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Raman Scattering from Superconductors*

F. G. DOS REIS and R. LUZZI
Instztuto de Física Gleb Wataghin , Universidade Estadual de Campinas, Campinas SP

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A study of the Raman spectrum of light scattered by a superwnductor is presented. The formalism described in previous article (Rev. Brasil. Fis. 2, 337 (1972)) is used. The dielectric constant of the superconducting media, which enters into the expression for the cross section, is approximated by the RPA result of Rickayzen It is shown that Coulomb interaction between electrons produces a sereening of the quast-elastic single-particle scattering and of the scattering from plasma waves The dependence of this spectra on the experimental geometry is discussed.

Apresenta-se um estudo do espectro Raman de luz espalhada por um supercondutor, utilizando-se um formalismo descrito em artigo anterior (Rev. Brasil. Fis. 2, 337 (1972)). A constante dielétrica do meio supercondutor, que entra na expressão da seção de choque, é aproximada pelo resultado de Rickayzen, obtido pela aproximação RPA. Mostra-se que a interação coulombiana entre os eletrons produz um ***screening*** do espalhamento quasi-elástico de partícula independente e do espalhamento por ondas de plasma. Discute-se a dependència desse espectro com a geometria.

1. Introduction

In a previous article', hereafter referred to as (I), a semiclassical study of surface Raman scattering was presented and the connection between the scattering cross section and the imaginary part of a generalized susceptibility was discussed. In this work we make a specific use of those results by studying Raman scattering by a superconducting sample. The response of superconductors to electromagnetic fields is of particular interest because it can produce information on the excitation spectra. However, up to present day, only infrared absorption experiments have been successful. Studies of photoluminescence and Raman scattering have not produced *clean* results[2,3]. However, it is believed that improvement in detection techniques could render this kind of experiments worthwhile.

Abrikosov and Falkovskii performed a calculation of Raman scattering upon reflection of light from the surface of a superconductor, by evaluating

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'Postal address: 13.100 – Campinas SP.

the relevant S-matrix using diagramatic techniques[4]. We reconsider here Raman scattering from a superconducting surface using the unified formalism described in (I). Electron-electrón interaction is included. This interaction produces screening effects on the portion of the Raman spectrum associated with scattering from single-particle excitations and an additional line at the plasma frequency ω_p. The first line, quasi-elastic scattering from excitations of the Cooper-pairs, predominates in the case of experimental geometnes that produce large momentum transfer. In this case, we show that our results go over to those of Ref. 4. On the other hand, in conditions of small momentum transfer, almost all scattered light is concentrated in the line at the plasma frequency and the line-shape is almost identical with that of a normal metal.

2. The Scattering Cross Section

Since charge density fluctuations are responsible for light scattering in charged materials, one needs to make in Eq. (3-2) of (I) the identifícations

$$\alpha_{\beta\gamma,\mu} \to \frac{\delta\varepsilon}{\partial\rho_0} = -\frac{1}{\rho_0}\frac{\omega_p^2}{\omega^2} \tag{2-1}$$

and

$$\langle Q_\mu^*(\mathbf{q})\, Q_\mu(\mathbf{q})\rangle_\omega \to \langle\rho(-\mathbf{q})\,\rho(\mathbf{q})\rangle_\omega , \tag{2-2}$$

where ρ_0 is the electron density, ω_p the plasma frequency and $\rho(\mathbf{q})$ the Fourier amplitude of the charge fluctuation of wavenumber q, the momentum transfer.

Next, we use the fluctuation-dissipation theorem [Eq. (3-13) of (I)] to obtain[5]

$$\frac{4\pi e^2}{q^2}\langle\rho^+(\mathbf{q})\,\rho(\mathbf{q})\rangle_\omega = \frac{1}{\pi}\,[1-e^{-\beta\omega}]^{-1}\,\mathrm{Im}\,\varepsilon^{-1}(\mathbf{q},\omega) \tag{2-3}$$

where $\varepsilon(\mathbf{q},\omega)$ is the space and time Fourier transform of the dielectric constant. Using the time-dependent Bogoliubov's average field approximation, Rickayzen[6] derived the dielectric constant $\varepsilon(\mathbf{q},\omega)$ of a superconductor described by the Bardeen-Cooper and Schrieffer theory[7]. Neglecting the fluctuations in the Cooper pairs density, it reads at T = 0°K:

$$\frac{1}{\varepsilon(\mathbf{q},\omega)} - 1 = \sum_{\mathbf{k}}\frac{1}{2}\left[1-\frac{\varepsilon_{\mathbf{k}}\,\varepsilon_{\mathbf{k}+\mathbf{q}}-\Delta^2}{E_{\mathbf{k}}\,E_{\mathbf{k}+\mathbf{q}}}\right]\left[\frac{1}{\omega-\nu_{\mathbf{k}}(\mathbf{q})}-\frac{1}{\omega+\nu_{\mathbf{k}}(\mathbf{q})}\right] \tag{2-4}$$

where $\varepsilon_{\mathbf{k}} = k^2/2m$ is the normal phase one-electron energy, $E_{\mathbf{k}} = [\varepsilon_{\mathbf{k}}^2 + \Delta^2]^{1/2}$ is the superconductor excitation energies, **A** being the energy gap and $\nu_{\mathbf{k}}(\mathbf{q}) = E_{\mathbf{k}} + E_{\mathbf{k}+\mathbf{q}}$.

Defining

$$G(\mathbf{q}, \omega) = \sum_{\mathbf{k}} \frac{1}{2} \left[1 - \frac{\varepsilon_{\mathbf{k}}\, \varepsilon_{\mathbf{k}+\mathbf{q}} - \Delta^2}{E_{\mathbf{k}}\, E_{\mathbf{k}+\mathbf{q}}} \right] \delta[\omega - \nu_{\mathbf{k}}(\mathbf{q})], \tag{2-5}$$

we finally obtain

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{V^2}{(2\pi)^3} \left(\frac{\omega_0}{c}\right)^4 \frac{\cos\theta_s}{c\,|E_0|^2} \int_{-\infty}^{+\infty} dq_z \,.$$

$$\sum_{\alpha} \left| \sum_{\beta\lambda} \Gamma_{\alpha\beta}\, (\mathbf{k}^s, k_z^s, \kappa_z^{s\,L}\, \omega_s) \frac{c\omega_0}{\omega_s^2} \cdot \frac{\partial\varepsilon}{\partial\rho_0} \cdot \frac{F_\beta^\lambda E_{0i}^\lambda}{(k_z^s - \varepsilon^0 k_z^s)(q_z + \kappa_z^s + k_{2z})} \right|^2 \times$$

$$\times \frac{1}{\pi} \frac{G(\mathbf{q}, \omega)}{|\varepsilon(\mathbf{q}, \omega)|^2}, \tag{2-6}$$

where the different quantites appearing in Eq. (2-6) are defined in I. Since T = **O°K,** only the Stokes line (**o** < 0) appears.

