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Transport properties of spin-glasses. Effect of including Kondo-like terms

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Transport properties in spin-glasses have been studied for the *s-d* model using the method of the double-time Green's function. The higher-order Green's functions have been decoupled to lower orders using Nagaoka's decoupling scheme. The self-energy has been obtained in a multiple-scattering approximation. A self-consistent expression for the *t* matrix has been obtained using Hamann's approach, and the temperature T_m, at which the resistivity is maximum, has been calculated. An expression for the Lorenz number has been obtained, following the procedure of Nam and Fullenbaum. The relative contribution to the Lorenz number $(\Delta L/L_0)$, where L is the contribution to the Lorenz number due to the exchange interaction J, is lower in the spin-glass system as compared to the Kondo system. The thermoelectric power has been calculated using the perturbation expansion of the self-energy to order J^3. It is found to contain values V_0J^2 and V_0J^3, where the second term is very large and dominates over the first term at low temperature, and the sign of the thermoelectric power is therefore decided by the sign of V_0 and J. The thermoelectric power involves a term such as $Q+\chi$, where Q is the spin-glass order parameter and χ is the spin-deviation correlation function. No abrupt change in the calculation of the thermoelectric power is found around T_f, which is supported by the experimental data. The thermoelectric power calculation agrees well with the experimental data at low temperatures but there is a systematic discrepancy between the two at high temperatures due to the neglect of the electron-phonon interaction in the present calculation.

I. INTRODUCTION

In a previous paper[1] the present authors calculated the magnetoresistance of the spin-glass alloys within the framework of Edwards-Anderson[2](EA) model, with the use of the method of the double-time Green's function.[3] For this we have used the decoupling approximation of Nagaoka[4]; however, we neglected the correlation functions of the type $\langle a^\dagger_{q'\downarrow}a_{q''\uparrow}s_j^- \rangle$ appearing in the higher-order Green's function. These correlation functions describe the quasibound states between the conduction electrons and the impurity spin. For dilute magnetic alloys Nagaoka's approach has been extensively studied by several authors[5-7] and it has been shown that such correlation functions give rise to the logarithmic divergence in the resistivity and a giant thermoelectric power in dilute magnetic alloys. These anomalous properties are known as the Kondo effect[8] and the corresponding dilute magnetic alloys as the Kondo systems. The transport properties in the dilute magnetic alloy problem has been studied by diverse methods. Abrikosov[9] used the diagramatic approach while Suhl[10] used the Chew-Low method. Later Hamann[7] generalized Nagaoka's approach and could show that all the three methods are closely related. It is to be noted that Nagaoka's formulation is easy to handle because only the lowest-order decoupling is involved. Recently the renormalization group and the scaling ideas have also been applied to the Kondo problem[11] and Bethe ansatz has been used to calculate, essentially, exactly the energy spectrum and the susceptibility of spin-$\frac{1}{2}$ Kondo problem.[12]

In this paper we shall study the transport properties of spin-glasses including the Kondo-like terms in the absence of the magnetic field by using Nagaoka's approach and its generalization by Hamann.[7] We shall study here spin-glass alloys of noble-metal hosts with transition-metal impurities. In these alloy systems there is interaction between the conduction electron and the isolated impurity spins called the *s-d* interaction at very low concentration of magnetic impurities (below 0.1 at. %) . It is argued that the Kondo effect in spin-glasses is washed out due to the presence of the internal magnetic fields. However, there are compelling experimental and theoretical evidences that the Kondo effect in spin-glasses may not be completely ignored. Larsen[13] has argued that the resistivity maximum temperature T_m, which is generally found to be greater than the spin-glass transition temperature T_f, can be explained by including the Kondo-like terms. The giant thermoelectric power in spin-glasses[14,15] is also reminiscent of the persistence of Kondo effect. Larsen[13] has derived the expression for T_m as a function of the Kondo temperature T_k in the parquet approximation with the use of the noise model. Recently Fischer[16] has studied the Kondo effect in spin-glasses and rederived Larsen's result for T_m in the modified form, with the use of the time-dependent perturbation theory by approximating the higher-order spin-deviation correlation functions to two-body correlation functions. Also there is a basic difficulty in his method in treating the spin operator $S_j(t)$ as an ordinary field operator.[17] Because of these objections in the earlier theories, we have here taken up the studies of the resistivity by the method of double-time Green's function and by retaining the Kondo-like terms. Some other transport properties like the thermopower and the Lorenz number have been studied in the spin-glass by the same method and by retaining the Kondo-like terms.

In Sec. II we write the equation of motion for the Green's functions and decouple the higher-order ones into the lower order and then average them over the impurity configurations. In Sec. III we obtain approximate solutions for the Green's functions and hence the self-energy to the first order in concentration. In Sec. IV the resistivity is obtained with the use of the self-consistent expression for the t matrix along the line of Hamann,[7] from which the expression for T_m is derived. The Lorenz number is calculated following closely the approach of Nam and Fullenbaum,[18] while we calculate the thermoelectric power using perturbation method and the self-consistent t-matrix approach. The last section is devoted to the conclusion.

II. FORMULATION

We consider a system of free electrons interacting with the magnetic impurities distributed randomly. The Hamiltonian of the system is given by[19]

$$\begin{aligned} H=\sum_{k,s}\epsilon_k a^\dagger_{ks}a_{ks}+(V_0/N)\sum_{k,k',s,j}\exp[i(\vec{\mathrm{k}}-\vec{\mathrm{k}}')\cdot\vec{\mathrm{R}}_j]a^\dagger_{ks}a_{k's} \\ -(J/N)\sum_{k,k',j}\exp[i(\vec{\mathrm{k}}-\vec{\mathrm{k}}')\cdot\vec{\mathrm{R}}_j][(a^\dagger_{k\uparrow}a_{k'\uparrow}-a^\dagger_{k\downarrow}a_{k'\downarrow})S^z_j+a^\dagger_{k\downarrow}a_{k'\uparrow}S^+_j+a^\dagger_{k\uparrow}a_{k'\downarrow}S^-_j]\ . \end{aligned} \tag{1}$$

The first term is the energy of the free electrons measured from the Fermi energy E_F. The second and third terms are the normal and exchange interactions with the strengths V_0 and J, respectively. For simplicity we assume that V_0 and J are independent of k and k'. The summation over j extends over all the impurity sites N_I. N is the total number of atoms. $a^\dagger_{ks}$ and a_{ks} are the creation and annihilation operators for an electron with the wave vector k and spin s. S^z and $S^\pm$ are the components of the impurity spin operator.

