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SOLUTION OF THE EXCHANGE-SCATTERING PROBLEM WITHOUT INADMISSIBLE COMPLEX POLES*

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Abstract

As previously demonstrated, the S-matrix formulation of the problem of exchange scattering of electrons in metals can lead to the appearance of inadmissible complex poles in the spin-flip scattering amplitude as the temperature falls below a certain value T_c. This amplitude then fails to satisfy the original scattering equations. In this paper, it is shown that such difficulties can be removed by making the proper analytic continuation in the temperature (or analytic continuation in the coupling strength for a fixed temperature). The scattering amplitudes, and with them such transport coefficients as conductivity, thermoelectric power, and Lorentz number are, in fact, smooth functions of temperature across T_c. Curves of these transport quantities versus temperature are plotted for a wide variety of values of the ordinary and exchange potentials.

1. Introduction

IN three previous publications [1-3] one of the authors developed an S-matrix formalism adapted to a certain scattering problem first brought to light by Kondo [4]. This problem concerns the scattering of a conduction electron in a metal by a paramagnetic impurity, to which it is coupled according to an interaction energy of the form

$$\int \left\{ V(\mathbf{r})\ \rho(\mathbf{r}) + J(\mathbf{r})\ \mathbf{S}\cdot\mathbf{s}(\mathbf{r}) \right\} d\mathbf{v}$$

Here S is the spin of the localized impurity, $\rho(\mathbf{r})$ is the density, and $\mathbf{s}(\mathbf{r})$ the spin-density of the conduction electrons. $J(r)$ is the exchange energy, and $V(r)$ is the ordinary potential due to the charge contrast between impurity and host metal.

In the most recent of the three publications [3], henceforth referred to as I, a solution of the equations for the s-wave projections of the spin flip and non-spin flip scattering amplitudes $\tau(z)$ and $t(z)$ as a function of complex energy z was presented which was essentially exact

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to within the neglect of certain boundary conditions. For the ferromagnetic sign of J (negative in the present notation), this solution was well behaved at all temperatures. However, for the antiferromagnetic sign of J(positive), the solution presented in I was well behaved only below a certain critical value of J for fixed temperature T, or above a certain critical value of T for fixed J. In particular, T_c is given by

$$kT_c \sim \varepsilon_f \exp -(J\rho_0)^{-1}$$

where ε_f is the Fermi energy and ρ_0 the density of states near the Fermi level. For $T < T_c$ the result presented in I develops an unacceptable shortcoming: the S-wave part of the spin flip amplitude acquires poles on the physical sheet of the complex energy plane. It then fails to be a solution of the original scattering equations. This conclusion was quite stable against various modifications in the conditions of the problem; in particular, it is insensitive to asymptotic behavior of the scattering amplitudes at energies remote from the Fermi level. However, it was noted that at the point where the poles passed from the unphysical sheet to the physical sheet the residue in the spin flip amplitude was actually zero.

In this paper, we show that for temperatures slightly above T_c, the residues of the complex poles in the unphysical sheet are also zero. By analytic continuation, the residues remain zero even after the poles migrate to the physical sheet. Explicit construction of the spin-flip and non-spin flip amplitudes are performed in the next section, and the passage through T_c is shown to be perfectly smooth. The existence of such a smooth, totally trouble-free solution calls into question the assertion often heard nowadays: that at T_c a kind of localized "phase transition" takes place in which the localized spin captures one or more electrons producing an antiparallel configuration and leading to the disappearance of the local moment at sufficiently low temperatures. However, to finally settle the question of a low-temperature compensation of S, it will still be necessary to include in the problem the electron-electron coupling, part of which has exchange character. A self consistent theory then arises, in which the exchange coupling J acquires corrections themselves dependent on the spin-flip scattering amplitude. These matters (including the question of a "bootstrap" solution when $J = 0$) will be discussed in a later publication.

The possession of a complete solution of the scattering problem allows us to calculate a set of curves for comparison with experimental data on the transport coefficients: conductivity and thermoelectric power, which should be relevant in any temperature range for low impurity concentrations.

2. Calculations of Scattering Amplitudes

The equations and solutions of I can be summarized thus:

$$t(z) = \frac{Vx_0}{z + x_0} + \int_{-\varepsilon_f}^{\infty} dx\ \rho(x)\ \frac{|t(x)|^2 + 4S(S+1)\ |\tau(x)|^2}{z - x} \tag{1}$$

$$\tau(z) = \frac{Jx_0}{4(z + x_0)} + \int_{-\varepsilon_f}^{\infty} dx\ \rho(x)\ \frac{\tau(x)t^*(x) + \tau^*(x)t(x) - 2|\tau(x)|^2 \tanh(\beta x/2)}{z - x} \tag{2}$$

where t is the non-spin-flip amplitude, and τ the spin flip amplitude for scattering of electrons of energy z above the Fermi surface. V and J are the respective coupling strengths for ordinary and spin-flip scattering, $(x_0 - \varepsilon_f)^{-1}$ is the range of the force, necessary as a cutoff parameter, $\rho(x) = \sqrt{x + \varepsilon_f}$, the density of states, and $\beta = 1/kT$. A number of subsidiary functions was introduced:

$$2\pi i\ \rho(z)t(z) = -(e^{2i\delta(z)} - 1), \tag{3}$$

$$\tau(z)\ e^{-2i\delta(z)} = \tau(z)/\left[1 - 2\pi i\ \rho(z)t(z)\right] \equiv F(z), \tag{4}$$

$$e^{-4\delta''(x)} \equiv 1 - a(x)\left|\tau(x)\right|^2 = \left[1 + a(x)\left|F(x)\right|^2\right]^{-1} \tag{5}$$

on the real axis with $a(x) = 16\pi^2\ \rho^2(x)\ S(S + 1)$ and

$$\delta(z) = \frac{\rho(z)}{\pi} \int_{-\varepsilon_f}^{\infty} dx\ \delta''(x)/\left[\rho(x)(x - z)\right] - \delta_v(z). \tag{6}$$

In these relations, $\delta_v(z)$ is the phaseshift for the elastic scattering problem with potential v. F is defined by (4). At fixed J, as the temperature is decreased to T_c, a (double) pole in F appears on the real axis at $z = z_0 = 0$ for the simplest models, and $e^{-2\delta''}$ is zero at that point. Therefore $(1 - 2\pi i\rho t)$ is also zero there. Thus, when the pole in $F(z)$ first appears, it may be ascribed to a zero in $(1 - 2\pi i\rho(z)t(z))$, and, as observed in I, $\tau(z)$ remains finite. However, for $T < T_c$, the double pole splits into a complex conjugate pair, the solution given in I does not satisfy $(1 - 2\pi i\rho(z_0)t(z_0)) = (1 - 2\pi i\rho(z_0^*)t(z_0^*)) = 0$, and so, according to equation (3) τ will then have complex poles with finite residues. In I, some ambiguity remained in F (the h-function following equations (11) and (23) of I, can be modified in a large number of ways, quite aside from the "CDD" ambiguity), because no attention was paid to the requirements that F approach a definite value as $z \to -x_0$ and that $(1 - 2\pi i\rho t)$ will have a zero in the vicinity of $-x_0$, so that F must have a pole there. None of these conditions have much qualitative or quantitative effect on the question of the complex poles, because this matter is decided mainly by conditions near the Fermi level, $z = 0$. We now demonstrate that as one continues the solution* from $T > T_c$ into a new one, valid for $T < T_c$, $(1 - 2\pi i\rho t)$ always vanishes at the poles of F. In so doing we shall first construct F for $T > T_c$ in such a way that it satisfies all the asymptotic conditions, so as to leave no obvious loopholes, and also in order to obtain more accurate numerical predictions.

