

ty space. The latter should strongly effect the peaks near $n\omega_c$ at high densities.⁹ Interactions higher than second-order have also been observed, and can be explained by an extension of the theory presented here. A detailed account of the present work is in preparation and will be published at a later date.

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TRANSPORT COEFFICIENTS IN DEGENERATE FERMI SYSTEMS*

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A method of calculating the transport coefficients of a degenerate Fermi system is described and compared with previous approaches. Applications to dilute mixtures of He³ in liquid He⁴ and to nearly ferromagnetic Fermi liquids are given.

It has become clear that the derivation of expressions for the transport coefficients of a degenerate Fermi system should be re-examined. At low temperatures, mean free times may be expanded in the form^{1,2}

$$1/\tau = aT^2 + bT^3, \quad (1)$$

where T is the absolute temperature and a and b are coefficients which depend upon the transport process. Two methods have been used to obtain τ . One is a direct approximate solution of the Boltzmann equation,^{2,3} the other a variational calculation,^{1,4} and they give different values of a and b . The discrepancy is particularly serious for the thermal conductivity κ .

In this Letter, we give the results of a more accurate approximation and discuss its relationship to the earlier approaches. During the course of this work, Brooker and Sykes⁵ and, independently, Jensen, Smith, and Wilkins,⁶ found a way

of calculating a exactly. The latter authors also applied their results to dilute mixtures of He³ in liquid He⁴, using the approximate scattering amplitude of Bardeen, Baym, and Pines. The method which will be described here is much easier to apply and gives simple explicit expressions for both a and b , with an error which is of the order of 1% for systems of physical interest.

The collision term in the linearized Boltzmann equation has the form of an integral operator $K_0(x, t)$ acting upon a function $q(t)$, which is proportional to the difference δn between the distribution function and its equilibrium value.³ Here t is the variable $(\epsilon - \mu)/k_B T$, where ϵ is a quasi-particle energy, μ is the chemical potential, and k_B is Boltzmann's constant. [See Eq. (7.19) of Abrikosov and Khalatnikov.³] The method which we have used is based upon the fact that, for the viscosity η and spin diffusion D , $q(t)$ is an even function of t and that the even eigenfunction of

$K_0(x, t)$ corresponding to the largest eigenvalue is a constant, independent of t . It turns out that, for the important values of t , $q(t)$ does not differ very much from a constant, and so its overlap with the other eigenfunctions is small. In addition, the eigenvalues of $K_0(x, t)$ form a decreasing set. Therefore, it should be a good approximation to replace $K_0(x, t)$ by a separable kernel which projects onto the principal eigenfunction. The same is true of the thermal conductivity, except that $q(t)$ is an odd function of t and the relevant eigenfunction is a constant times t .

The Boltzmann equation may then be solved explicitly and, to lowest order in the temperature, it is found that $q(t) = Q(t)$ for D and η and $q(t) = tQ(t)$ for κ , where

$$Q(t) = \tau_{\text{QP}} \left[\frac{1}{1+t^2/\pi^2} + \left(\frac{1}{\tau_{\text{QP}}} - \frac{1}{\tau_A} \right) \frac{\tau_A}{\langle 1+t^2/\pi^2 \rangle} \right]. \quad (2)$$

Here τ_A is the mean free time calculated by Abrikosov and Khalatnikov³ or Hone³ and τ_{QP} is the lifetime of a quasiparticle on the Fermi surface—both evaluated to lowest order in T . Expressions for these quantities are given in Ref. 2. The factors $1+t^2/\pi^2$ come from integrals of Fermi functions, as usual, and the average $\langle f(t) \rangle$ is defined to be

$$\langle f(t) \rangle = \frac{\int_{-\infty}^{\infty} dt n(t) [1-n(t)] h(t) f(t)}{\int_{-\infty}^{\infty} dt n(t) [1-n(t)] h(t)}, \quad (3)$$

where $n(t)$ is a Fermi function and $h(t) = 1$ for D and η and $h(t) = t^2$ for κ .