To investigate the transport properties in the spin-glass phase we follow the two-time Green's-function method. We define the retarded double-time single-particle Green's function for $s=s'=\uparrow$ as[3]

$$G_{kk'}(t)=-i\Theta(t)\langle[a_{k\uparrow}(t),a^\dagger_{k'\uparrow}(0)]\rangle\ , \tag{2}$$

where $\langle\ \rangle$ is the thermal average and $\Theta(t)$ is the unit step function. Its Fourier transform is given by

$$G_{kk'}(\omega)=\int_{-\infty}^{\infty}G_{kk'}(t)e^{i\omega t}dt\ . \tag{3}$$

As usual let us write the equation of motion of the Fourier transform of $G_{kk'}(t)$ as follows:

$$(\omega-\epsilon_k)G_{kk'}(\omega)=\delta_{kk'}+(V_0/N)\sum_{q,j}\exp[i(\vec{\mathrm{k}}-\vec{\mathrm{q}})\cdot\vec{\mathrm{R}}_j]G_{qk'}(\omega)-(J/N)\sum_{q,j}\exp[i(\vec{\mathrm{k}}-\vec{\mathrm{q}})\cdot\vec{\mathrm{R}}_j]\Gamma^j_{qk'}(\omega)\ . \tag{4}$$

$\Gamma^j_{qk'}(\omega)$ is the Fourier transform of the higher-order Green's function defined by

$$\Gamma^j_{qk}(t)=-i\Theta(t)\langle[(a_{q\uparrow}(t)S^z_j(t)+a_{q\downarrow}(t)S^-_j(t),a^\dagger_{k\uparrow}(0)]_+\rangle\ . \tag{5}$$

$\Gamma^j_{qk'}(\omega)$ obeys the equation of motion,

$$\begin{aligned} (\omega-\epsilon_q)\Gamma^j_{qk'}(\omega)=\delta_{qk'}\langle S^z_j\rangle+(V_0/N)\sum_{q',j'}\exp[i(\vec{\mathrm{q}}-\vec{\mathrm{q}}')\cdot\vec{\mathrm{R}}_{j'}]\Gamma^{j'}_{q',k'}(\omega) \\ +(J/N)\sum_{q',j'}\exp[i(\vec{\mathrm{q}}-\vec{\mathrm{q}}')\cdot\vec{\mathrm{R}}_{j'}]\{\langle\langle a_{q'\downarrow}(t)[S^z_{j'}(t)S^-_j(t)-S^-_{j'}(t)S^z_j(t)]\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega \\ -\langle\langle a_{q'\uparrow}(t)[S^z_j(t)S^z_{j'}(t)+S^+_{j'}(t)S^-_{j'}(t)]\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega\} \\ -(J/N)\sum_{q',q''}\exp[i(\vec{\mathrm{q}}'-\vec{\mathrm{q}}'')\cdot\vec{\mathrm{R}}_j]\{\langle\langle a_{q\downarrow}(t)a^\dagger_{q'\downarrow}(t)a_{q''\uparrow}(t)S^+_j(t)\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega \\ -\langle\langle a_{q\uparrow}(t)a^\dagger_{q'\uparrow}(t)a_{q''\downarrow}(t)S^-_j(t)\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega \\ +\langle\langle a_{q\downarrow}(t)[a^\dagger_{q'\uparrow}(t)a_{q''\uparrow}(t)-a^\dagger_{q'\downarrow}(t)a_{q''\downarrow}(t)]S^-_j(t)\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega \\ -2\langle\langle a_{q\downarrow}(t)a^\dagger_{q'\downarrow}(t)a_{q''\uparrow}(t)S^z_j(t)\,|\,a^\dagger_{k'\uparrow}(0)\rangle\rangle_\omega\}\ , \end{aligned} \tag{6}$$

where we have used the notation $\langle\langle\ \rangle\rangle_\omega$ for the Fourier transform of the corresponding Green's function and used the commutation relation

$$[S_j^z,S_{j'}^{\pm}]=\pm S_j^{\pm}\delta_{jj'}\ ,$$
$$[S_j^{+},S_{j'}^{-}]=2S_j^z\delta_{jj'}\ . \tag{7}$$

To solve Eqs. (4) and (6) we have to approximate the higher-order Green's functions appearing in (6). For this we shall use the decoupling scheme of Nagaoka,[4]

$$\begin{aligned}
&\langle\langle a_{q\uparrow}a_{q'\downarrow}^{\dagger}a_{q''\uparrow}S_i^{+}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle=\langle a_{q'\downarrow}^{\dagger}a_{q''\uparrow}S_i^{+}\rangle\langle\langle a_{q\uparrow}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle+\langle a_{q\uparrow}a_{q'\downarrow}^{\dagger}S_i^{+}\rangle\langle\langle a_{q''\uparrow}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle\ ,\\
&\langle\langle a_{q\downarrow}a_{q'\downarrow}^{\dagger}a_{q''\uparrow}S_i^{z}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle=\langle a_{q\downarrow}a_{q'\downarrow}^{\dagger}\rangle\langle\langle a_{q''\uparrow}S_i^{z}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle+\langle a_{q\downarrow}a_{q'\downarrow}^{\dagger}S_i^{z}\rangle\langle\langle a_{q''\uparrow}S_i^{z}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle\ ,\\
&\langle\langle a_{q'\uparrow}S_{j'}^{+}S_j^{-}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle=\langle S_{j'}^{+}S_j^{-}\rangle\langle\langle a_{q'\uparrow}\,|\,a_{k'\uparrow}^{\dagger}\rangle\rangle\ ,
\end{aligned} \tag{8}$$

etc. In the absence of the magnetic field, we have

$$\begin{aligned}
&\langle a_{q\uparrow}^{\dagger}a_{q'\uparrow}\rangle=\langle a_{q\downarrow}^{\dagger}a_{q'\downarrow}\rangle\ ,\\
&\langle a_{q\uparrow}^{\dagger}a_{q'\downarrow}S^{-}\rangle=\langle a_{q\downarrow}^{\dagger}a_{q'\uparrow}S^{+}\rangle=2\langle a_{q\uparrow}^{\dagger}a_{q'\uparrow}S^{z}\rangle=-2\langle a_{q\downarrow}^{\dagger}a_{q'\downarrow}S^{z}\rangle\ .
\end{aligned} \tag{9}$$