As in I, the function $F^{-1}(z)$ has particularly simple analytic structure. According to (1), (2) and (4) (with η denoting the step function),

$$\operatorname{Im} F^{-1}(x) = -2\pi\rho(x)\ \tanh\left(\frac{\beta x}{2}\right) \eta(x + \varepsilon_f), \tag{7}$$

$$F^{-1}(-x_0) = 8\pi\ V\ \sqrt{x_0 - \varepsilon_f}/J, \tag{8}$$

* By using the freedom supplied by the CDD ambiguity.

$$F^{-1}(z) = 0(z), \quad z \to \infty. \tag{9}$$

From (7), (8) and (9), one can immediately construct the function

$$F(z) = \left[\frac{8\pi\ V \sqrt{x_0 - \varepsilon_f}}{J} + c(z + x_0) - (z + x_0) \int_{-\varepsilon_f}^{\infty} dx \frac{2\rho(x) \tanh(\beta x/2)}{(x + x_0)(x - z)} \right]^{-1} \tag{10}$$

where c is a real parameter whose numerical value is to be determined later.

Let us now turn to the non-spin slip amplitude $t(z)$ and make the ansatz of Froissart [5]:

$$2\pi i\ \rho(z) t(z) = -\left(R(z) e^{-2i\delta_{\bar{V}}(z)} - 1 \right) \tag{11}$$

where

$$R(z) = \exp\left[\frac{2i\ \rho(z)}{\pi} \int_{-\varepsilon_f}^{\infty} \frac{\delta''(x)}{\rho(x)(x - z)} \right] \tag{12}$$

$\delta''(x)$ is related to $F(x)$ by equation (5):

$$\delta''(x) = (1/4) \log\left[1 + a(x)\ |F(x)|^2 \right] \tag{13}$$

and $\delta_{\bar{V}}(z)$ is the phaseshift due to an ordinary potential scattering problem

$$\bar{t}(z) \equiv -\left(e^{-2i\delta_{\bar{V}}} - 1 \right) / 2\pi i \rho, \tag{14}$$

$$\bar{t}(x) = \frac{\bar{V} x_0}{z + x_0} + \int_{-\varepsilon_f}^{\infty} dx \frac{|\bar{t}(x)|^2\ \rho(x)}{z - x}. \tag{15}$$

The potential $\bar{V}$ is not quite equal to V (a finer point which was also neglected in I). Rather, from the fact that

$$2\pi i \rho \bar{t} = -\left(e^{-2i\delta_{\bar{V}}(z)} - 1 \right),$$

it follows that

$$R(z) = \left(1 - 2\pi i\ \rho(z)\ t(x) \right) / \left(1 - 2\pi i\ \rho(z)\ \bar{t}(z) \right), \tag{16}$$

so that near $z = -x_0$

$$\frac{\bar{V}}{V} = \frac{1}{R(-x_0)} \tag{17}$$

Equation (15) is identical in form to equation (22) of I and can be solved by the standard method. It gives

$$\bar{t}(z) = \frac{\bar{V}x_0}{(z + x_0)\left[1 + \bar{V}x_0(z + x_0)\int_{-\varepsilon_f}^{\infty} dx \frac{\rho(x)}{(x + x_0)^2(x - z)}\right]} \tag{18}$$

Now from (4), (11) and (14)

$$\tau(z) = R(z)\left[1 - 2\pi i\ \rho(z)\ \bar{t}(z)\right] F(z) \tag{19}$$

By explicitly evaluating the integral in (18), one finds that $(1 - 2\pi i\rho\bar{t})$ has a zero at

$$z = -\bar{x}_0 = -x_0 + (x_0 - \varepsilon_f)\left[1 - \left(\frac{2\sqrt{x_0 - \varepsilon_f} + \pi\bar{V}x_0}{2\sqrt{x_0 - \varepsilon_f} - \pi\bar{V}x_0}\right)^2\right] \tag{20}$$

On the other hand $\tau(z)$ does not necessarily have a zero at $-\bar{x}_0$. In particular, in the weak coupling limit, the perturbative solutions of (1) and (2) does not produce such a zero in $\tau(z)$. In order to have a solution joining analytically to the perturbative results for weak coupling, we must adjust the parameter c in (10) so that $F(z)$ has a pole at $-\bar{x}_0$. The function $F(z)$ can now be rewritten as

$$F(z) = \frac{\bar{J}}{(z + \bar{x}_0)\left[1 - 2\bar{J}(z + x_0)\int_{-\varepsilon_f}^{\infty} dx \frac{\rho(x)\tanh(\beta x/2)}{(x + x_0)(x + \bar{x}_0)(x - z)}\right]} \tag{10$'$}$$

where

$$\bar{J} = \left(\frac{J}{V}\right)\left(\frac{\bar{x}_0 - x_0}{8\pi\sqrt{x_0 - \varepsilon_f}}\right) \tag{21}$$

For practical calculations, it is more convenient to take $\bar{V}$ and $\bar{J}$ rather than V and J as input parameters of the problem. Starting with (18), one calculates $\bar{t}(z)$ and $\delta_{\bar{V}}(z)$. Then one evaluates $\bar{x}_0$ by (20) and calculates $F(z)$ by (10$'$). Using (13), (12) and (11) one obtains successively $\delta''(x)$, $R(z)$ and $t(z)$. Finally $\tau(z)$ is determined by (19).

Now we come to the central question of complex poles. At given J, for all temperatures above a certain critical one, T_c, the expression (10$'$) contains a series of complex poles on the unphysical sheet. At T_c, two of these poles meet, at $z = 0$, and then proceed to the physical sheet for $T < T_c$. For the discussion of these poles, it is more convenient to consider the complex variable $\rho(\rho = (z + \varepsilon_f)^{1/2})$ rather than z. The physical sheet becomes the upper half-plane of ρ and the unphysical sheet, the lower half-plane.

Considered as a function of β (for fixed $\bar{J}$) the positions of the complex poles in the ρ-plane for β in the neighborhood of $\beta_c = 1/kT_c$ are given by

$$P(\beta) = \pm P_r(\beta) + iP_i(\beta) \tag{22}$$

where

$$P_i(\beta) = \begin{cases} > 0, & \beta > \beta_c\,, \\ 0, & \beta = \beta_c\,, \\ < & \beta < \beta_c\,, \end{cases}$$

and $P_r(\beta_c) = (\varepsilon_f)^{1/2}$.