Equation (2) may be understood as follows. As a quasiparticle, with energy $k_{\text{B}}Tt$ above the Fermi surface, moves through the medium, it undergoes a series of two-body collisions. If the background quasiparticles are assumed to be in thermal equilibrium, $Q(t)$ is given by $\tau_{\text{QP}}(1+t^2/\pi^2)^{-1}$, which is the same as the relaxation time for a single quasiparticle added to the system. This is the first term on the right-hand side of Eq. (2). In a transport process, the disturbance of the distribution function of the background particles, which is proportional to $\tau_A/\langle 1+t^2/\pi^2 \rangle$, may not be neglected and this gives rise to the second term in $Q(t)$. By definition, τ_A^{-1} contains a contribution from the incident particle which has already been included, and τ_{QP}^{-1} is

there to remove it. The mean free time is given by

$$\begin{aligned} \tau_0 &= \langle Q(t) \rangle \\ &= \tau_{\text{QP}} \left\langle \frac{1}{1+t^2/\pi^2} \right\rangle + \frac{\tau_A^{-1} \tau_{\text{QP}}}{\langle 1+t^2/\pi^2 \rangle}. \end{aligned} \quad (4)$$

This expression is for the lowest order in temperature, corresponding to aT^2 in Eq. (1).

The variational approximation^{1,4} amounts to replacing $1+t^2/\pi^2$ by $\langle 1+t^2/\pi^2 \rangle$ in Eq. (2) and then $Q(t)$ is $\tau_A/\langle 1+t^2/\pi^2 \rangle$, which is the same as the averaged value for the background particles. In this approximation, Eq. (4) gives

$$\tau_{\text{var}} = \tau_A / \langle 1+t^2/\pi^2 \rangle. \quad (5)$$

Abrikosov and Khalatnikov³ and Hone³ additionally neglect t^2/π^2 .

It should be noticed that τ_{QP} , unlike τ_A , is independent of the transport process. Thus, for example, according to Eq. (4), the spin-diffusion coefficient D depends upon parallel spin scattering (through τ_{QP}) although, in the earlier approximations, it did not.

On evaluating the averages in Eq. (4), it is found that

$$\tau_0 = \frac{1}{12\pi^2} \tau_{\text{QP}} + \frac{3}{4} (\tau_A^{-1} \tau_{\text{QP}}) \quad (6)$$

for D and η and

$$\tau_0 = \left(3 - \frac{\pi^2}{4} \right) \tau_{\text{QP}} + \frac{5}{12} (\tau_A^{-1} \tau_{\text{QP}}) \quad (7)$$

for κ .

Since $\tau_{\text{QP}} > 0$, it can be seen that $\tau_0 > \tau_{\text{var}}$. From the definitions of τ_{QP} and τ_A , it is easy to show that τ_{QP}/τ_A has upper limits of 3 for η , 4 for D , and $\frac{4}{3}$ for κ , whatever the quasiparticle scattering amplitude. It follows that τ_0/τ_A is less than 0.97 for η , 1.04 for D , and 0.57 for κ , so that τ_0 can come close to τ_A for D and η , but it is always considerably less than τ_A for κ . The upper limits for τ_{QP}/τ_A are extreme cases and, in practice, $\tau_{\text{QP}} \approx \tau_A$, so that $\tau_0/\tau_A \approx \frac{1}{12}\pi^2$ for D and η and $\tau_0/\tau_A \approx (3 - \frac{1}{4}\pi^2)$ for κ .

Equation (4) agrees with the exact solution,⁵ when $\tau_{\text{QP}} = \tau_A$. The maximum error occurs when τ_{QP}/τ_A is a maximum, and it is 4.6% for η , 7.9% for D , and 1.8% for κ . Once again, these are extremes and, since usually $\tau_{\text{QP}} \approx \tau_A$, the typical error in Eq. (4) is much smaller, perhaps 1%.