From Eqs. (8) and (9), Eq. (6) reduces to

$$\begin{aligned}
(\omega-\epsilon_q)\Gamma_{qk'}^{j}=&\langle S_j^z\rangle\delta_{qk'}+(V_0/N)\sum_{q'',j'}\exp[i(\vec{q}-\vec{q}\,'')\cdot\vec{R}_{j'}]\Gamma_{q''k'}^{j'}-(J/N)\sum_{q'',j'}\exp[i(\vec{q}-\vec{q}\,'')\cdot\vec{R}_{j'}]\langle\vec{S}_j\cdot\vec{S}_{j'}\rangle G_{q''k'}\\
&+(2n_q^j-1)(J/N)\sum_{q''}\exp[i(\vec{q}-\vec{q}\,'')\cdot\vec{R}_j]\Gamma_{q''k'}^{j}+(J/N)m_q^j\sum_{q''}\exp[i(\vec{q}-\vec{q}\,'')\cdot\vec{R}_j]G_{q''k'}\ ,
\end{aligned} \tag{10}$$

where

$$n_q^j=\sum_{q'}\langle a_{q'}^{\dagger}a_q\rangle\exp[i(\vec{q}\,'-\vec{q})\cdot\vec{R}_j]$$

and

$$m_q^j=3\sum_{q'}\exp[i(\vec{q}\,'-\vec{q})\cdot\vec{R}_j]\langle a_{q'\uparrow}^{\dagger}a_{q\downarrow}S_j^{-}\rangle\ . \tag{11}$$

Nagaoka[20] has studied the anomalous scattering of conduction electrons in alloys with a moderate concentration of magnetic impurities. Our equations are very similar to his equations. In fact one can easily check that our Eq. (10) reduces to Eq. (12) of Nagaoka[20] for $j'=j$, $V_0=0$, $S=\frac{1}{2}$, and $\langle S^z\rangle=0$.

Equations (4) and (10) are the two basic equations which have been studied by many workers for single impurity in various approximations. The problem is quite involved in the spin-glass phase because of the random distribution of the magnetic impurities. The random distribution of the impurities obviously causes the exchange interaction among the impurity magnetic moments to vary randomly. These spins do not have a long-range correlation with no overall magnetization. We have to introduce this feature of the spin-glass phase into Eq. (10). The correlation term $\langle\vec{S}_j\cdot\vec{S}_{j'}\rangle$ between the spins at j and j' is to be evaluated from the first principles keeping in mind the random distribution of impurities. We have simplified this by resorting to an approximation where we replace $\langle\vec{S}_j\cdot\vec{S}_{j'}\rangle$ by its average over all the impurity configurations, that is we write for $\langle\vec{S}_j\cdot\vec{S}_{j'}\rangle$ in (10),

$$\begin{aligned}
[\langle\vec{S}_j\cdot\vec{S}_{j'}\rangle]_{\text{av}}&=[\langle\vec{S}_j\rangle\langle\vec{S}_{j'}\rangle]_{\text{av}}+[\langle\delta\vec{S}_j\cdot\delta\vec{S}_{j'}\rangle]_{\text{av}}\\
&=(Q+\mathcal{X})\delta_{jj'}\ ,
\end{aligned}$$

where $[\ ]_{\text{av}}$ denotes the average over the impurity configurations,[16] and

$$Q=[\langle S_j\rangle^2]_{\text{av}}$$

and

$$\mathcal{X}=[\langle\delta\vec{S}_j\cdot\delta\vec{S}_j\rangle]_{\text{av}}$$

are the spin-glass order parameter and the spin-deviation correlation functions, respectively. With the above approximation Eq. (10) reduces to

$$\begin{aligned}
(\omega-\epsilon_q)\Gamma_{qk'}^{j}=&(V_0/N)\sum_{q',j'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_{j'}]\Gamma_{q'k'}^{j'}-(J/N)(2n_q^j-1)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j]\Gamma_{q'k'}^{j}\\
&+(J/N)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j](m_q^j-Q-\mathcal{X}_{jj})G_{q'k'}\ ,
\end{aligned} \tag{12}$$

where G_{qk}, Γ^j_{qk}, etc. are to be understood as configurationally averaged.

III. APPROXIMATE SOLUTION FOR $G_{kk'}$ AND $\Gamma_{kk'}$

Equations (4), (11), and (12) are the set of coupled equations to be solved self-consistently. These equations are still quite involved and hence it is necessary to resort to some approximations. With $V_0=0$, similar equations were solved in a t-matrix approximation by Nagaoka[20] for a normal alloy by replacing n^j_q and m^j_q by their averages $\bar{n}^j_q = n_q$ and $\bar{m}^j_q = m_q$. Such an approximation is equivalent to neglecting some of the diagrams with intersections of interaction lines in the calculation of $G_{kk'}(\omega)$. The presence of V_0 in Eq. (12) makes our task more difficult. Let us solve Eq. (12) in the t-matrix approximations. For this we set

$$\alpha^j_{qk'} = -(2n_q-1)(J/N)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j]\Gamma^j_{q'k'} + (J/N)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j](m_q-Q-\chi)G_{q'k'}\,, \tag{13}$$

and write Eq. (12) in a more familiar form,

$$\Gamma^j_{qk'} = G^0_q\alpha^j_{qk'} + (G^0_q V_0/N)\sum_{q',j'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_{j'}]\Gamma^{j'}_{q'k'}\,, \tag{14}$$

where

$$G^0_q = \frac{1}{\omega-\epsilon_q}\,. \tag{15}$$

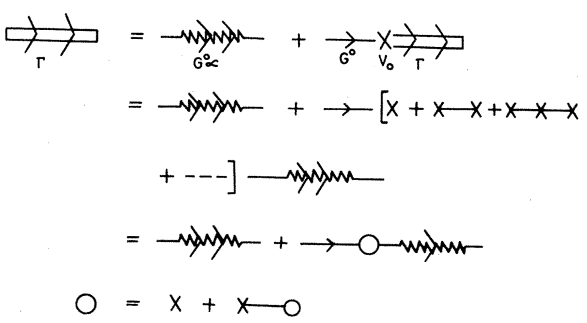

FIG. 1. Graphical representation of the multiple scattering approximation and the iterated form.