Define*

$$G(z) = \frac{1}{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)} \tag{23}$$

$$R_0(z) = \exp\left\{\frac{i\rho(z)}{\pi}\int_{-\varepsilon_f}^{\infty} dx\,\frac{\log[1 + a(x)|G(x)|^2]}{2\rho(x)(x - z)}\right\} \tag{24}$$

For $\beta < \beta_c(T > T_c)$, a straightforward evaluation of the integral in (24) gives

$$R_0(z) = \bar{R}(z) \equiv \frac{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)}{(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)} \tag{25}$$

where

$$\alpha_\pm = \sqrt{\gamma \pm \sqrt{\gamma^2 - (P_r^2 - P_i^2)^2}}\,,$$

$$\gamma = 4\pi^2\, S(S + 1) - P_r^2 + P_i^2\ .$$

As the temperature decreases through T_c, $R_0(z)$ as given by the integral representation (24) no longer agrees with the analytic continuation of $\bar{R}(z)$ given by (25). In fact, as explained in the Appendix, they differ by a unimodular factor

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* In this paper we actually work in dimensionless units with $\varepsilon_f = 1$. Hence $a|G|^2$ in (24) is dimensionless. If one does not work in dimensionless units, the numerator of G must be supplied with a factor of dimension $\sqrt{\text{energy}}$. This does not affect the result (see H. SUHL, *Varenna Lectures*, June 1966, to be published).

$$R_0(z) = \frac{(\rho(z) - P_r + iP_i)(\rho(z) + P_r + iP_i)}{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)} \quad \bar{R}(z); \; P_i > 0) \tag{26}$$

Now, in the place of the integral representation (12), we define $R(z)$ to be

$$\begin{aligned} R(z) &= \bar{R}(z)\, R_0^{-1}(z) \exp\left[\frac{2i\rho(z)}{\pi} \int_{-\varepsilon_f}^{\infty} dx \frac{\delta''(x)}{\rho(x)(x-z)}\right] \\ &= \bar{R}(z)\, A(z) \;. \end{aligned} \tag{27}$$

It is clear that $A(z)$ contains no complex poles or zeros in the neighborhood of $z = 0$ and the integral representations for $A(z)$ gives the proper analytic continuation from $T > T_c$ to $T < T_c$. Furthermore, $\bar{R}(z)$ as given explicitly by (25) is trivially the analytic continuation as P_i goes from negative to positive values. Hence $R(z)$ as defined by (27) is equal to the Froissart function (12) for $T > T_c$ and gives the analytic continuation in T for $T < T_c$. It contains a pair of complex zeros which exactly cancels the poles of $F(z)$.

The calculational procedure for $T < T_c$ is essentially the same as described above except that now we must evaluate P_r and P_i before calculating $R(z)$. A simple method for finding P_r and P_i is as follows:

Define

$$H(z) = 1 - 2\bar{J}(z + x_0) \int_{-\varepsilon_f}^{\infty} dx \frac{\rho(x)\tanh(\beta x/2)}{(x + x_0)(x + \bar{x}_0)(x - z)} \tag{28}$$

$$H'(z) = \exp\left\{\frac{z + x_0}{\pi} \int_{-\varepsilon_f}^{\infty} dx \frac{\tan^{-1}[\,\mathrm{IM}\, H(x)/\mathrm{Re}\, H(x)\,]}{(x + x_0)(x - z)}\right\} \tag{29}$$

Since H and H' are separately real analytic functions, the quotient (H/H') is also a real analytic function. However, by construction, (H/H') is real along the entire real axis. Hence, it has no branch point and can only be a polynomial in z (H' also has no zeros). This polynomial must contain the zeros of H:

$$\frac{H(z)}{H'(z)} = \frac{(z + \varepsilon_f + P_r^2 + P_i^2)^2 - 4P_r^2(z + \varepsilon_f)}{(-x_0 + \varepsilon_f + P_r^2 + P_i^2)^2 - 4P_r^2(-x_0 + \varepsilon_f)} \tag{30}$$

The constant factor in the denominator restores the normalization $(H(-x_0)/H'(-x_0)) = 1$ as required by (28) and (29). Now, by evaluating (28) and (29) for H and H' at any two points in the z-plane, we obtain two algebraic equations for the two unknown P_r and P_i using (30). These equations can be solved easily; thus the calculational procedure is complete.

As noted above, R_0 and $\bar{R}$ differ by a factor, unimodular along $x > -\varepsilon_f$, for $\beta > \beta_c$. One might question whether it would be possible to supply additional factors of this kind as long as they only produce poles on the lower half ρ-plane (unphysical sheet in z). As far as the original equations (1) and (2) are concerned, this is indeed possible and the arbitrariness associated with it is the well-known CDD ambiguity. On the other hand, if one accepts the perturbative solution as the desired solution for the range of β where the series converges, then our solution for $\beta > \beta_c$ is the analytic continuation from the region of small β, and is the only acceptable one within the present model.

3. Computation of Transport Coefficients

It is customary to write the total resistivity in the form

$$\rho_{\text{total}} = \rho_{\text{lattice}} + \rho_{\text{impurities}} . \tag{31}$$

Such a decomposition is questionable when one or both of the corresponding collision cross-sections are markedly energy-dependent near the Fermi level. A correct theory would require solution of a complicated integral equation. We have therefore calculated the transport coefficients for impurity scattering alone, and thus accept equation (31) in the hope that it is approximately correct. At temperatures sufficiently far below the Kondo resistance minimum, equation (31) is, of course, correct since the lattice scattering is very small there. We assume, furthermore, that in the limit of very low concentration, Boltzmann transport theory applies in the present problem.

The rate of change of the electron distribution function $f(\varepsilon_k)$ due to collisions is then given by

$$\left.\frac{\partial f(\varepsilon_k)}{\partial t}\right|_{\text{coll.}} = \frac{\Omega}{8\pi^3}\frac{2\pi}{\hbar}\int \delta(\varepsilon_k - \varepsilon_{k'})\, p_{kk'} \Big[f(k')(1 - f(k)) - f(k)(1 - f(k')) \Big]\, d^3k'$$

where $p_{kk'}$ is essentially the imaginary part of the non-spinflip scattering amplitude:

$$P_{kk'} = |t_{kk'}|^2 + 4S(S+1)|\tau_{kk'}|^2$$

and Ω is the sample volume.