Transforming the variables (k, θ, ϕ) to the new set $\varepsilon_{\mathbf{k}} = E$, $\varepsilon_{\mathbf{k}+\mathbf{q}} = E'$ and ϕ, the Jacobian of the transformation being m^2/k^2q, one obtains

$$G(\mathbf{q}, \omega) = \frac{m^2}{2\pi^2 q} \int_{\Delta}^{\omega-\Delta} dE \frac{E(\omega - E)}{\sqrt{E^2 - \Delta^2}\sqrt{(\omega - E)^2 - \Delta^2}} \left[1 + \frac{\Delta^2}{E(\omega - E)} \right]. \tag{2-7}$$

Performing the infegration in Eq. (2-7) results

$$G(\mathbf{q}, \omega) = \begin{cases} 0 & \text{for} \quad \omega < 2\Delta, \\ (m^2/2\pi^2 q)\Delta\, F(\alpha) & \text{for} \quad \omega > 2\Delta, \end{cases} \tag{2-8}$$

where

$$F(\alpha) = (\alpha + 4)\, E\,(\alpha/\alpha + 4) - 4\left(\frac{\alpha + 2}{\alpha + 4}\right) K[\alpha/(\alpha + 4)], \tag{2-9}$$

with **a** = (**o** − 2Δ)/Δ. **E** and **K** are elliptic functions. In the limit **A** → 0, one recovers the result for a normal metal namely,

$$G_N(\mathbf{q}, \omega) = m^2\omega/2\pi q. \tag{2-10}$$

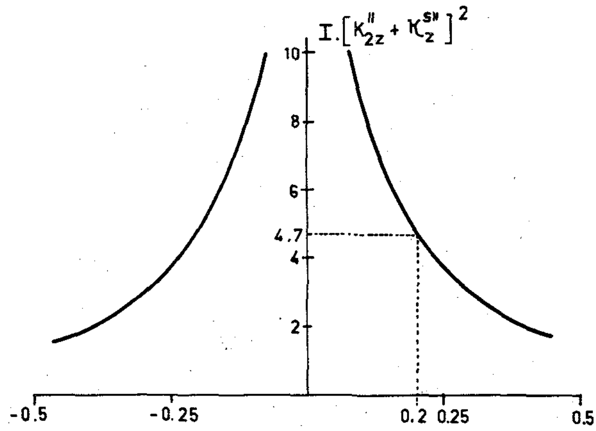

Fig. 1 - The function I of **Eq.** (2-11) times $|K^{\|}_{2z} + \kappa^{s\|}_z|^2$ vs. $\lambda = q_{\|}/|\kappa^{s\|}_z + K^{\|}_{2z}|$. Doted lines refer to the values to be roughly expected in case of normal incidence.

Eq. (2-8) clearly shows that scattering can only occur at frequencies above the absorption edge at $w = 2\Delta$. Another important factor in **Eq.** (2-6) is the scattering coherence length [see (I), Eq. (3-4)]. Taking into account the fact that the imaginary parts of κ^s_z and k_{2z} are much larger than their real parts, one gets the approximate result

$$I = \int_{-\infty}^{\infty} \frac{dq_z}{q[(\kappa_z^{\|s})^2 + k_{2z}^{\|2} + q_z^2]} \approx$$

$$= [\kappa_z^{s\|} + k_{2z}^{\|}]^{-2} (1-\lambda^2)^{-1/2} \ln \frac{1+(1+\lambda^2)^{1/2}}{1-(1-\lambda^2)^{1/2}}, \qquad (2.11)$$

where $\lambda = q_{\|}/[\kappa_z^{s\|} + k_{2z}^{\|}]$. The function I is displayed in Fig. 1.

3. Discussion and Conclusions

Had we neglected Coulomb correlation between electrons in the calculation of the dielectric constant, we would have obtained a formula similar to **Eq.** (2-6) except that $|\varepsilon|^2$ in the denominator would not be present. This factor produces a screening of the single-particle scattering cross section and introduces a new line in the spectrum at the frequency ω_p at which $\varepsilon(\mathbf{q}, \omega_p) = 0$, due to scattering by plasma oscillations.

The single particle scattering arises from the individual motion of Cooper-pairs, and is nearly elastic. In the limit of $\omega \sim 0$, one has

$$\varepsilon(q, \omega) = 1 + (J_s/q)^2, \tag{3-1}$$

where the screening factor J_s^2 is given by

$$J_s^2 \doteq 4\pi e^2 \sum_{\mathbf{k}} \left[1 - \frac{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k}+\mathbf{q}} - \Delta^2}{E_{\mathbf{k}} E_{\mathbf{k}+\mathbf{q}}} \right] v_{\mathbf{k}}^{-1}(\mathbf{q}). \tag{3-2}$$

If $q^2 \gg J_s^2$, the dielectric constant is nearly unity and one recovers Abrikosav and Falkovskii result[4]:

$$\frac{(d^2\sigma/d\Omega d\omega)_S}{(d^2\sigma/d\Omega d\omega)_N} = \frac{\Delta}{\omega} F(\alpha). \tag{3-3}$$

Since $F(0) = \pi/2$, $F(\infty) = 1$ and $F(\alpha) = \frac{\pi}{2}\left(1 - \frac{\alpha}{4}\right)$ in $0 < a < 1$, the shape of this function will be like that shown in Fig. 2. For incident light entering normal to the surface and using typical values for the parameters involved, it can be estimated that $(d\sigma/d\Omega)_S \sim 10^{-26}$ cm^2. Since the skin depth is of the order of 10^{-5} cm the scattering efficiency is small, roughly 10^{-8}.