Equation (14) can be solved by using the usual technique of the multiple scattering theory. For this we treat the first term in (14) as the inhomogeneous term and iterate it in powers of V_0. A graphical representation to it and its iterated form is given in Fig. 1. In this approximation we get

$$\Gamma^j_{qk'} = G^0_q\alpha^j_{qk'} + (G^0_q t/N)\sum_{p}\exp[i(\vec{q}-\vec{p}\,)\cdot\vec{R}_j]G^0_p\alpha^j_{pk'}\,, \tag{16}$$

where $t = V_0/(1-V_0F)$ is the t matrix for the scattering by a single impurity, and

$$F = (1/N)\sum \frac{1}{\omega-\epsilon_k}\,. \tag{17}$$

We now substitute (13) into (14) and get

$$\Gamma^j_{qk'} = G^0_q[-(2n_q-1)-2tg(\omega)](J/N)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j]\Gamma^j_{q'k'} + G^0_q[(m_q-Q-\chi)+t\Gamma(\omega)](J/N)\sum_{q'}\exp[i(\vec{q}-\vec{q}\,')\cdot\vec{R}_j]G_{q'k'}\,, \tag{18}$$

where

$$g(\omega) = (1/N)\sum_q \frac{n_q-\frac{1}{2}}{\omega-\epsilon_q}$$

and

$$\Gamma(\omega) = (1/N)\sum_q \frac{m_q-Q-\chi}{\omega-\epsilon_q}\,. \tag{19}$$

Now we multiply Eq. (18) by $\exp[i(\vec{k}-\vec{q}\,)\cdot\vec{R}_j]$ and sum over q and j, so that

$$\sum_{q,j}\exp[i(\vec{k}-\vec{q}\,)\cdot\vec{R}_j]\Gamma^j_{qk'} = \frac{J_{\text{eff}}\Gamma(\omega)}{1+2J_{\text{eff}}g(\omega)}\sum_{q',j'}\exp[i(\vec{k}-\vec{q}\,')\cdot\vec{R}_{j'}]G_{q'k'} \tag{20}$$

where $J_{\text{eff}} = J[1+tF(\omega)]$ may be considered as the effective exchange interaction. Substituting Eq. (20) into Eq. (4) we find

$$G_{kk'} = \delta_{kk'}G^0_k + (G^0_k V^*/N)\sum_{q,j}\exp[i(\vec{k}-\vec{q}\,)\cdot\vec{R}_j]G_{qk'}\,, \tag{21}$$

where

$$V^{*}=V_0\frac{J\Gamma(\omega)J_{\text{eff}}}{1+2J_{\text{eff}}g(\omega)} \;. \tag{22}$$

Equation (21) is the well-known equation and can be solved graphically. Equation (15) of Nagaoka[20] is the same as our Eq. (21) with the exception that we have V^{*} instead of V'. Henceforth we shall closely follow his work.

We average over the impurity positions in Eq. (21) and get

$$\overline{G}_{kk}(\omega)=[\omega-\epsilon_k-\Sigma(\omega)]^{-1} \;, \tag{23}$$

where the overbar represents the average over the impurity positions. The self-energy $\Sigma(\omega)$, to the first order in concentration, is given by

$$\Sigma(\omega)=\frac{cV^{*}}{1-V^{*}F(\omega)}=\frac{c[t+2tJ_{\text{eff}}g(\omega)-J_{\text{eff}}^{2}\Gamma(\omega)]}{1+2J_{\text{eff}}g(\omega)+J_{\text{eff}}^{2}\Gamma(\omega)F(\omega)} \;. \tag{24}$$

In order to calculate n_k and m_k we have to find out the following averages:

$$\overline{G}_k=\left[\sum_{k'}\exp[i(\vec{k}\,'-\vec{k}\,)\cdot\vec{R}_j]G_{kk'}\right]_{\text{av}}$$

and (25)

$$\overline{\Gamma}_k=\left[\sum_{k'}\exp[i(\vec{k}\,'-\vec{k}\,')\cdot\vec{R}_j]\Gamma_{kk'}\right]_{\text{av}} \;.$$

$\overline{G}_k$ and $\overline{\Gamma}_k$ can be easily obtained by the procedure of Ref. 20. The final result is

$$\overline{G}_k(\omega)=G_k^0(\omega)\frac{1+2J_{\text{eff}}g(\omega)}{1+2J_{\text{eff}}g(\omega)-F(\omega)\{V_0[1+2J_{\text{eff}}g(\omega)]-JJ_{\text{eff}}\Gamma(\omega)\}} \tag{26}$$

and

$$\overline{\Gamma}_k(\omega)=\frac{J_{\text{eff}}F(\omega)G_q^0(\omega)}{1+2J_{\text{eff}}g(\omega)+J_{\text{eff}}^{2}F(\omega)\Gamma(\omega)}\{[m_k-Q-\chi+t\Gamma(\omega)][1+2J_{\text{eff}}g(\omega)]-[2n_k-1+2tg(\omega)]J_{\text{eff}}\Gamma(\omega)\} \;. \tag{27}$$

With the use of the spectral representation of the Green's functions, n_k and m_k are given by

$$n_k=-\pi^{-1}\int_{-\infty}^{\infty}d\omega f(\omega)\,\text{Im}\overline{G}_k(\omega)$$

and (28)

$$m_k=-2\pi^{-1}\int_{-\infty}^{\infty}d\omega f(\omega)\,\text{Im}\overline{\Gamma}_k(\omega) \;,$$

where $f(\omega)=(e^{\beta\omega}+1)^{-1}$ and $\beta=(k_BT)^{-1}$. Thus we get Eqs. (23), (24), and (26)—(28) as our basic set of equations which should be solved simultaneously in a self-consistent manner.

In the absence of ordinary scattering V_0, Hamann,[7] Falk and Fowler,[5] and Bloomfield and Hamann[21] studied Nagaoka's equations self-consistently and derived an expression for the scattering matrix which is true for all temperatures ($T\gtrless T_k$). Subsequently Kondo[22] and Nagaoka[23] incorporated the ordinary scattering V_0 and obtained the self-consistent expression for the scattering matrix. If we assume that the spin-deviation correlation function χ in (24) is a constant and not affected by the scattering mechanism, Hamann's method may be applied to the present case also in a straightforward manner. In analogy with the work of Hamann[7] and Nagaoka[23] we have

$$\Sigma(\omega)=ct(\omega)=\frac{c}{2\pi i\rho}\left[1-\exp[2i\eta+i\Delta(\omega)]\times\frac{X(\omega)}{[X^2(\omega)+(Q+\chi)\pi^2]^{1/2}}\right], \tag{29}$$