The Boltzmann equation is solved in the usual way: f is taken in the form

$$f(\varepsilon) = f_0(\varepsilon) + \vartheta(\varepsilon)\, v \frac{\partial f}{\partial \varepsilon}\left(eE + T\frac{\partial}{\partial x}\frac{\varepsilon_f}{T} + \frac{\varepsilon}{T}\frac{\partial T}{\partial x}\right)$$

where E is the electric field, T the temperature, ε_f the fermi energy, and f_0 the Fermi distribution function. The reciprocal relaxation time ϑ is given by

$$\vartheta^{-1}(\varepsilon) = \frac{\pi\rho(\varepsilon)}{\hbar}\int_0^{\pi} p_{kk'}(1 - \cos\theta_{kk'})\sin\theta_{kk'}\, d\theta_{kk'}\Big|_{\varepsilon_k=\varepsilon_{k'}=\varepsilon}$$

here $\theta_{kk'}$ is the angle between k and k'. Defining the usual moments

$$K_n = \int \vartheta(\varepsilon)\ \varepsilon^n \frac{\partial f}{\partial \varepsilon}\ \rho(\varepsilon)\ d\varepsilon$$

e have, for the ratio of the conductivity at finite J to the ordinary residual resistance at ero J

$$\frac{\sigma_J}{\sigma_0} = \frac{K_1(J,\ V)}{K_1(0,\ V)}\ ,$$

$_0$ is of course practically independent of temperature. The thermoelectric voltage per °K is

$$\Theta(J,\ V) = \left(K_2 - \varepsilon_f K_1\right) / e\ T\ K_1$$

nd the ratio of Lorentz numbers at J finite and $J = 0$ is $L(J,\ V)/L(J,\ 0)$ where

$$L(J,\ V) = \left(\frac{K_1 K_3 - K_2{}^2}{K_1}\right)_{J,V}$$

n the computation, the Fermi-level is taken as the energy zero, and all energies are measured n units of ε_f. Then

$$K_n = \varepsilon_f{}^n \int \rho(x)\ \vartheta(x)\ (1 + x)^n \frac{\partial f}{\partial x}\ dx$$

o that the thermoelectric voltage may be written

$$\frac{k}{e}\ \beta\ \frac{I_1 + I_2}{I_0 + I_1}$$

here

$$I_n = \int \rho(x)\ \vartheta(x)\ x^n \frac{\partial f}{\partial x}$$

nd $\beta = \varepsilon_f / kT$.

In the evaluation of the relaxation time ϑ, the s-wave parts of t and τ were taken into ccount exactly, the higher partial waves only in Born approximation. This was done by contructing that potential $V_{kk'}$ whose s-wave part has a single pole on the real axis below $-\varepsilon_f$.

We write,

$$t_{kk'}(x) = V_{kk'} - \frac{V x_0}{x + x_0} + t(x)$$

where

$$V_{kk'} = \frac{4x_0(x_0 - \varepsilon_f)\ V}{\left[2(x_0 - \varepsilon_f) + (x + \varepsilon_f)(1-\cos\theta_{kk'})\right]^2}$$

and similarly for $J_{kk'}$. In configuration space, such a potential has exponential form. The amplitude $t(x)$ is still only approximate, in the sense that even for an exponential potential, $t(z)$ (as distinct from the s-wave part of V) has a whole series of discrete poles (not just a single one) on the left hand real axis.

4. Discussion

Figures 1 a-d) show σ_J/σ_0 for a variety of values of V and J, for $S = ½$, and for a force range $x_0 = 2$ (i.e. $1/k_f$ in the usual units). Wherever "T_c" occurs within the range of the graph, we have marked it by an open circle, and we note that the curves are quite smooth there. The qualitative character of the curves is summarized in Fig. 2. For a given V, the conductivity is more or less constant at high temperatures. As the temperature is decreased it eventually begins to decline, linearly on a log-scale over several decades, and gradually flattens off again in the vicinity of T_c. From then on, it stays virtually constant down to absolute zero. The smaller J, the lower the temperature at which the decline begins, but the low temperature

FIGURE 1

The ratio σ_J/σ_0 for various V and J.

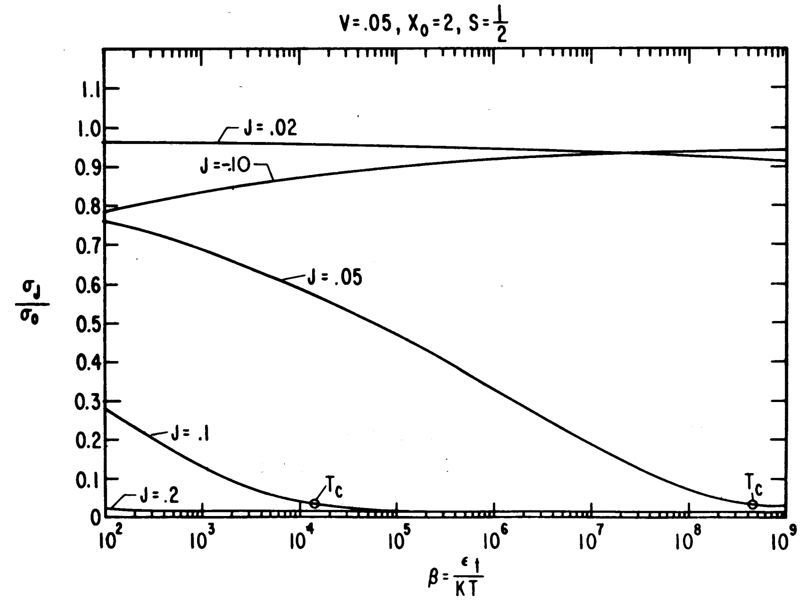

Fig. 1a.

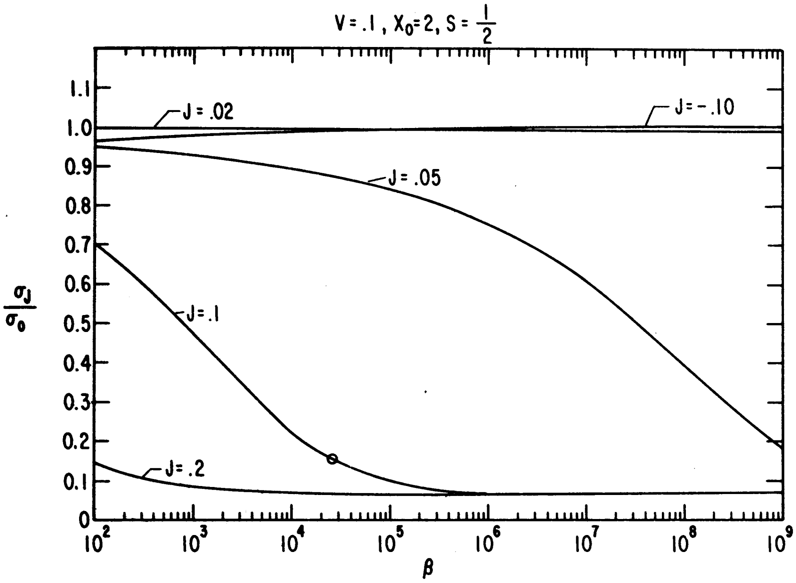
V = .1, X_0 = 2, S = $\frac{1}{2}$
J = .02
J = -.10
J = .05
J = .1
J = .2
$\frac{\sigma_J}{\sigma_0}$
β

Fig. 1*b*.

