\right)\ .\end{aligned} \tag{F4}$$

From (F2) we get $(\varphi_n, J\varphi_n) = -\lambda_n(\varphi_n, L\varphi_n)$, which together with (F1b) and (F1c) shows that $\lambda_n > 0$. Similarly $(\varphi_n, H\varphi_n) = (1-\lambda_n)(\varphi_n, L\varphi_n)$ together with (F1a) and (F1c) implies that $(1-\lambda_n) \geq 0$. Hence, (F4) is either negative or zero, and H' therefore, negative semidefinite.

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[9] The authors are indebted to N. D. Mermin for stressing this point of view.

[10] An equivalent, but less convenient form, is $T \geq (U, X)$ provided U satisfies the normalization condition $(U, X) = (U, HU)$.

[11] It might appear that the smallest eigenvalue of H for the case of the Boltzmann equation is zero, since the original collision integral (see Appendix B) conserves number, momentum, and energy. However, we only consider distortions of the Fermi distribution which correspond to quantities which are *not* conserved by the collision integral. Accordingly, the zero eigenvalues have already been projected out when the operator H is introduced.

[12] Arthurs and Robinson considered an integral equation of the type (2.1) with $f = 1$ and a positive-definite symmetric F. Their result [Eq. (47) in Ref. 4] is identical to (2.13) with $f = 1$.

[13] A. A. Abrikosov and I. M. Khalatnikov, Rept. Progr. Phys. 22, 329 (1959), henceforth referred to as AK.

[14] The result (3.15) is due to G. Baym (see Ref. 8) and is obtained with the customary choice of trial function $\psi_p(t)$ (see Appendix B for definition). We have introduced $Q(t)$ so that $\psi_p(t) \propto \cosh\frac{1}{2}t\, Q(t)$. This means that a trial function $U(t) \propto t/(\cosh\frac{1}{2}t)$ corresponds to a (trial) $\psi_p \propto t$, which is in fact the usual choice made (Ref. 1).

[15] The maximum value of $\alpha = 6$ corresponds to the special case of forward scattering in which the colliding particles have parallel momenta.

[16] P. Morel and P. Nozieres, Phys. Rev. 126, 1909 (1962).

[17] From (B15) we observe that the range of α is $-2 < \alpha < 6$. Since negative values of α correspond to rather pathological $w(\theta, \varphi)$, we have focused our attention on the range $0 < \alpha < 6$ in the discussion of the bounds on the thermal conductivity in Sec. III. However, the bounds apply to the region of negative α as well, although some of them change from upper to lower ones and vice versa at $\alpha = 0$ (cf. Sec. II).

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[22] A. J. Bennett and M. J. Rice (unpublished) have used this set to obtain the exact solution for all values of β. These authors expand the solution Q itself rather than $Q - X/f$ as in the present work and Ref. 6 [cf. (C3)]. Their resulting series for the transport coefficient converges therefore much slower than (C9)–(C11) and the similar expression for arbitrary β.

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Fluctuations and the Onset of Superfluidity

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The onset of superfluidity in thin (~ 20 Å) He II films is discussed in terms of fluctuations on the Ginzburg-Pitaevskii free-energy functional. The response of the system to an external force is presented in a linearized form. Fluctuations of quantum origin are included explicitly. The theory indicates that the onset thickness is proportional to the coherence length, in agreement with experimental observations. An outline for a method for the calculation of the superfluid density in the bulk within the same simple approximation is given.

I. INTRODUCTION

Mass flow,[1,2] heat flow,[3-5] and third sound[6,7] experiments in thin He II films indicate that for any given temperature $T (T < T_\lambda)$, the film loses its superfluid properties when the film thickness becomes less than a certain characteristic thickness $d_c(T)$. These results were summarized recently in Ref. 7 where the unsaturated vapor pressure at the onset of superfluidity was plotted against the onset temperature (Fig. 2, Ref. 7). Thermodynamics relates the film equilibrium thickness $d(T)$ to the unsaturated vapor pressure P by[7]

$$d^3(T) = \frac{87\,°\mathrm{K}}{T \ln(P_0/P)} \quad . \tag{1}$$

In Eq. (1), d is given in atomic layers (1 a.l. $= 3.6 \times 10^{-8}$ cm) and P_0 is the saturated pressure at the temperature in question. We shall work exclusively with the film thickness $d(T)$ rather than the experimental parameter P_0/P.

The onset of dissipation in thin films is a familiar phenomenon in superconductivity. There it is widely accepted[8,9] that superconductivity does not exist in two dimensions (2D henceforth). Nonetheless very thin films of superconductor materials exhibit a very high conductivity.[10,11] The theoretical reasonings which interpret these results were pioneered by Aslamazov and Larkin.[12] These reasonings were refined and greatly simplified by several authors.[13-16] The theory as presented in this paper is closely analogous to those advanced for 2D superconductors, in particular to those considerations[14-16] that were given in terms of the Ginzburg-Landau equation. Our considerations shall proceed in terms of the Ginzburg-Pitaevskii equation (G-P henceforth; the equation is given in Sec. II) which is formally equivalent to the Ginzburg-Landau equation. [In either case, superconductors (SC henceforth) or superfluids (SF henceforth), the use of these equations is justified inasmuch as we are interested in the behavior of the system near the transition.] There are two important differences between the SC and SF cases.[17] The first is that in SF one does not measure the energy dissipation ("resistance") as a function of temperature for a fixed film thickness; while this is what is measured in the SC case. Rather, one observes in the case of He II the appearance of appreciable dissipation for a fixed temperature as a function of film thickness. The second difference is in the meaning of "two dimensional." For SC a 2D film is one whose thickness d is smaller than the