where

$$\begin{aligned}
X(\omega)&=-\frac{1}{\widetilde{\gamma}}\left[1-(Q+\chi)(\pi\widetilde{\gamma}\,)^2\cos^2\eta+\widetilde{\gamma}\int_{-D}^{D}\frac{f(\omega')-\frac{1}{2}}{\omega-\omega'+i\delta}d\omega'\right],\\
\Delta(\omega)&=\frac{1}{2\pi i}\int\frac{dx}{\omega-x+i\delta}\ln|H(X)| \;,\\
H(x)&=\frac{|X(x-i\delta)|^2+(Q+\chi)\pi^2}{X(x-i\delta)^2+(Q+\chi)\pi^2} \;,\\
e^{2i\eta}&=\frac{1+i(\pi\rho_FV_0)}{1-i(\pi\rho_FV_0)} \;,\quad F(\omega)=-i\pi\rho_F \;,\\
\widetilde{\gamma}&=2\widetilde{J}\rho_F \;,\\
\widetilde{J}&=J\cos^2\eta \;,
\end{aligned} \tag{30}$$

where D is the width of the conduction band and η is the phase shift due to the ordinary potential V_0 only. In the following discussions we shall neglect $\Delta(\omega)$ because it plays little role in the calculation of the transport coefficients. The Kondo temperature T_k is obtained by setting $X(0)=0$. This leads to

$$T_k=T_k^0\exp\{-\pi^2[Q(T_k)+\chi(T_k)]\tilde{\gamma}\}\ , \tag{31}$$

where $T_k^0=D\exp(1/\tilde{\gamma})$ is the Kondo temperature for noninteracting spins.

The self-energy expression (29) is not reliable below the Kondo temperature because in this region the localized interaction between isolated impurity and conduction electrons become dominant causing fluctuation in the d- or f-electron spin S of the impurities. Also for $T \ll T_k$, the Kondo effect prevents strong impurity-impurity interactions which are the basic ingredient of spin-glass state. Hence the transition temperature T_f must be higher than T_k. Moreover, our calculation for Q and χ for the "good-moment" system would not be reliable for $T \ll T_k$.

IV. TRANSPORT COEFFICIENTS

We assume that the usual Boltzmann transport theory may be applied to the spin-glass system. The transport coefficients require the evaluation of the integrals[24]

$$K_n=-\int d\epsilon\,\rho(\epsilon)v^2\epsilon^n\sum_\sigma\tau_\sigma(\epsilon)\frac{\partial f(\epsilon)}{\partial\epsilon}\ , \tag{32}$$

where $\rho(\epsilon)$ is the density of states of the host electrons, v the electron velocity, τ_σ the relaxation time for an electron with spin σ, and $f(\epsilon)$ the Fermi-distribution function. τ_σ is related to the imaginary part of the self-energy Σ_σ of the Green's function $\bar{G}_{kk}(\omega)$ through

$$\tau_\sigma^{-1}=-(1/h)\,\mathrm{Im}\Sigma_\sigma(\omega)\ . \tag{33}$$

The electrical resistivity ρ, thermal resistivity W, thermoelectric power S, and the Lorenz number L are given by

$$\begin{aligned}
&\rho=3/e^2K_0\ ,\\
&W=3TK_0/(K_2K_0-K_1^2)\ ,\\
&S=K_1/eTK_0\ ,\\
&L=\rho/WT=(K_2K_0-K_1^2)/(eTK_0)^2\ .
\end{aligned} \tag{34}$$

A. Resistivity

In the absence of the magnetic field $\tau_+=\tau_-$ and the conductivity σ assumes the form

$$\sigma=\frac{2e^2\rho_F}{3}v_F^2\int\tau(\epsilon)\left[-\frac{\partial f}{\partial\epsilon}\right]d\epsilon\ , \tag{35}$$

where we have replaced the energy-dependent $\rho(\epsilon)$ and $v(\epsilon)$ by their values ρ_F and v_F, respectively, at the Fermi surface. σ can be calculated to any desired order in J and V_0. In the Born approximation τ can be easily obtained from (24) and (33) if one sets $m_q=0$ and all the terms higher than J_{eff}^2 are neglected. A simple calculation to order V_0^2 and J^2 yields

$$\tau^{-1}=\frac{c\pi\rho_F}{\hbar}[V_0^2+J^2(Q+\chi)]\ , \tag{36}$$

as obtained by Fischer[25] and also by us.[1]

In this way one can find out τ^{-1} to any desired order in J and V_0 with the use of the perturbation approach. Our main interest is to obtain here the resistivity maximum temperature T_m. For this we use the self-consistent expression (29) for the self-energy and obtain

$$\rho=\frac{3c}{2\pi e^2\rho_F^2v_F^2}\times\left[1-\cos2\eta\frac{\ln(T/T_k)}{[\ln^2(T/T_k)+(Q+\chi)\pi^2]^{1/2}}\right]. \tag{37}$$

For most of the spin-glasses the resistivity maximum temperature T_m is greater than T_f. Hence to calculate T_m, we put $Q=0$ in (37). From the condition $d\rho/dT=0$, simple algebra leads to

$$T_m=T_k\exp\left[\frac{2}{T}\frac{\chi}{\chi'}\right]_{T_m}\ , \tag{38}$$

where $\chi'=d\chi/dT$.

The result (38) is similar to that of Fischer.[16] We observe that T_m is dependent on the spin-deviation correlation function χ. To evaluate it, let us define the Green's function,

$$G_{jj}(t)=\langle\langle\delta\vec{S}_j(t)\,|\,\delta\vec{S}_{j'}(0)\rangle\rangle\ . \tag{39}$$

The spin-deviation correlation function χ_{jj} is related to it through the spectral representation,

$$\begin{aligned}
&[\langle\delta\vec{S}_j\cdot\delta\vec{S}_j\rangle]_{\mathrm{av}}\\
&\quad=\frac{1}{2\pi}\int\frac{d\omega}{e^{\beta\omega}-1}[G_{jj}(\omega+i\epsilon)-G_{jj}(\omega-i\epsilon)]_{\mathrm{av}}\\
&\quad=\frac{1}{\pi}\int\frac{d\omega}{e^{\beta\omega}-1}[\,\mathrm{Im}G_{jj}(\omega+i\omega)]_{\mathrm{av}}\ .
\end{aligned} \tag{40}$$

Now we write[25]

$$[\,\mathrm{Im}G_{jj}(\omega)]_{\mathrm{av}}=\frac{1}{N}\sum_q\frac{\omega\epsilon_q}{\omega^2+\epsilon_q^2}\chi_q\ ,$$

with $\chi_q=\chi$ for an ideal spin-glass and $\epsilon_q=\Lambda q^2$ or $\epsilon_q=\text{const}$. Λ is the diffusion constant. We shall assume that $\epsilon_q=\epsilon_0$ is a constant, which in fact means a single-mode behavior. Evaluating (40) in high-temperature approximation we obtain

$$\chi\simeq\frac{\bar{\chi}}{1+(\beta\epsilon_0/\pi)\ln2} \tag{41}$$

with $\bar{\chi}=(1/\beta)\chi_0$ which is independent of temperature.[25] From Eqs. (38) and (41) we finally obtain

$$d=x_0-\ln(x_0-2)+\ln2\ , \tag{42}$$

where

$$\chi_0=\ln(T_m/T_k),\ \ d=\ln(\bar{\epsilon}_0/k_BT_k)$$

and

$$\bar{\epsilon}_0=\frac{\epsilon_0}{4\ln 2} .$$

This result is the same as obtained by Fischer[16] but there is a difference in the value of $\bar{\epsilon}_0$. In the above treatment it has been assumed that $\mathrm{Im}G_{jj}(\omega)$ is independent of Kondo temperature T_k. It is to be noted that the single-mode approximation for the excitation spectrum used here is crude. To compare with the experimental data one requires the spectrum of excitation modes. From the above discussions it is obvious that T_m is mode dependent.