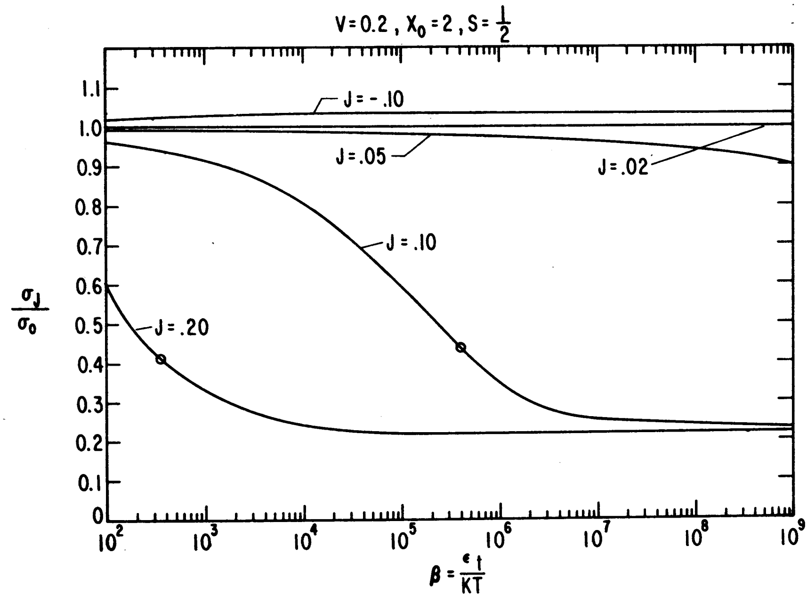
V = 0.2, X_0 = 2, S = $\frac{1}{2}$
J = -.10
J = .05
J = .02
J = .10
J = .20
$\frac{\sigma_J}{\sigma_0}$
$\beta = \frac{\epsilon_t}{KT}$

Fig. 1*c*.

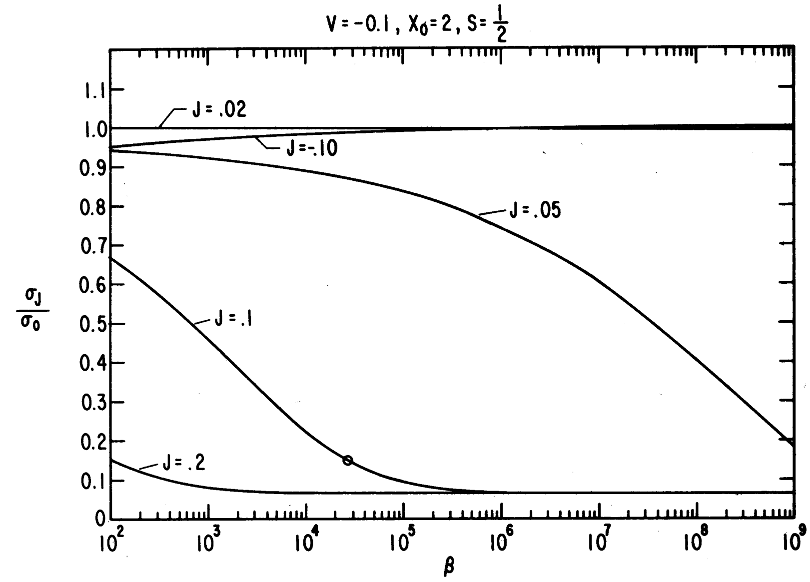

Fig. 1*d*.

plateau value is independent of J. Finally, for $J = 0$, the decline does not set in until $T = 0$ (see Fig. 2); for any finite T, no matter how small, we simply get the usual temperature independent impurity resistance due to ordinary potential scattering alone. At $T = 0$ and $J = 0$, equations (1) and (2) have a bootstrap solution (see Fig. 2), i.e. there is a solution with a finite τ although $J = 0$; however, no such solution exists at any arbitrarily small temperature. A negative value of J (ferromagnetic coupling) has also been considered; it appears that the conductivity will then actually increase slightly at low temperatures. That all the curves must reach a high temperature plateau is easily seen by noting that as $\beta \to 0$, equations (1) and (2)

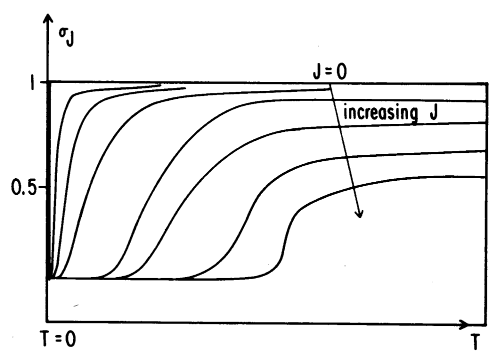

FIGURE 2

Qualitative summary of the conductivity curves as a function of J.

reduce to ordinary potential scattering problems for two new amplitudes

$$u_{\pm} = t \pm 2 \sqrt{S(S+1)}\ \tau$$

in potentials of the form

$$\frac{x_0}{z + x_0} \left\{ V \pm \tfrac{1}{2} \sqrt{S(S+1)}\ J \right\}$$

In that limit $\rho_{kk'} = |u_+|^2 + |u_-|^2$, and the energy dependence of $u_{\pm}$ near $z = 0$ is so weak that the resistivity is then virtually temperature independent. Figure 3 shows a comparison with a 3rd order perturbation calculation, and with a solution in which the correct analytic continuation is not made, and complex poles remain. The 3rd order conductivity does not initially decrease as sharply with temperature as does the exact result, but since it contains the Kondo

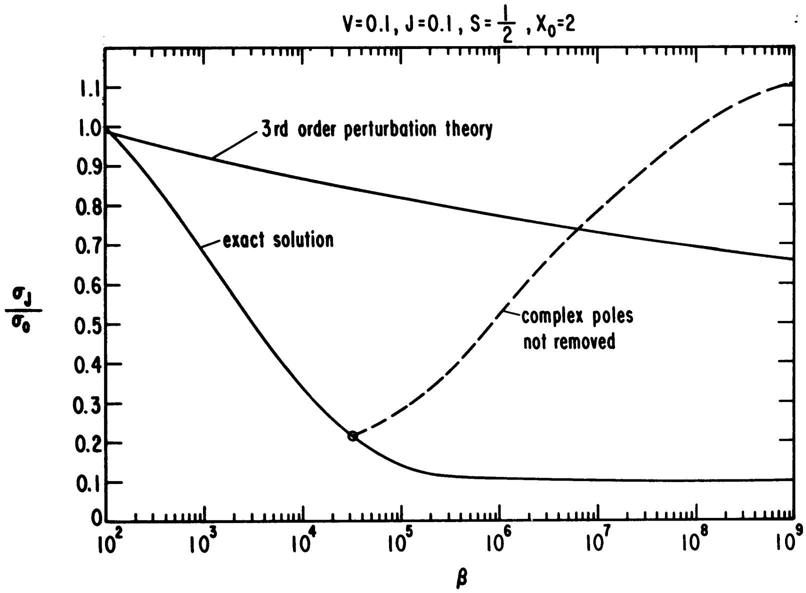

FIGURE 3

Comparison with perturbation theory and with the improperly continued solution.

singularity it must eventually go to zero at infinite β. The thermoelectric voltage shows some fairly spectacular behavior (Figs. 4 *a-d*). For $V > 0$ (repulsive potential) and $J > 0$ (antiferromagnetic coupling), it shows a change in sign and a low temperature maximum comparing favorably with its magnitude in the range $\beta \sim$ a few hundred, which (for ordinary ε_F's) is the room temperature range. At small β's, the thermoelectric voltage varies as β^{-1}, just as for potential scattering. For $V < 0$, no change in sign seems to occur, but the low temperature maximum in thermoelectric power remains. In all cases, the maximum shifts rapidly towards lower temperature with decreasing J. For a rather unrealistically large J of order 0.2, the peak occurs in the room temperature range. For $V > 0$ and $J < 0$, no change in sign or peak seems to occur.