The most interesting systems for applications of Eq. (4) are dilute mixtures of He³ in liquid He⁴, for which the experiments have been carried out in most detail at He³ concentrations of 1.3 and 5%, and analyzed⁶ in terms of an effective He³-He³ interaction, assumed to be a hard core with a longer range attractive square well. The potential parameters were chosen to fit the spin-diffusion data using τ_A , and other quantities were predicted. We have now repeated these calculations using τ_0 instead. The required change in the potential is rather small, and the equilibrium properties are substantially as before.⁶ The values of κT in erg/cm sec changed from 19.1 at 1.3% and 64 for 5% using τ_A to 12.1 at 1.3% and 33.3 at 5% using τ_0 . Experimentally,⁷ κT is 11 at 1.3% and 24 at 5%, so that the new solution constitutes a considerable improvement. There is still a disagreement between theory and experiment for κT at 5% concentration, but there is little doubt that this could be removed by varying the shape of the potential from the original

form, which was chosen for ease of calculation. It does not seem to be worthwhile to do so at present, since the existing data clearly are far from being sufficient to determine the potential uniquely.

We now consider the calculation of the coefficient b in Eq. (1). This depends upon scattering with small energy and momentum transfer,² and it is particularly important for nearly ferromagnetic systems.¹ The integral operator in the collision term of the Boltzmann equation has to be calculated to first order in T and becomes $K_0(x, t) + TK_1(x, t)$. An expansion in powers of T corresponds to an expansion in $K_1(x, t)$ and it is sufficient to work to first order. Then the approximation described above may be applied to $K_0(x, t)$, but it is not necessary to use it for $K_1(x, t)$. The assumption that $Q(t)$ does not differ too much from a constant turns out to be just as good as before, so that the errors should be small. For the present, we shall merely quote the results for a nearly ferromagnetic system.^{1,2}

For the spin diffusion,

$$\frac{1}{\tau} - \frac{1}{\tau_0} = \frac{3}{4} \zeta(3) \pi^3 \frac{k_B T^3}{h T_F^2} \left| \frac{\frac{1}{4} Z_0}{1 + \frac{1}{4} Z_0} \right|^3 \left\{ 1 - \frac{\pi^2}{6 \zeta(3)} [\zeta(3) - 1] \frac{\tau_{QP}}{\tau_0} + 0.0663 \frac{\tau_{QP}^2}{\tau_0^2} \right\}. \quad (8)$$

For the viscosity,

$$\frac{1}{\tau} - \frac{1}{\tau_0} = -0.056 \pi^3 \frac{k_B T^3}{h T_F^2} \left| \frac{\frac{1}{4} Z_0}{1 + \frac{1}{4} Z_0} \right|^3 \frac{\tau_{QP}}{\tau_0^2}. \quad (9)$$

For the thermal conductivity,

$$\frac{1}{\tau} - \frac{1}{\tau_0} = -\frac{135 \pi \zeta(5)}{8} \frac{k_B T^3}{T_F^2} \left| \frac{\frac{1}{4} Z_0}{1 + \frac{1}{4} Z_0} \right|^3 \left[1 - 0.1642 \frac{\tau_{QP}}{\tau_0} + 0.0808 \frac{\tau_{QP}^2}{\tau_0^2} \right]. \quad (10)$$

Here, Z_0 is an average forward-scattering amplitude and appears in the same way in Ref. 6. The degeneracy temperature is denoted by T_F and $\zeta(\nu)$ is Riemann's zeta function of argument ν . All of the coefficients of τ_{QP}^2/τ_0^2 and the coefficient of τ_{QP}/τ_0 in Eq. (10) were obtained by numerical integration.

The variational approximation gives Eqs. (8)-(10) with $\tau_{QP} = 0$. The numerical coefficients differ from those obtained by Rice,¹ since he made additional assumptions.² The method of Ref. 2 is an extension of that of Abrikosov and Khalatnikov³ and it too omits terms involving τ_{QP} and gives different numerical coefficients.

Otherwise, the main qualitative differences

from the previous results^{1,2} are that (a) now there is a term proportional to T^3 in τ^{-1} for the viscosity, and (b) since τ_{QP} and τ_0 appear, the coefficients of the T^3 terms do not depend only upon the forward-scattering amplitudes.²

Within the allowed range of values of τ_{QP}/τ_A , the corrections from the terms involving τ_{QP} for D in Eq. (7) are less than 35% and, typically, are about 20%. For κ they are less than 10%. For η , $1/\tau - 1/\tau_0$ is about $0.03 \tau_{QP}^2/\tau_0^2$ times $1/\tau - 1/\tau_0$ for κ . Thus, usually, the T^3 term in η will not be large, although it could be significant if τ_{QP}/τ_0 took on its extreme value of 3.1.