B. Lorenz number

The Lorenz number for metals containing a low concentration of magnetic impurities has been calculated algebraically by Nam and Fullenbaum[18] using Hamman's[7] expression for the t matrix. They have shown that the Lorenz number L shows a maximum at certain temperature T_0 which may be smaller or greater than T_k. In the previous section we have seen that the form of the t matrix in the spin-glass phase is similar to the normal Kondo systems. The Lorenz number L may be calculated, therefore, using the approach of Nam and Fullenbaum.[18] If we write $\Sigma(\omega)=\Sigma_{V_0}(\omega)+\Sigma_J(\omega)$, where $\Sigma_J(\omega)$ does not contain any contribution from the ordinary scattering potential V_0, the rest of the calculation is then analogous to Nam and Fullenbaum and we get

$$L/L_0=1+0.6666G(1,y) , \tag{43}$$

where $L_0=K(0)/\sigma(0)T$ is the Lorenz number when $J=0$ and $G(1,y)$ is given by (44) below. It is to be mentioned here that in principle one can calculate the Lorenz number using the self-energy expression (29) without splitting it into two parts. We did this mainly to compare our result with the normal Kondo system as follows:

$$\begin{gathered} G(1,y)=-\frac{C_0}{1+C_0 g(0,y)}\frac{\partial g(0,y)}{\partial y} , \\ C_0=C/[2\pi\rho_F(\mathrm{Im}t_n)] . \end{gathered} \tag{44}$$

t_n is the t matrix with $J=0$, and

$$g(0,y)=1-\frac{y}{[y^2+(Q+\chi)\pi^2]^{1/2}} , \tag{45}$$

where

$$y=\ln(T/T_k) .$$

It is to be noted here than unlike the Kondo system, we get an extra temperature dependence to L through $(Q+\chi)$. The temperature T_0 at which L shows a maximum in the Kondo system is around T_k which is near 1 or 2 K. To study L in the spin-glass phase and around T_k, the knowledge of low-temperature excitation modes become important. Several authors have studied the low-temperature excitation modes and their effects[25] on the resistivity and specific heat. Rivier[26] and also we ourselves[1] have shown the $T^{3/2}$ behavior of the resistivity at low temperature in spin-glasses using Rivier's modes.[27] The spin-deviation correlation function χ calculated by these modes is

$$\chi=\frac{\Omega_{\mathrm{at}}S^2}{6\sqrt{2}\pi^2\Lambda^{3/2}}(k_B T)^{3/2}J_{3/2} , \tag{46}$$

where $J_{3/2}=\Gamma(\frac{5}{2})\zeta(\frac{3}{2})$ with $\Gamma(z)$ as the Γ function and $\zeta(n)$ as the Riemann ζ function. Ω_{at} is the atomic volume and Λ is the diffusion constant. At low temperatures the spin-glass order parameter $Q(T)$ is given by[2]

$$Q(T)=S^2(1-T/T_f)\simeq S^2 , \tag{47}$$

for sufficiently small temperatures. Substituting (47) and (46) into (45) we get

$$g(0,y)=1-\frac{y}{\{y^2+\pi^2S^2[1+b\exp(\frac{3}{2}y)]\}^{1/2}} , \tag{48}$$

where b is a constant given by

$$b=\frac{\Omega_{\mathrm{at}}S(S+1)}{6\sqrt{2}\pi^2\Lambda^{3/2}}(k_B T_k)^{3/2}J_{3/2} . \tag{49}$$

In Fig. 2 we have plotted $\Delta L/L_0$ vs temperature for a normal Kondo system (dashed curved lines) and a spin-glass system (solid curved lines) for $\pi\rho V_0=3.29$ (curves I_S and I_K), $\pi\rho V_0=1.0$ (curves II_S and II_K), and $\pi\rho V_0=0.5$ (curves III_S and III_K), where the subscripts S and K stand for the spin-glass and Kondo systems, respectively. The value of $b=0.1$ has been arbitrarily taken because the value of the diffusion constant Λ in (49) is difficult to calculate. From the figure we observe that the value of $\Delta L/L_0$ is lower in the spin-glass system as compared to the Kondo system and also the maximum in the former system is more pronounced and shifted towards lower-temperature values as compared to that in the latter system. On physical ground the result looks sensible because the role of J for the s-d interaction becomes less important for the spin-glass system. For $T/T_k \ll 1$ we find more pronounced deviation between III_S and III_K as compared to other sets of curves. In the first place the deviation is expected because the calculation of Q and χ for the good-moment system breaks down in this temperature region. Secondly, the curves III show much pronounced deviation, which is also expected because the value of $\pi\rho V_0$ in this case is smaller and hence the role of the s-d interaction strength is more dominant.