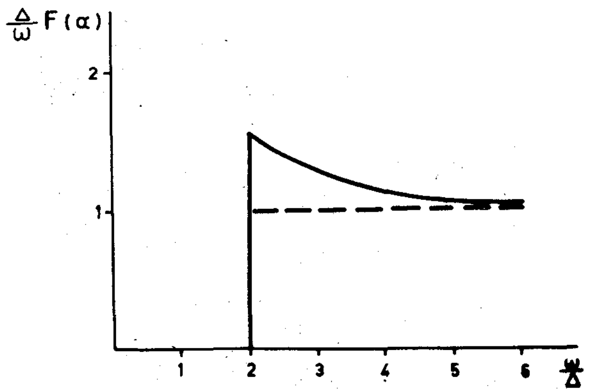

Fig. 2 - The function $\frac{\Delta}{\omega}F(\alpha)$, which measures the ratio of cross sections in the superconducting and normal states [cf. Eqs. (3-3) and (2-9)].

On the other hand, if the momentum transfer is much smaller than the screening parameter, the dielectric constant, for values of ω in the single-particle range, is large and the scattering cross section is greatly reduced

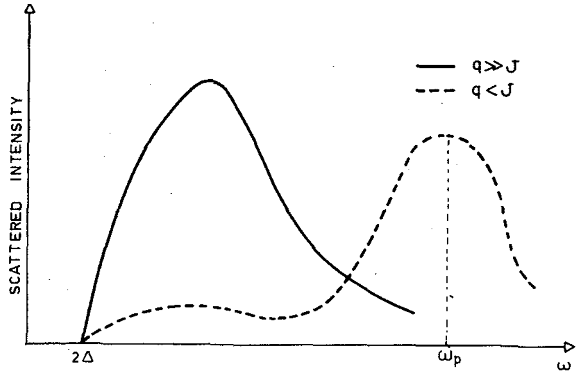

Fig. 3 - Typical qualitative Raman spectra to be expected for light scattered from a superconductor under different experimental geometries as explained in the tert.

by a factor of $(q/J_s)^4$. Since the integrated cross section is roughly $(e^2/mc^2)^2\,(q/J_s)^2$, in the small q limit most of the intensity of the scattered light will be collected at frequencies around the plasma frequency. Fig. 3 shows the qualitative form of the Raman spectra in both cases. It should be remarked that in the limit of $A = 0$ one recovers the results obtained for the case of a normal plasma[S].

In conclusion, we may say that inelastic scattering of light may provide an additional way to study a superconctucting plasma. However, as previously mentioned, the scatteríng efficiency is small, requiring a good experimental resolution for a proper observation. Futhermore, this observation can be greatly impaired by a background of luminescence and by strong absorption.

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References

1. F. G. Reis and R. Luzzi, Rev. Brasil. Fís. 2, 337 (1972).
2. L. M. Fraas, P. F. Williams and S. P. S. Porto, Solid State Comm. 8 2113 (1970).
3. M. S. Khaikin and V. P. Bykov, Soviet Physics – **JEPT** 3, 119 (1956);S. P. S. Porto *et al.*, private communication.
4. A. A. Abrikosov and L. A. Falkovskii, Soviet Physics – JETP 13, 179 (1961). See also S. Y. Tong and A. A. Maradudin, Mat. Res. Bull. 4, 563 (1969).
5. C. Kittel, ***Quantum Theory of Solids,*** Ch. 6, p. 107 ***et seq.*** John Wiley and Sons, Inc. (1963).
6. G. Rickayzen, Phys. Rev. 115, 795 (1959).
7. J. Bardeen, L. Cooper and R. Schrieffer, Phys. Rev. **108**, 1175 (1957).
8. P. A. Wolff in ***Light Scattering Spectra of Solids*** I, G. B. Wright Ed., Springer-Verlag (1970).

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The Magnetic Properties of Ideal Quantum Gases'

S. GOULART ROSA Jr.
Departamento de Física e Ciência dos Materiais,
Instituto de Fisica e Química de São Carlos*, *USP*
W. T. **GRANDY,** Jr.
Phvsics Department, *Universitv* of Wvoming, Laramie, Wvoming

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A review of the magnetic properties of Ideal Quantum Gases is given. The use of the Mellin transform representation for the logarithm function allows us to give a mathematically unified treatment of the magnetic properties of fermion and boson gases. In this formulation, all the thermodynamical phenomena are determined by the analytical behavior of the integrand of a contour integral which defines the logarithm of the grand partition function. The main advantage of our formulation is its extreme simplicity, but yet it is rigorous and elegant. The known results are quickly obtained by simple mathematical procedures.

Faz-se uma resenha das propriedades magnéticas de gases ideais. O uso da transformada de Mellin para representar a função logaritmo nos permite dar um tratamento unificado das propriedades magnéticas de gases de bosons e fermions. Nessa formulação, todos os fenômenos termodinâmicos são determinados pelo comportamento analítico do integrando de uma integral de linha que define o logarítmo da função de grande partição. A principal vantagem de nossa formulação é sua extrema simplicidade, sendo, ainda rigorosa e elegante. Os resultados conhecidos são obtidos por procedimentos matemáticos simples.

1. Introduction

One of the early achievements of the new-born quantum mechanics was the study of the magnetic properties of matter. The unsuitability of classical physics for analysing magnetism was amply demonstrated by Miss Van Leewen's[1] theorem, which proved that when classical physics is used to study the magnetic properties of any dynamical system, the magnetic susceptibility is identically zero. The conflict between experimental facts and the theoretical predictions of classical physics is obvious. However, it has been possible to explain the experimental results in a logical and consistent way with the help of quantum mechanics. We mention here

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*Postal address: Caixas Postais 359-378, 13560 – São Carlos SP.

some. important breakthroughs in the understanding of magnetic properties of matter, from which one can see clearly the quantum nature of magnetism.

In 1927, Pauli[2] applied Fermi-Dirac statistics to the free-electron theory of metals and showed that the spin susceptibility was small and almost temperature independent, in agreement with experimental results. Thr second important breakthrough was made in 1930 bv Landau[3], who evaluated the correct diamagnetism of a free electron gas. The non-zero result for the Landau diamagnetism can be traced back to the quantization of the orbits of the electron in a magnetic field. Because quantum mechanics makes a definitive selection of the possible orbits, there is an average current at each point and a magnetic behavior of the system is possible.