A detailed account of these calculations will be

published later.

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LATTICE VIBRATIONS IN SILICON: MICROSCOPIC DIELECTRIC MODEL*†

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The phonon-dispersion curves in silicon are calculated from a microscopic model by a dielectric screening theory. The part of the dynamical matrix arising from the diagonal part of the inverse dielectric-function matrix is calculated just as in metals; the off-diagonal part is approximated by interactions of ions and bonds treated as point charges in Phillips's bond-charge model.

Neutron-scattering experiments have measured the phonon dispersion curves $\omega(\vec{q})$ in diamond,¹ silicon,² and germanium³ for wave vector \vec{q} along the principal symmetry directions [100], [111], and [110]. So far the data have been analyzed only in terms of classical spring models. A successful analysis was carried out for diamond by McMurry et al.⁴ using only bond-stretching and -bending force constants derived from hydrocarbons. However, in order to fit the dispersion curves for Si and Ge,⁵ distant neighbor forces must be introduced requiring many parameters. Even the most successful model, the Cochran shell model,⁶ requires 11 adjustable parameters² to fit $\omega(\vec{q})$ along all the symmetry directions in Si. In this Letter we report the results of the first microscopic calculation of $\omega(\vec{q})$ for Si. The approach utilizes ion-core properties based on free-ion quantum term values as well as valence screening properties based on the quantum electronic spectrum of the crystal. One parameter affecting only longitudinal modes is used in the present calculation.

The microscopic dielectric theory for the covalently bonded crystals closely resembles the dielectric-screening approach^{7,8} which has been used in metals such as Na and Al. In the calculations for metals, the dielectric function is that of the free-electron gas, and the ion-core potential is represented by a model potential based on free-ion spectroscopic term values.⁹ An identical approach using free-electron screening theory is not satisfactory in covalent crystals as is indicated by the fact that such loosely packed structures are not stable against shear in the presence of nearest-neighbor central forces only.¹⁰ This instability against shear has been verified by one of our calculations for Si which used the free-electron dielectric function to screen the ion-ion interactions. As expected, all TA-mode frequencies were found to be imaginary.

A general expression,¹¹ valid in any crystal, for the dynamical matrix in terms of the complete inverse dielectric-function matrix $\epsilon^{-1}(\vec{q} + \vec{G}, \vec{q} + \vec{G}')$ is

A general expression,¹¹ valid in any crystal, for the dynamical matrix in terms of the complete inverse dielectric-function matrix $\epsilon^{-1}(\vec{q} + \vec{G}, \vec{q} + \vec{G}')$ is

$$D_{\alpha\beta}(\vec{q}) = \bar{D}_{\alpha\beta}(\vec{q}) - \delta_{\alpha\beta} \sum_{\gamma=1}^s \bar{D}_{\alpha\gamma}(0) \left(\frac{M_\gamma}{M_\beta} \right)^{1/2}, \quad (1a)$$

where

$$\begin{aligned} \bar{D}_{\alpha\beta}(\vec{q}) = & \frac{1}{(M_\alpha M_\beta)^{1/2}} \frac{\Omega}{4\pi e^2} \sum_{\vec{G}, \vec{G}'} \frac{(\vec{q} + \vec{G})(\vec{q} + \vec{G}')}{|\vec{q} + \vec{G}'|^2} |\vec{q} + \vec{G}|^2 v_i^\alpha(|\vec{q} + \vec{G}|) \exp(i\vec{G} \cdot \vec{R}_\alpha) \\ & \times \epsilon^{-1}(\vec{q} + \vec{G}, \vec{q} + \vec{G}') |\vec{q} + \vec{G}'|^2 v_i^\beta(|\vec{q} + \vec{G}'|) \exp(-i\vec{G}' \cdot \vec{R}_\beta). \end{aligned} \quad (1b)$$