C. Thermoelectric power

We shall calculate the thermoelectric power from Eqs. (24), (32), and (34). For this we shall assume that v^2 and $\rho(\epsilon)$ in (32) are energy independent and replace them by their values at the Fermi surface. It is then clear that only those terms in $\tau(\epsilon)$ which are odd in ϵ will contribute to the thermoelectric power. Kondo[28] has demonstrated that a giant thermopower in zero field appears in the fourth order of the perturbation series for the relaxation time. The thermoelectric power was found to be proportional to J^3V_0. To calculate the thermoelectric power for the spin-glass system, we shall resort to the perturbation expansion of the self-energy (24) to the fourth order in J and V_0. This is achieved by restricting the values of $\Gamma(\omega)$ to order

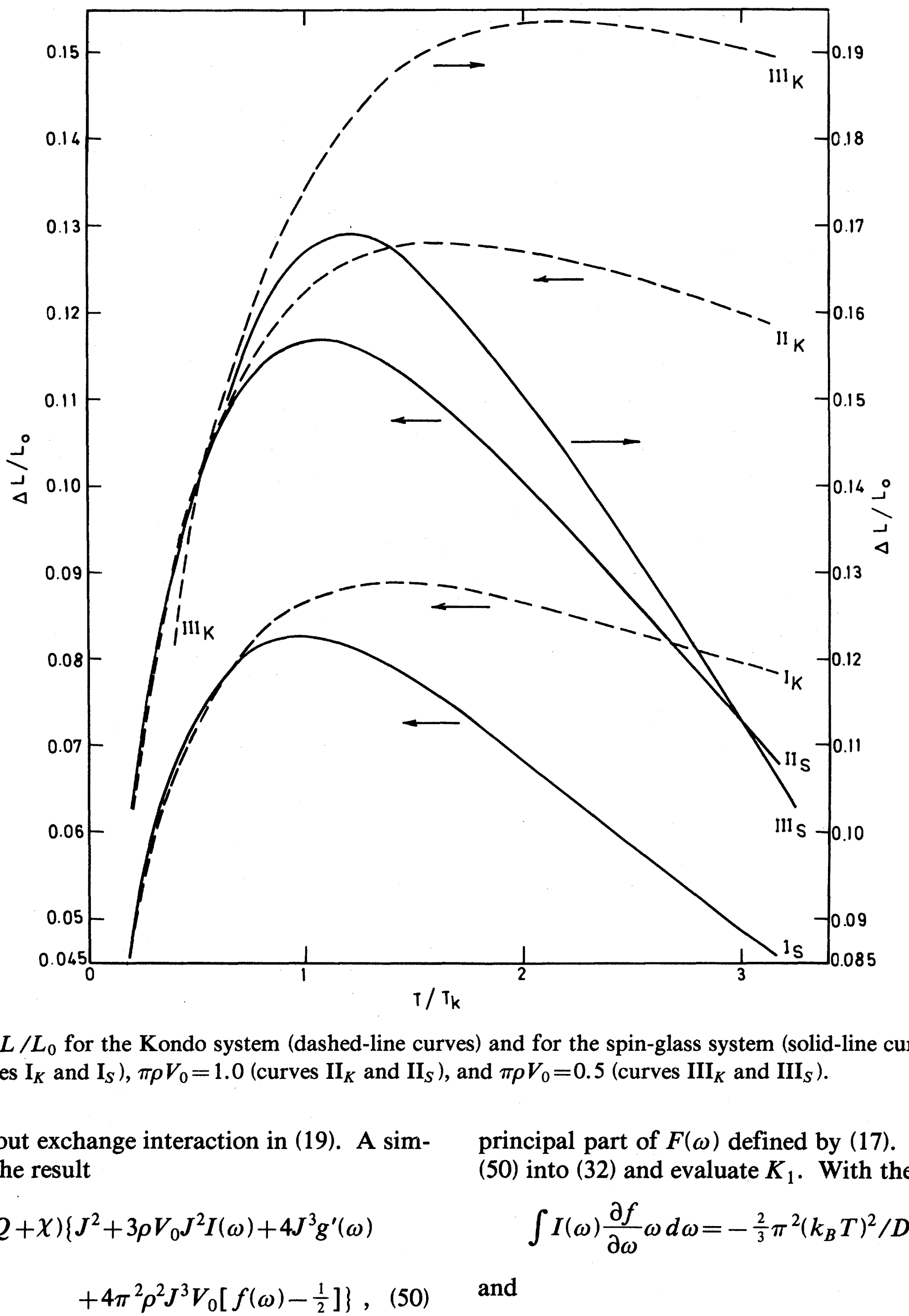

FIG. 2. Plot of $\Delta L/L_0$ for the Kondo system (dashed-line curves) and for the spin-glass system (solid-line curves) with the values of $\pi\rho V_0=3.29$ (curves I_K and I_S), $\pi\rho V_0=1.0$ (curves II_K and II_S), and $\pi\rho V_0=0.5$ (curves III_K and III_S).

J_{eff} and $g(\omega)$ without exchange interaction in (19). A simple algebra yields the result

$$\tau^{-1}=\tau_n^{-1}+\frac{c}{h}\pi\rho(Q+\mathcal{X})\{J^2+3\rho V_0J^2I(\omega)+4J^3g'(\omega)+4\pi^2\rho^2J^3V_0[f(\omega)-\tfrac{1}{2}]\}\;, \qquad (50)$$

where

$$I(\omega)=\int\frac{P}{\omega-\epsilon_k}d\epsilon_k=-\ln\left|\frac{\omega-D}{\omega+D}\right|\simeq\frac{2\omega}{D}$$

and (51)

$$g'(\omega)=\rho\int_0^D P\frac{f(\omega)}{\omega-\epsilon_k}d\omega\;.$$

In (50) we see that the terms in V_0J^2 and V_0J^3 are odd in ω and terms in J^2 and J^3 are even in ω. Hence the contribution to the thermopower will come from the terms V_0J^2 and V_0J^3 only. It is to be mentioned here that Kondo did not get the V_0J^2 term because he neglected the principal part of $F(\omega)$ defined by (17). We now substitute (50) into (32) and evaluate K_1. With the use of the results

$$\int I(\omega)\frac{\partial f}{\partial\omega}\omega\,d\omega=-\tfrac{2}{3}\pi^2(k_BT)^2/D$$

and (52)

$$\int[f(\omega)-\tfrac{1}{2}]\left[\frac{\partial f}{\partial\omega}\right]\omega\,d\omega=\pi^2/12(k_BT)\;,$$

we find

$$S=+\frac{\pi^2}{3}\left[\frac{k_B}{e}\right]\pi^2\rho^2(Q+\mathcal{X})\times\left[\frac{6k_BT}{\pi^2\rho D}V_0J^2+V_0J^3\right]\Big/[V_0^2+(Q+\mathcal{X})J^2]\;. \qquad (53)$$