In 1930, de Hass and van Alphen[4] (denoted hereafter by dHvA) found an oscillatory variation with the field in the magnetic susceptibility of bismuth at low temperature and they verifed that the amplitude of the oscillations decreased rapidly as the temperature was raised; the effect disappeared for temperatures above 40°K. A few years later, Peierls[5] proposed a very simple model to explain the physical origin of the dHvA effect. Using the quantized energy-level of a single particle, he calculated the zero-temperature total energy of a two dimensional free electron gas in a uniform magnetic field, the field being perpendicular to the plane of the system. The plot of total energy against the inverse field strength shows a periodic discontinuity in the slope of the graph, as a consequence of a periodic magnetization. Even this unrealistic model reproduces remarkably well the important observed features, namely the periodicity of the magnetization and the constancy of the period of the oscillations.

Several attempts have been made to generalize the theory of free electrons in order to interpret in a better quantitative way the measured magnetic susceptibility of metals[6]. The contnbution of the electron spin has been taken into account. Although the spin paramagnetism does not show a dHvA oscillatory behavior, it modifies the phase of the oscillatory terms of the diamagnetic susceptibility. A discussion of the effects of the collisions of the electrons with impurities as well as the finite volume of the sample, on the magnetic properties of a system of free electrons, was given by Dingle[7] and more recently the impurity problem has been studied by Hebborn and March[8]. Also, the anisotropy of the dHvA effect and the lattice field of the crystal have been consistently introduced in the free electron theory by considering an effective mass tensor for the electron as did Landau in 1938, assuming an ellipsoidal constant energy surface.). However, the first approach introducing the anisotropy of the effect was done by Blackman as a tentative generalization of Peierls' theory.

A much more profound discovery, however, was made by Onsager[9], who was able to show a connection between the dHvA oscillations in the magnetic susceptibility and the electronic structure of metals. He showed that the period of oscillations should be proportional to the inverse of the extremal area of the Fermi surface normal to the direction of the field. Therefore, the measurements of the period of oscillations, for different orientatioris with respect to the field, give information about the size and form of the Fermi surface. For this reason, the dHvA effect became very importarit in the studies of electronic properties of metals. It should be mentioned that Onsager's result was also obtained independently by Lifshitz and Kosevich[10]

The first completely rigorous mathematical treatment of the magnetic properties of a free electron gas was given by Sondheimer and Wilson[11]. The generalization to take into account the effect of the electron spin and the binding of the electrons, by introducing an effective mass, was made. A detailed discussion of the precaution needed in quantitatively interpreting the measured magnetic susceptibility using the free electron model was also presented.

The studies of the magnetism of a free charged Bose gas are more recent, but no less spectacular, than those of an electron gas. For instance, as Schafroth[12] has shown, the most remarkable feature of a Bose gas, the Bose-Einstein condensation, is destroyed by the presence of the uniforrn magnetic field. Also, as long as the temperature is less than T_c (the transition temperature for the gas in the absence of the field), the system completely expels a uniform magnetic field weaker than a certain field H,, and allows a uniform penetration for fields strongerthan H,. We must emphasize that this effect occurs even when there is no condensation into the ground state of the system. Above T_c, the system has a normal behavior; i.e., the magnetization has a linear field (B) dependence and for $T \gg T_c$ the diamagnetic susceptibility is inversely proportional to T.

More recently, May[13] considered the magnetic properties of an "n" dimensional charged ideal quantum gas in a uniform magnetic field. The purpose of his studies was to investigate to what extent the magnetic behavior depends on the dimensionality of the system. He observed that a fermion gas is diamagnetic (neglecting the spin contribution to the magne tic susceptibility) for all "n". For a boson system, however, the dimensionality plays a more crucial role: for n < 2, the Bose gas is diamagnetic and the susceptibility becomes very large as the temperature approaches zero, but does not show a perfect diamagnetism. For 4 > n > 2, the Bose gas exhibits a Meissner-Ochsenfeld effect below its transition temperature, although there is no condensation into the ground state, as shown by Schafroth. For n > 4, the presence of the uniform magnetic field has no effect on the condensation, and below the transition temperature T_c the condensed bosons can expel all fields weaker than the critical field.

2. The Grand Potential

From the theory of the grand canonical ensemble, the grand potential "f" of an ideal quantum gas is given by

$$\Omega f = P\Omega\beta = -\varepsilon \sum_j \log\left[1 - \varepsilon \exp \beta(\xi - E_j)\right], \tag{2-1}$$

where E_j is the energy of the single particle in its j^{th} state, 5 is the chemical potential, $\beta^{-1} = kT$, k being the Boltzmann constant and T the absolute temperature, E $= 1$ for bosons, E $= -1$ for fermions, P is the pressure, R is the volume of the system, and the summation over j runs over all single particle states. For Bose statistics, we have always the constraint that $\xi < E_j$ for all j, which is equivalent to $\xi <$ E MINIMUM, in order Eq. (2-1) to be true.

Other thermodynamic properties of the system can be evaluated by appropriate derivatives of f. For instance the density p, the magnetization M and the magnetic susceptibility χ are given respectively by

$$\beta\rho = \left.\frac{\partial f}{\partial \xi}\right|_{\beta,\Omega,B}, \tag{2-2}$$

$$\beta M = \left.\frac{\partial f}{\partial B}\right|_{\beta,\xi,\Omega}, \tag{2-3}$$

$$\beta B\chi = \left.\frac{\partial f}{\partial B}\right|_{\beta,\xi,\Omega} = \beta M, \tag{2-4}$$

B being the magnetic induction field.

The Mellin transform representation of the logarithm function[14]

$$\log[1 - \varepsilon \exp \beta(\xi - E_j)] =$$

$$= \frac{1}{2\pi i} \int_{\alpha - i\infty}^{\alpha + i\infty} \pi[\cos(\pi t)]^{\varepsilon'} t^{-1} \csc(\pi t) \exp[\beta t(\xi - E_j)]\, dt, \qquad (2\text{-}5)$$

where $\varepsilon' = (1 + \varepsilon)/2$ and $0 < \alpha < 1$, is now used in combination with Eq. (2-1). Thus we have:

$$\Omega f = -\frac{\varepsilon}{2\pi i} \int_{\alpha - i\infty}^{\alpha + i\infty} \pi[\cos(\pi t)]^{\varepsilon'} t^{-1} \csc(\pi t) \exp(\beta \xi t) \cdot \sum_j \exp(-\beta E_j t)\, dt. \qquad (2\text{-}6)$$

The one-particle partition function, $Z = \sum_j \exp(-\beta E_j)$, for a charged particle in a uniform magnetic field has been evaluated by Sondheimer and Wilson[14]. We emphasize that we are working in the Landau gauge in which the vector potential $A = (0, Bx, 0)$. $\mathbf{B} = \nabla \times \mathbf{A}$ is therefore parallel to the z-axis. Z is related to the one-particle density matrix which satisfies a Bloch equation and an initial condition. They solved the differential equation without using the explicit knowledge of the Landau energy levels $E_{r p_z \sigma} = (r + \frac{1}{2})\hbar\omega + p_z^2/2m - g\sigma\mu B$. There are $(2S + 1)$ possible values for σ, all with magnitude less than or equal to the particle spin S. The harmonic oscillator quantum number is r.