FIGURE 4

The thermoelectric power. Θ is in $V/°K$.

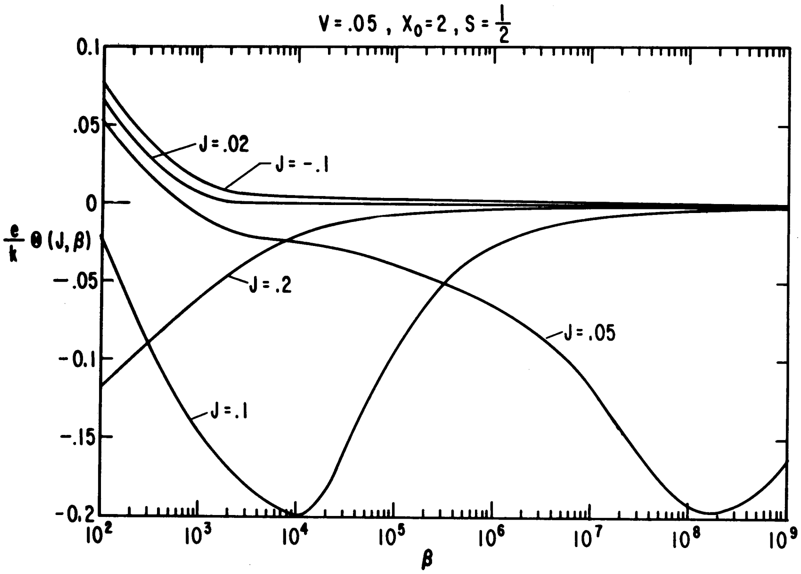

Fig. 4*a*.

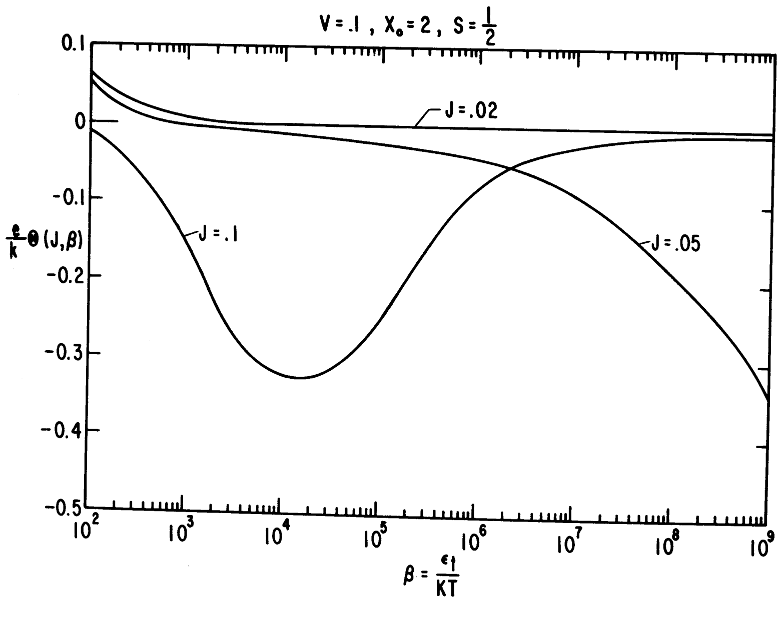

Fig. 4*b*.

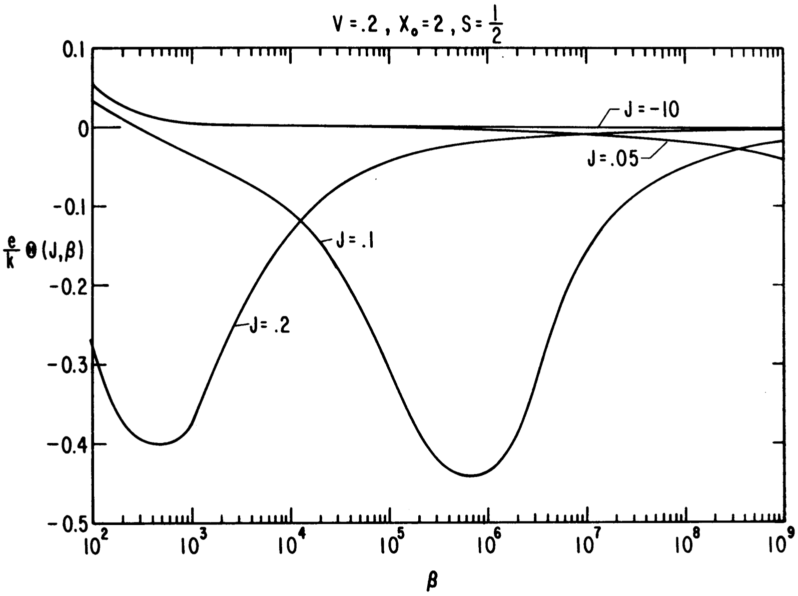
V = .2 , X₀ = 2 , S = 1/2
0.1
0
-0.1
-0.2
-0.3
-0.4
-0.5
e/k Θ (J, β)
J = -10
J = .05
J = .1
J = .2
10²
10³
10⁴
10⁵
10⁶
10⁷
10⁸
10⁹
β

Fig. 4*c*.