In the evaluation of K_0, we have used the Born approximation for τ. Thus as expected we get a giant thermopower, the sign of which depends upon the sign of J and V_0. This was also noted by Kondo for the normal alloys. However, in the spin-glass system the thermoelectric power depends on $Q+X$ also, is temperature dependent. There is another term V_0J^2 present in our calculation which might have been present in Kondo's calculation, if he could have taken principal value of $F(\omega)$ in (17). This term, at high temperature will become important and hence there will be a decrease in the absolute value of the thermopower. At sufficiently high temperature the V_0J^2 term may dominate over the V_0J^3 term and this will give rise to positive thermoelectric power. Since the term $(Q+X)$ smoothly varies around the temperature T_f, we do not expect any abrupt change in the thermoelectric power around this temperature. This is also supported by the experimental data.[14] One point must be noted here that Eq. (53) is the high-temperature result. Following the argument of Kondo,[29] one should multiply the right side of (53) by $T/(T+T_0)$ to make it applicable for the whole temperature range, and the resistivity term $[V_0^2+(Q+X)J^2]$ should include the phonon contribution also. Here T_0 is an arbitrary constant to be determined from experimental points. Q and X have been calculated for low temperature from Eqs. (47) and (46), respectively, for $S=\frac{5}{2}$. Above T_f, X has been calculated from Eq. (41). The values of $\pi\rho V_0$ and T_0 have been determined from the two points of the experimental data of *Au*Fe (5 at. %).[14] We get $\pi\rho V_0=1.104$ and $T_0=29.82$. The value of $J/V_0=-0.2$ has been taken. The phonon contribution of the resistivity has been ignored, due to which our result deviates from the experimental curve at high temperature (see Fig. 3). But at low temperature our result agrees well with the experimental data.

As we have obtained a closed expression (29) for the self-energy $\Sigma(\omega)$, it is worthwhile to calculate the thermoelectric power from this expression which will be valid for all temperatures. We have evaluated the two integrals K_1 and K_0 following Maki[30] and have obtained

$$S=-\frac{\pi}{2e}\frac{\sin(2\eta)}{1-\cos(2\eta)\{\ln(T/T_k)/[\ln^2(T/T_k)+\pi^2(Q+X)]^{1/2}\}}\frac{\pi^2(Q+X)}{[\ln^2(T/T_k)+\pi^2(Q+X)]^{3/2}}\ . \tag{54}$$

We see that the dependence of the sign of the thermopower on V_0 and the dependence on temperature coming through $Q+X$ remains the same as found by the perturbation method. It is not difficult to see that for $T\gg T_k$, (54) reduces to (53) except the term proportional to V_0J^2 which is absent in (54) because in Hamann's treatment[7] of the self-energy, $F(\omega)$ is approximated by $-i\pi\rho$.

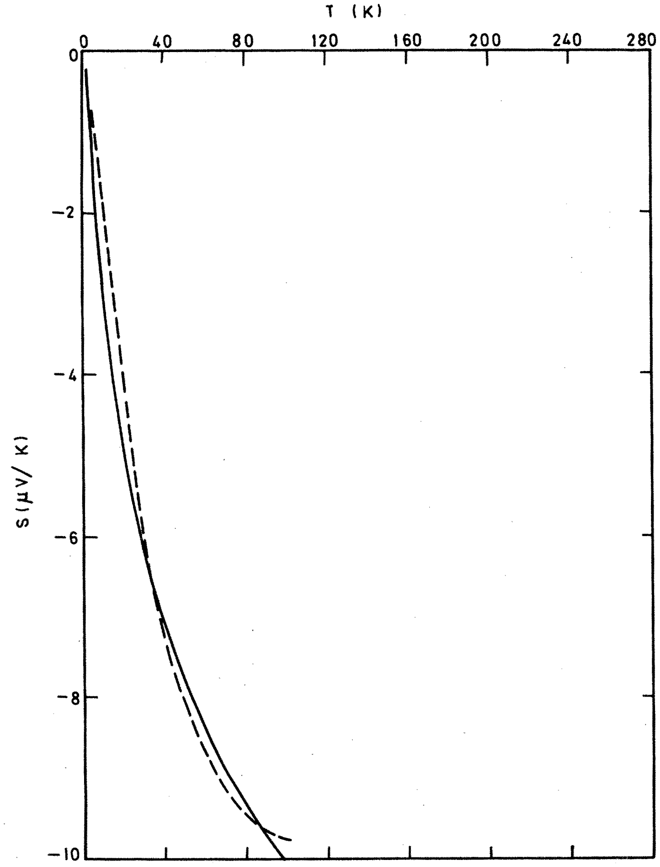

FIG. 3. Plot of the thermoelectric power of spin-glasses. The solid-line curve represents our calculation and the dashed-line curve denotes the experimental results for $T_f=22$ K (Ref. 14).

V. CONCLUSION

We have studied the transport properties in spin-glasses using the method of double-time Green's function for the *s-d* model. The higher-order Green's function has been decoupled to the lower order with the use of Nagaoka's decoupling scheme and retaining the terms representing quasibound states. The self-energy of the Green's function for the spin-glass has been obtained in multiple scattering approximation. Using Hamann's[7] approach, we have obtained a self-consistent expression for the t matrix and thereby calculated the resistivity maximum temperature T_m. This temperature T_m is higher than T_f which is supported by the experiments. Following the procedure of Nam and Fullenbaum[18] we have calculated the Lorenz number L for the spin-glass system. Unlike the Kondo system, we get an extra temperature dependence through $Q+X$. With the use of Rivier's modes at low temperature, for X, we find that $\Delta L/L_0$, where ΔL is the contribution to the Lorenz number due to the *s-d* interaction, is lower in the spin-glass system as compared to the Kondo system and also the maximum of $\Delta L/L_0$ in the former system is more pronounced and shifted towards lower temperature values as compared to that in the latter system. On physical ground the result looks sensible because the role of J for the *s-d* interaction becomes less important for the spin-glass system. At temperature $T/T_k\ll 1$, the deviation in the calculation of $\Delta L/L$ for Kondo and spin-glass systems is thought to be due to the fluctuation in the impurity moments which is not being taken care of in the calculation of Q and X.

The thermoelectric power has been calculated using the perturbation expansion of the self-energy to order J^3V_0.

We get an expression for the thermoelectric power involving the terms V_0J^2 and V_0J^3, where the second term is very large and dominates over the first at low temperature. Hence the sign of the thermopower is determined by the sign of J and V_0 in the small temperature range. Owing to the presence of the term V_0J^2 which becomes substantial at high temperature, there will be a decrease in the absolute value of the thermoelectric power. At sufficiently high temperature the V_0J^2 term may dominate over the V_0J^3 term and this will reverse the sign of the thermoelectric power. Our expression for the thermoelectric power also involves a term $Q+X$ which arises due to the spin-glass phase. Since the term $Q+X$ smoothly varies around the temperature T_f, we do not expect any abrupt change in the thermoelectric power around this temperature. This is also supported by the experimental data.[14] Our calculation for the thermoelectric power agrees well at low temperatures, but at high temperatures there is a systematic deviation which is thought to be due to the neglect of contribution arising from the electron-phonon interaction.

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