Their result for Z, generalized to particles with any spin $S(S = 0, 1/2, 1 \ldots)$, is

$$Z = \frac{\sinh[(2S + 1)\beta\mu Bg/2]}{\sinh(\beta\mu Bg/2)} \frac{\lambda^{-3}\,\Omega(\beta\hbar\omega/2)}{\sinh(\beta\hbar\omega/2)} \qquad (2\text{-}7)$$

where $\mu = q\hbar/2mc$ is the particle magnetic moment, $\omega = qB/mc$ is the cyclotron frequency, $\lambda = (2\pi\hbar^2/mkT)^{1/2}$ is the thermal wavelength and g is the particle Landé factor. The other symbols have their traditional meaning. We note that the factors in Eq. (2-7) are due respectively to the spin and orbital parts of the energy E_{LANDAU}.

The advantage of writing Z in this form, since eventually μB can be equal to $\hbar\omega/2$, is because we can identify easily at any step the spin and orbital contributions in all forthcoming thermodynamic functions.

The substitution of Eq. (2-7) into Eq. (2-6) gives us

$$f = \frac{-\varepsilon\lambda^{-3} a}{2i} \int_{\alpha}^{\alpha + i} \frac{[\cos(\pi t)]^{\varepsilon'} e^{\beta\xi t} \sinh[(2S + 1)bt]}{\sin(\pi t)\, t^{3/2} \sinh(bt)} \frac{dt}{\sinh(at)}, \qquad (2\text{-}8)$$

where we have introduced the dimensionless expansion parameters a $= \beta\hbar\omega/2$ and $b = \beta\mu Bg/2$. We observe that the spin factor

$$\sinh[(2S + 1)\,bt]/\sinh(bt)$$

is an entire function of t. The integrand has a branchpoint at the origin, the real negative axis being the branch cut; it also has simple poles at all real positive integers $n = 1, 2, 3 \ldots$ and at $t_p = \pi pi/a$, $p = \pm 1, \pm 2, \ldots$ The procedure to solve **Eq.** (2-8) will be to complete the straight line contour with the arc of a circle and a loop around the origin in order to close it (see Figs. 1 and 2), such that the integrand satisfies all the conditions for the

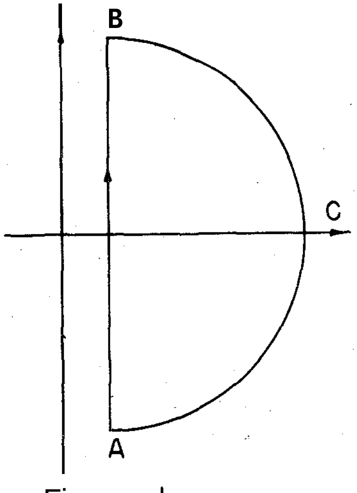

Figure 1

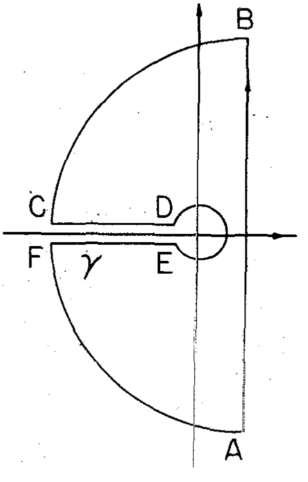

Figure 2

application of the residue theorem. The requirements for the vanishing of the integrals taken along the arcs in the limit of infinite radius, and the singularities of the integrand, which are important, will be different if we choose to close to the left or to the right for both boson or fermion systems. We can this way rederive in a systematic manner all the results already published in the literature[1,5].

3. The Classical Limit

Consider the closed contour in the t-plane given by Fig. 1. Let Γ be a circle with its center at the origin with radius R $= n + \frac{1}{2}$, so that the circle does not pass through any of the poles at $t = \mathrm{n}$ of the integrand, which are due to the factor $\csc(\pi t)$. In the limit of n going to infinity, the integral Eq. *(2-8)* taken along the arc BCA of Fig. 1 tends to zero if $\xi \leq$ a, 2Sb for fermions and $\beta\xi < a-2Sb$ for bosons. Thus we can replace the integration along the straight line by the limit when $n \to \infty$ of the integral over the closed contour ABCA, which can be easily obtained evaluating the residues of the integrand at $t = n$.

Therefore,

$$f = \lambda^{-3} a \sum_{n=1}^{\infty} \varepsilon^{n+1} e^{n\beta\xi} n^{-3/2} \{\sinh[(2S+1)nb]\}/\{\sinh(nb)\sinh(na)\}. \quad (3\text{-}1)$$

If we specialize to a system of electrons ($S = 1/2$, $\varepsilon = -1$, $a = b$), Eq. (3-1) reduces to that series obtained by Stephen[15]. The resultant series was summed up in the limit of low temperature by expanding the $\coth(nb)$ in powers of $\exp(nb)$, and the steady terms of the susceptibility are then obtained. Stephen's series does not have an oscillatory behavior as he implies because of the restriction on ξ. The dHvA oscillation occurs only at extremely low temperatures and high fields, which correspond to positive values of Γ, and are not included in the region of validity of Eq. (3-1).

In the case of a spinless Bose gas ($S = 0$, $\varepsilon = 1$), Eq. (3-1) gives the expression obtained by Schafroth.