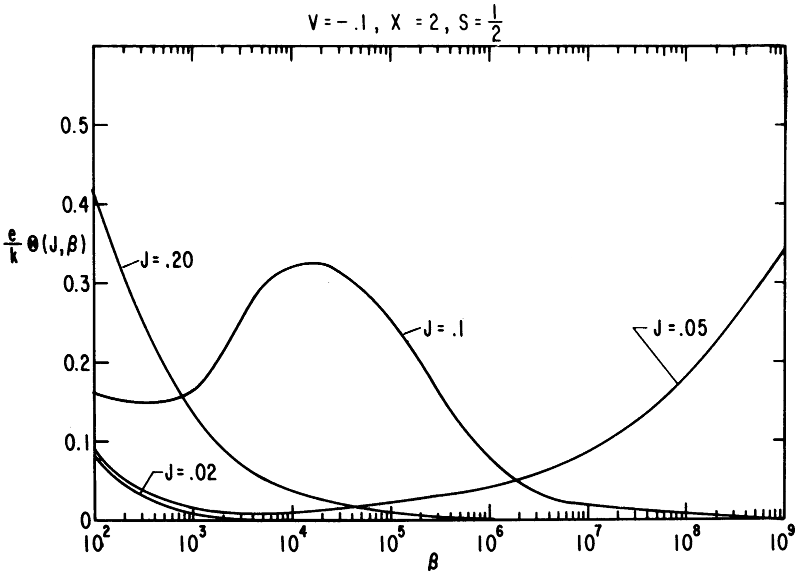
V = - .1 , X = 2 , S = 1/2
0.5
0.4
0.3
0.2
0.1
0
e/k Θ (J, β)
J = .20
J = .1
J = .05
J = .02
10²
10³
10⁴
10⁵
10⁶
10⁷
10⁸
10⁹
β

Fig. 4*d*.

Such "giant" thermoelectric power effects have previously been discussed by Kondo using perturbation theory [6].

Finally, we note that no spectacular variations seem to occur in the Lorentz number L as a function of temperature (Figs. 5 *a-c*)). This number has a broad, low temperature peak extending

FIGURE 5

Ratio of Lorentz numbers at finite to zero J.

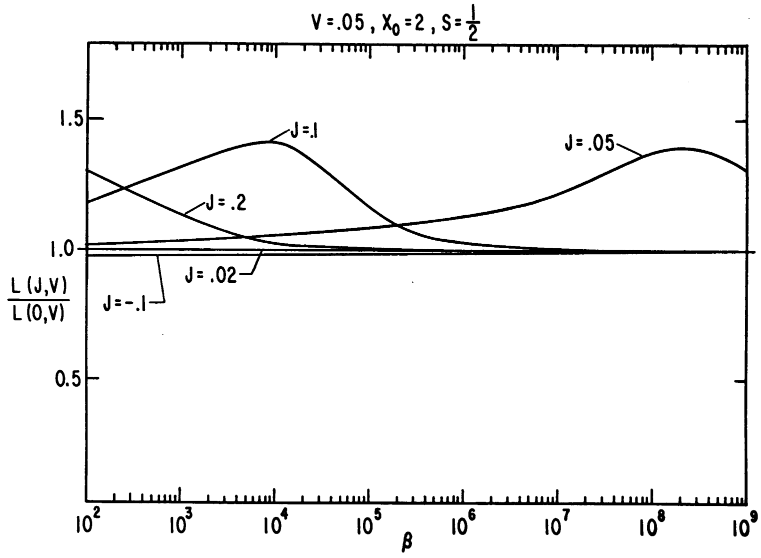

Fig. 5*a*.

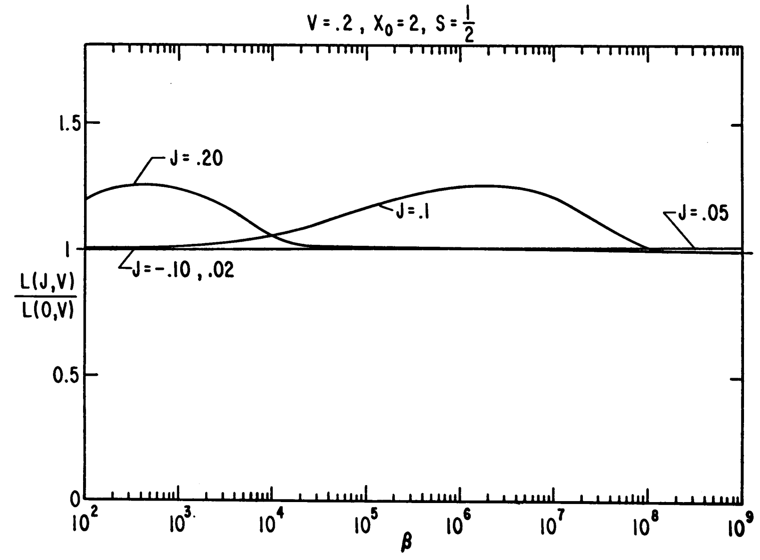

Fig. 5*b*.

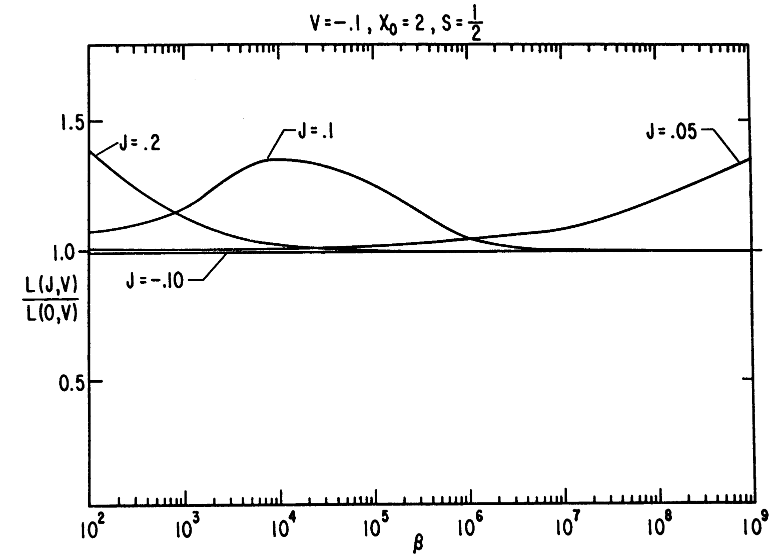

Fig. 5*c*.

over two to three decades and reaching about 40 per cent above the (apparently equal) high and low temperature plateau values. Hence the thermal conductivity $\kappa = \sigma TL$ should diminish at low temperatures somewhat in the same way as the electrical conductivity.

FIGURE 6

Resonance in the non-spin flip scattering amplitude.

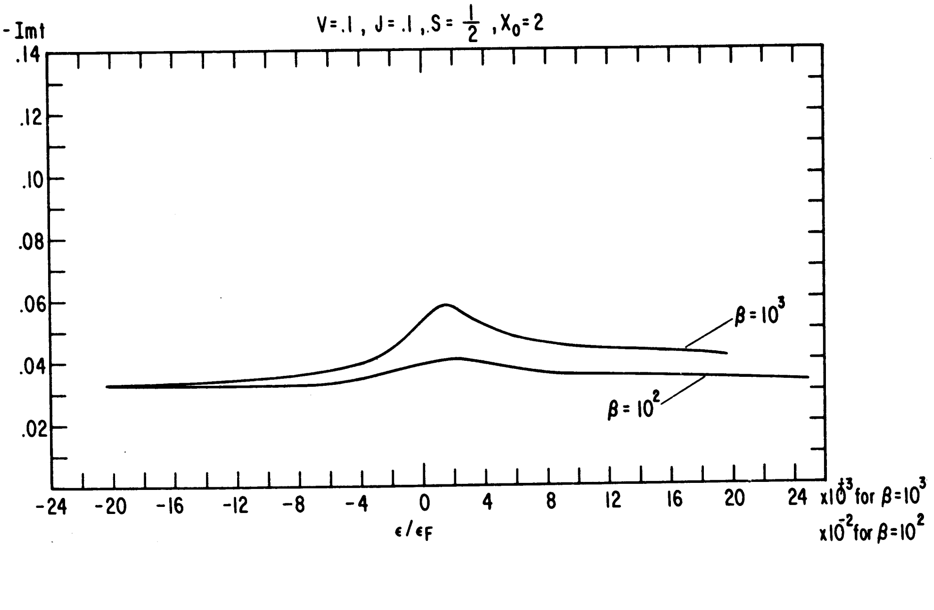

Fig. 6*a*.