As an application of Eq. (3-1), we discuss here the weak field strength and high temperature limits on an electron and spinless Bose gas. In this regime $a \ll 1$, $b \ll 1$ and the high temperature limit implies that $\exp(\beta\xi) \ll 1$, so the series for f converges extremely rapidly. We only keep the first term in Eq. (3-1) which gives the dominant contribution. Then, for the spinless Bose gas, we have

$$f = \lambda^{-3} e^{\beta\xi} a \operatorname{csch}(a) \simeq \lambda^{-3} e^{\beta\xi}\left(1 - \frac{1}{6}a^2\right), \quad (3\text{-}2)$$

$$\rho \simeq \lambda^{-3} e^{\beta\xi}\left(1 - \frac{1}{6}a^2\right). \quad (3\text{-}3)$$

The chemical potential ξ is now eliminated from Eq. (3-2) by using a expression for the density with no field dependence i.e., we substitute $\rho = \lambda^{-3} \exp(\beta\xi)$ in the equation for "f". The diamagnetic magnetization and susceptibility are then obtained by using Eqs. (2-3) and (2-4):

$$M = \frac{\rho\mu^2 B}{3kT}, \quad (3\text{-}4)$$

$$\chi = -\rho\mu^2/3kT. \quad (3\text{-}5)$$

The relation $\mu B = \hbar\omega/2$ has also been used.

For the electron gas, we have made the approximations:

$$f = 2\lambda^{-3}\, a e^{\beta\xi} \cosh(b)/\sinh(a) \simeq 2\lambda^{-3}\, e^{\beta\xi}\left(1 + \frac{b^2}{2} - \frac{a^2}{6}\right), \tag{3-6}$$

$$\rho \simeq 2\lambda^{-3}\, e^{\beta\xi}\left(1 + \frac{b^2}{2} - \frac{a^2}{6}\right). \tag{3-7}$$

The total magnetization and total susceptibility are obtained similarly for the Bose gas:

$$M = \frac{\rho}{\beta B}\left(b^2 - \frac{a^2}{3}\right) = \frac{2\rho\mu^2 B}{3kT}, \tag{3-8}$$

$$\chi = \frac{\rho}{\beta B^2}\left(b^2 - \frac{a^2}{3}\right) = \frac{2\rho\mu^2}{3kT}. \tag{3-9}$$

The last equality in both equations is obtained by putting a = b.

We can see clearly the advantage of keeping both a and b different up to the end. The total magnetic susceptibility for the electron gas is positive, the diamagnetic (orbital) contribution being additive and equal to minus one third of the term due to the spin.

4. Low Temperature Limit

As was mentioned above, in evaluating the integral in **Eq.** (2-8) we can close the path to the left as in Fig. 2. The radius R $= (p + 1/2)\pi/a$ of the large arc of circle Γ centered at the origin has been chosen so that the integrand is an analytic function on the countour. When p tends to infinity and the radius of the small circle tends to zero, the integral over BC and FA will go to zero when $\beta\xi \geq 2Sb - a$ for bosons and $\beta\xi > 2Sb - a$ for fermions; hence the value of the integral in **Eq.** (2-8) is equal to $(-\varepsilon\lambda^{-3}$ na) times the sum of the residues of the integrand at $t_p = \pi pi/a$ plus the integral around the contour FEDC (denoted by y). The residues are easily evaluated because the integrand is a ratio of two functions: $f(t) = h(t)/q(t)$, where $q(t) = \sinh(at)$ and $h(t)$ is the remaining part. Moreover $q(t)$ and

$h(t)$ are analytic at t_p, $q(t_p) = h(t_p) = 0$ and $q'(t_m) \neq 0$. Therefore, the residue b_p is given by the expression

$$b_p = \frac{-a^{1/2}[\cosh(\pi^2 p/a)]^{\varepsilon'} \sin[(2S+1)\pi pb/a] \exp[i\pi(p\beta\xi/a - 1/4)]}{\sinh(\pi^2 p/a)\sin(\pi pb/a)(\pi p)^{3/2}\cos(p\pi)}. \tag{4-1}$$

Therefore,

$$\begin{aligned} f &= -\frac{\varepsilon\lambda^{-3}}{2i}\int_\gamma \frac{[\cos(\pi t)]^{\varepsilon'} e^{\beta\xi t}}{\sin(\pi t)\, t^{3/2}} \times \frac{\sinh[(2S+1)bt]\,dt}{\sinh(bt)\sinh(at)} \\ &+ \frac{2\varepsilon a^{3/2}}{\pi^{1/2}\lambda^3}\sum_{p=1}^{\infty}\frac{(-1)^p[\cosh(\pi^2 p/a)]^{\varepsilon'}}{p^{3/2}\sinh(\pi^2 p/a)} \\ &\times \frac{\sin[(2S+1)\pi pb/a]}{\sin(\pi pb/a)}\cos\left(\frac{p\beta\xi}{a} - \frac{1}{4}\right)\pi \\ &= f_1 + f_2 \end{aligned} \tag{4-2}$$

where we combined the residues at t_p and t_{-p} and them summed from 1 to infinity.

For the sake of clarity, we will proceed in evaluating the contour integral in the last expression for the cases of electrons and spinless bosons.

For the fermion system, the leading contribution to the integral comes from the region of small $|t|$. Therefore, expanding the circular and hyperbolic functions, we find that f_1 can be approximated by

$$f_1 = 2a\pi\lambda^{-3}\frac{1}{2\pi i}\int_\gamma e^{\beta\xi t}\left[\frac{1}{\pi a t^{7/2}} + \left(\frac{b^2}{2\pi} + \frac{\pi}{6}\right)\frac{1}{at^{3/2}} - \frac{a}{6\pi t^{3/2}}\right]dt. \tag{4-3}$$

The next term is of order of $t^{1/2}$. The integrals above can be performed with the aid of Hankel's formula for the gamma function. After an easy algebric manipulation, we have

$$\begin{aligned} f &= \frac{16}{15}\frac{\lambda^{-3}}{\pi^{1/2}}(\beta\xi)^{5/2}\left\{1 + \frac{15}{8}\left[\left(\frac{b}{\beta\xi}\right)^2 - \frac{1}{3}\left(\frac{a}{\beta\xi}\right)^2\right] + \frac{5\pi^2}{8}\left(\frac{1}{\beta\xi}\right)^2\right. \\ &\left. - \frac{15}{4a}\left(\frac{a}{\beta\xi}\right)^{5/2}\sum_{p=1}^{\infty}\frac{(-1)^p\cos(\pi pb/a)}{p^{3/2}\sinh(\pi^2 p/a)}\cos\left(\frac{p\beta\xi}{a} - \frac{1}{4}\right)\pi\right\} \end{aligned} \tag{4-4}$$