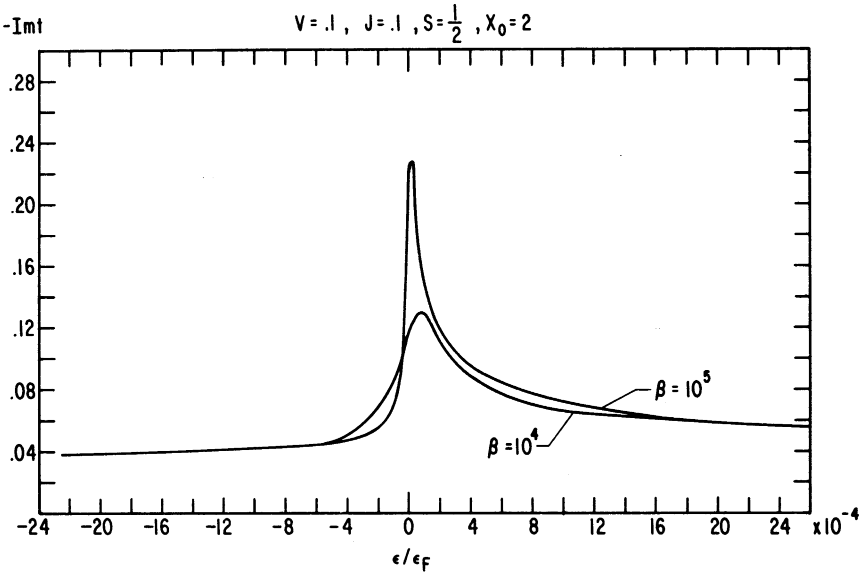

Fig. 6*b*.

It is of some interest to note that Im $t(\varepsilon)$, the quantity that determines single particle state density in a simple multiple scattering approximation [2], for negative J does exhibit a maximum slightly above the Fermi level. The maximum is the narrower and larger the lower the temperature (see Figs. 6*a* and *b*).

References

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4. J. KONDO, *Progr. Theoret. Phys., Kyoto* 32, 37 (1964).

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APPENDIX

Evaluation of the integral in equation (24)

The integral (including the factor $1/\pi$) may be written

$$L(z) = \frac{1}{\pi} \int_{-\varepsilon_f}^{\infty} dx \ln \left[\frac{(\rho - i\alpha_+)(\rho + i\alpha_+)(\rho - i\alpha_-)(\rho + i\alpha_-)}{(\rho - P_r - iP_i)(\rho - P_r + iP_i)(\rho + P_r - iP_i)(\rho + P_r + iP_i)} \right] / 2\rho(x)(x - z)$$

where $\rho(x) = \sqrt{x + \varepsilon_f + i0}$, and the square root is defined as in I. The imaginary part of $L(z)$ just above the real axis is

$$\operatorname{Im} L(x + i0) = \frac{1}{2\rho} \ln \frac{(\rho - i\alpha_+)(\rho + i\alpha_+)(\rho - i\alpha_-)(\rho + i\alpha_-)}{(\rho - P_r - iP_i)(\rho - P_r + iP_i)(\rho + P_r - iP_i)(\rho + P_r + iP_i)}$$

for $x > -\varepsilon_f$ and zero for $x < -\varepsilon_f$. Now consider the following function:

$$J(z) = \frac{i}{2\rho(z)} \ln \frac{(\rho(z) - i\alpha_+)(\rho(z) + i\alpha_+)(\rho(z) - i\alpha_-)(\rho(z) + i\alpha_-)}{(\rho(z) - P_r - iP_i)(\rho(z) - P_r + iP_i)(\rho(z) + P_r - iP_i)(\rho(z) + P_r + iP_i)}$$

We have

$$\operatorname{Im} J(x + i0) = \operatorname{Im} L(x + i0)$$

for $x > -\varepsilon_f$. For $x < -\varepsilon_f$, $\rho = i\sqrt{|x| + \varepsilon_f}$, and the lograrithm is real, therefore $\operatorname{Im} J(x + i0) = 0$ for $x < -\varepsilon_f$. Furthermore, like $L(z)$, $J(z)$ tends to zero as $z \to \infty$. Hence L would be equal to J, were it not that $J(z)$ has singularities on the physical sheet, whereas $L(z)$ has none.

These singularities are at $\rho(z) = \alpha_+$, α_-, and, for $T > T_c$, at $\rho = \pm P_r + iP_i$. They can be removed by multiplying the argument of the logarithm in $J(z)$ by the following so-called "Blaschke product":

$$B(z) = \frac{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)}{(\rho(z) - P_r + iP_i)(\rho(z) + P_r + iP_i)(\rho(z) - i\alpha_+)(\rho(z) - i\alpha_-)}$$

Now $B(x + i0)$ is unimodular for $x > -\varepsilon_f$, and so does not change $\operatorname{Im} J(x + i0)$. Also, for $x < -\varepsilon_f$ $B(x)$ is real, and again does not change $J(x + i0)$. Thus the value of the integral is

$$L(z) = \frac{i}{\rho(z)} \ln \frac{(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)}{(\rho(z) - P_r + iP_i)(\rho(z) + P_r + iP_i)}, \quad \beta < \beta_c$$

from which (25) follows. When $T < T_c$, a similar procedure applies, but then the singularities of J are at α_+, α_- and $\pm P_r + iP_i$. The signs of the P_i in the Blasche product must then be reversed, and so

$$L(z) = \frac{i}{\rho(z)} \ln \frac{(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)}{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)}, \quad \beta > \beta_c$$

According to (24), R_0 will thus have a discontinuity in slope:

for $T > T_c$, it is $\dfrac{(\rho(z) - P_r - iP_i)(\rho(z) + P_r - iP_i)}{(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)}$ and

for $T < T_c$, it is $\dfrac{(\rho(z) - P_r + iP_i)(\rho(z) + P_r + iP_i)}{(\rho(z) + i\alpha_+)(\rho(z) + i\alpha_-)}$. The correct result, for all T, is $\bar{R}(z)$

as defined by (25). But the expression (24), below T_c, differs from the analytic continuation of (25) to $T < T_c$ by only a unimodular factor, and so the equation Im $t = \pi\rho|t|^2 + 4S(S+1)|\tau|^2$ continues to hold, with R given by (27).