Using Eqs. (2-2) through (2-4), we obtain for the density, magnetizatiori and susceptibility, the following expressions:

$$\rho = \frac{8\lambda^{-3}}{3\pi^{1/2}} (\beta\xi)^{3/2} \left[1 + \frac{3\pi}{2a} \left(\frac{a}{\beta\xi} \right)^{3/2} \times \sum_{p=1}^{\infty} \frac{(-1)^p \cos(\pi p b/a)}{p^{1/2} \sinh(\pi^2 p/a)} \sin \left(\frac{p\beta\xi}{a} - \frac{1}{4} \right) \pi \right], \tag{4-5}$$

$$M = \frac{4\lambda^{-3}}{\pi^{1/2}} (\beta\xi)^{1/2} \left(\frac{kT}{B} \right) \left[\left(b^2 - \frac{1}{3} a^2 \right) - \pi(\beta\xi a)^{1/2} \times \sum_{p=1}^{\infty} \frac{(-1)^p \cos(\pi p b/a)}{p^{1/2} \sinh(\pi^2 p/a)} \sin \left(\frac{p\beta\xi}{a} - \frac{1}{4} \right) \pi \right], \tag{4-6}$$

$$\chi = \frac{M}{B}. \tag{4-7}$$

Eq. (4-5) gives the complete dependence of the chemical potential in terms of *p*, T and B. It consists of a series of oscillatory terms as well as a steady term. Since $\mu B \ll \xi$, the series gives a negligible contribution to *p*, compared with the first term, and the particle density can be approximated by

$$\rho = \frac{8\lambda^{-3}}{3\pi^{1/2}} (\beta\xi)^{3/2}. \tag{4-8}$$

This is the relation used to remove ξ from all final formulae of interest.

We see clearly that the branch point is responsible for the steady term in f and that the poles on the imaginary axis give rise to the oscillatory (with B^{-1}) series.

Wilson and Sondheimer's results for the particle density, magnetization and magnetic susceptibility, are quickly reproduced if we put

$$a = \frac{\beta q \hbar B}{2m^* c} \quad \text{and} \quad b = \frac{\beta q \hbar B}{2mc} \tag{4-9}$$

in Eqs. (4-5), (4-6) and (4-7), where m* is an effective mass of the electron.

The treatment of the electron gas given by Isihara, Tsai and Wadati[16] is identical to ours and their results are obtained with the substitution of a $= \beta\mu B$, b $= ga/2$ and the use of a system where $\hbar = 1$, 2m $= 1$.

Finally, we turn our attention to the spinless Bose gas, in which case Eq. (4-2) becomes equal to

$$\lambda^3 f = (ai/2) \int_\gamma t^{-3/2} \cot(\pi t)\, e^{\beta\xi t} \times \operatorname{csch}(at)\, dt$$

$$+ 2\pi^{-1/2} a^{3/2} \sum_{p=1}^{\infty} (-1)^p p^{-3/2} \coth(\pi^2 p/a) \cos\left(\frac{p\beta\xi}{a} - \frac{1}{4}\right)\pi. \qquad (4\text{-}10)$$

In the regime of weak field strength and finite (low) temperature, we have $\hbar\omega \ll kT$, which implies also $\xi \ll kT$ (as a consequence of the restriction $\xi < E_{MINIMUM} \equiv \frac{1}{2}\hbar\omega$). Thus, after expanding the exponential and hyperbolic functions and keeping leading contributions we obtain the following expression for the grand potential:

$$\lambda^3 f \simeq (i/2) \int_\gamma t^{-5/2} \cot(\pi t)(1 + \beta\xi t)\, dt - 2\pi^{-1/2} a^{3/2}$$

$$\times \sum_{p=1}^{\infty} p^{-3/2} \sin\left(ps - \frac{1}{4}\right)\pi, \qquad (4\text{-}11)$$

where we have introduced the dimensionless parameter $s = 1 - \dfrac{\xi}{\mu B}$ in order to compare our results with those of Ref. (12).

The integrals are evaluated by using a contour integral representation of the Riemann Zeta function (see Appendix), namely,

$$\zeta(z) = (i/2) \int_\gamma \cot(\pi t)\, t^{-z}\, dt. \qquad (4\text{-}12)$$

Then, we have

$$\lambda^3 f = \zeta(5/2) + \xi\beta[\zeta(3/2)] - 2\pi^{-1/2} a^{3/2} \sum_{p=1}^{\infty} p^{-3/2} \sin\left(ps - \frac{1}{4}\right)\pi. \qquad (4\text{-}13)$$

We notice that the last term in the expression above for "f" is proportional to the Hurwitz formula of the generalized Rieman Zeta function (Ref. 17) $\zeta(-1/2, 5/2)$.

The density ρ is immediately obtained,

$$\rho = \zeta(3/2) + 2(\pi a)^{1/2} \sum_{p=1}^{\infty} p^{-1/2} \cos\left(ps - \frac{1}{4}\right) \text{n}. \qquad (4\text{-}14)$$

These expressions for f and p were first obtained by Schafroth after an involved sequence of calculations. Once again we can verify the power of our approach in studying the magnetic properties of ideal gases.

The above expression can be rewritten as

$$\rho\lambda^3\left[1-\left(\frac{T}{T_c}\right)^{3/2}\right] = 2(\pi a)^{1/2} \sum_{p=1}^{\infty} p^{-1/2} \cos\left(ps-\frac{1}{4}\right)\pi, \tag{4-15}$$

where we have introduced the transition temperature T_c for the system in a free field situation, defined by the relation

$$\zeta(3/2) = \rho\left(\frac{4\pi\hbar^2}{2mkT_c}\right)^{3/2} = \rho\lambda^3\left(\frac{T}{T_c}\right)^{3/2}. \tag{4-16}$$

The system magnetization is also easily obtained

$$\lambda^3 M = -2(\pi a)^{1/2}\,\mu\left[\frac{3}{2\pi}\sum_{p=1}^{\infty} p^{-3/2}\sin\left(ps-\frac{1}{4}\right)\pi\right.$$

$$\left. + (1-s)\sum_{p=1}^{\infty} p^{-1/2}\cos\left(ps-\frac{1}{4}\right)\pi\right. . \tag{4-17}$$

Now a final form for M is obtained after the elimination of s in the term of the density. This can be done expanding in a series the expressions for M and ρ, for small s, using the relation[18]

$$F_\sigma(\alpha) = \sum_{n=1}^{\infty} \frac{e^{-n\alpha}}{n^\sigma} = \frac{\pi}{\sin\pi\sigma}\,\frac{\alpha^{\sigma-1}}{\Gamma(\sigma)} + \sum_{m=0}^{\infty}\frac{(-1)^m}{m}\zeta(\sigma-m)\,\alpha^m. \tag{4-18}$$

We write the series of interest as real or imaginary parts of $F_\sigma(\alpha)$. Thus,

$$\sum_{p=1}^{\infty} p^{-3/2}\sin\left(ps-\frac{1}{4}\right)\pi \simeq -\frac{\zeta(3/2)}{\sqrt{2}} + 2\pi s^{1/2} + 0(s), \tag{4-19}$$

$$\sum_{p=1}^{\infty} p^{-1/2}\cos\left(ps-\frac{1}{4}\right)\pi \simeq s^{-1/2} + \frac{(1/2)}{\sqrt{2}} + 0(s). \tag{4-20}$$

Therefore, the expressions for p and M are approximated by

$$\lambda^3\rho\left[1-\left(\frac{T}{T_c}\right)^{3/2}\right] \simeq 2(\pi a)^{1/2} s^{-1/2}, \quad \lambda^3 M = -2(\pi a)^{1/2} s^{-1/2}\mu, \tag{4-21}$$

or

$$M = -\rho\mu\left[1-\left(\frac{T}{T_c}\right)^{3/2}\right] \tag{4-22}$$

Thus, below the transition temperature there is a spontaneous magnetization. For temperatures T $< T_c$, a better approximation in the evaluation of Eq. (4-11) is needed.

5. Conclusion

We have shown how to obtain the grand potential of a free gas in all different domains of temperature and fieldstrength. The known results are always quickly and directly evaluated as particular cases of the more general and exact equations Eq. (3-1) and Eq. (4-2).

The spin contribution was taken into account from the very beginning in Eqs. (2-7) and we identify its effect through the parameter ***h***. Also the equivalence of Eqs. (4-13) and (3-1) (with c $= 1, S = 0$) shown by Schafroth, after somewhat difficult mathematical manipulations, can now be inferred at the outset without any further assumption.

Concerning the Fermi system, an alternative rigourous treatment of the degenerate electron gas was performed, where the' simplification of the mathematical machinery is better illustrated.

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Appendix - A contour-integral representation of the Riemann Zeta function

The integral

$$i/2\int_{-\infty}^{0} \cot(\pi t)\, t^{-z} dt$$

can be shown to be equal to the Zeta function of argument z. $\zeta(z)$. The limits of integration $[-\infty, +0]$ signify that thepath of integration starts at "infinity" on the negative part of the real axis, encircles the origin in the positive sense and returns to the starting point; i.e., identical to the path γ in the text.

Consider the integral

$$(i/2) \int_C \cot(\pi t)\, t^{-z}\, dt$$

taken in the positive sense around the countour C which starts at the point $-[N + (1/2)]$ and consists of a circle Γ centered at the origin with a radius $R = [N + (1/2)]$ and a loop $[-(N + 1/2), +0]$ of which the contour $[-\infty, +0]$ is a limiting form The integral is an analytic and single-valued function of t inside and on C, except at $t = n$, $n = 1, 2, \ldots N$, where it has simple poles. Hence, after applying the residue theorem to evaluate the integral, we get

$$(i/2) \int_C \cot(\pi t)\, t^{-z}\, dt = \sum_{n=1}^{N} R_n = \sum_{n=1}^{N} \frac{1}{n^z}$$

where R_n are the residues of the integrande at $t = n$ Now, the integral taken around Γ goes to zero as $N \to \infty$ if Re $z > 1$. Making $N \to \infty$, we obtain the contour integral representation of the Riemann Zeta function:

$$(i/2) \int_{-\infty}^{0} \cot(\pi t)\, t^{-z}\, dt = \zeta(z).$$

References and Notes

1. J. H. van Leewen, dissertation, Leiden (1919).
2. W. Pauli, Z. Physik **41,** 81 (1927).
3. L. Landau, Z. Physik 64, 629 (1930).
4. W. J. de Haas and P. M. van Alphen, Comm. Phys. Lab. Univ. Leiden, 212a (1930). An excellent review on the dHvA effect is given by D. Schoenberg in ***Progress in Lorv** Temperature Physics* vol. **II** North Holland (1957).
5. R. Peierls, Z. Physik **81,** 186 (1933).
6. See, for instance, the bibliography of Ref. 7.
7. R. B. Dingle, Proc. R. Soc. **A211**, 500 (1952).
8. J. E. Hebborn and N. H. March, Proc. R. Soc. **A280**, 85 (1964).
9. L. Onsager, Phil. Mag. 43, 1003 (1952).
10. I. M. Lifshitz and 4. M. Kosevich, Doklady Akad. Nauk. USSR **96,** 963 (1954).
11. E. H. Sondheimer and A. H. Wilson, Proc. R. Soc. **A210**, 173 (1951).
12. M. R. Schafroth, Phys. Rev. 100, 463 (1955).
13. R. M. May, J. Math. Phys. *6,* 1462 (1965).
14. See, for instance, H. Erdélyi (Editor) ***Table of Integral** Transforms*, Vol. *I* McGraw-Hill (1954) page 315 Eqs. 15 and 18. The use of the Mellin transform to calculate the grande partition function of an ideal electron gas has been made independently by Isihara,Tsai, Wadati (Ref. 16), and by one of us (S. G. R.): Ph. D. Thesis, Univ. of Wyoming (1972), unpublished.
15. Results of Refs. 11, 12, 13 as well as those of M. J. Stephen, Proc. R. Soc., A265, 215 (1962) are obtained by the present treatment.
16. A. Isihara, J. Tsai and Wadati, Phys. Rev. **A3,** 990 (1971).
17. E. T. Whittaker and N. Watson, ***A Course of** Modern Analysis*, Cambridge Univ. Press. Fourth Ed. (1969).
18. See, for insfance, Ref. 12.