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Relativistic formulation for the nuclear-spin-lattice relaxation rate in metallic systems: Applications to $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$

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The nuclear-spin-lattice relaxation rate $(T_1T)^{-1}$ in metallic systems is formulated in a relativistically correct form, which is applicable to pure metals as well as to alloys. As an example, the results of relativistic Korringa-Kohn-Rostoker coherent-potential approximation calculations for the alloy system $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$ are used to calculate the relaxation rates of Ag and Pt in this system.

I. INTRODUCTION

Within the framework of charge self-consistent nonrelativistic Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) calculations, in a recent paper Ebert *et al.*[1] have determined the theoretical nuclear-spin-lattice relaxation rates $(T_1T)^{-1}$ of Ag and Cu in the alloy systems $\mathrm{Ag}_x\mathrm{Pd}_{1-x}$ and $\mathrm{Cu}_x\mathrm{Pd}_{1-x}$, respectively. For both systems it has been found that, for the noble-metal-rich side, the contact term is the dominating part of $(T_1T)^{-1}$, while with decreasing noble-metal content the *d*-electron contributions grow, and in the case of Cu in $\mathrm{Cu}_x\mathrm{Pd}_{1-x}$ finally are larger than the contact term. Although the concentration dependence of the calculated rates is in agreement with experiment, the theoretical values are up to 40% smaller than the experimental ones as long as the contact term is the main contribution to $(T_1T)^{-1}$ and the familiar formula for the contact hyperfine field B_s^{nr} is used. This discrepancy is much more pronounced for Ag than for Cu, and therefore indicates that it might be of relativistic origin. Indeed, the formula for B_s^{nr} has been derived by Fermi[2] using approximations that only apply for atomic numbers which are not too high. If, however, instead of B_s^{nr}, the relativistic counterpart of the contact hyperfine field is used, the theoretical relaxation rates are in good agreement with the experimental results for Ag in $\mathrm{Ag}_x\mathrm{Pd}_{1-x}$ as well as for Cu in $\mathrm{Cu}_x\mathrm{Pd}_{1-x}$.[1]

To avoid this mixing of a relativistic hyperfine field and a nonrelativistic band-structure approach, and to get an expression for $(T_1T)^{-1}$ which is applicable also for other contributions to $(T_1T)^{-1}$ influenced by relativistic effects, we have developed a relativistically correct formula for the relaxation rate in metallic systems. The Hamiltonian which describes the relaxation process caused by magnetic dipole interactions is given in Sec. II, together with a short description of the mechanism of the nuclear-spin-lattice relaxation process in metallic systems. In Sec. III, a formula for $(T_1T)^{-1}$ is derived, applicable not only to pure metals, but also to alloys. This is demonstrated in Sec. IV, where results for the theoretical relaxation rates of Ag and Pt in $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$ are compared with experimental results.

II. MECHANISM OF NUCLEAR-SPIN-LATTICE RELAXATION PROCESSES IN METALLIC SYSTEMS

The nuclear-spin-lattice relaxation process in metals is caused by magnetic and electric (quadrupolar) interactions between the nuclei and conduction electrons. This process consists of an exchange of energy between the nuclear-spin and electronic systems, and is only possible because the spectrum of the conduction electrons is continuous.

The magnetic interaction between a nucleus and an electron to which we will restrict our considerations is described in relativistically correct form by the following Hamiltonian:[3]

$$H_{\mathrm{hf}}=e\,\boldsymbol{\alpha}\cdot\mathbf{A}\ . \tag{2.1}$$

In Eq. (2.1), $-e$ is the electronic charge, $\boldsymbol{\alpha}$ is the vector of the 4×4 Dirac matrices related to the Pauli spin matrices, and $\mathbf{A}$ is the vector potential due to the magnetic moment $\boldsymbol{\mu}$ of the nucleus,

$$\mathbf{A}=\boldsymbol{\mu}\times\mathbf{r}_0/r^2\ ,\ \mathbf{r}_0=\mathbf{r}/|\mathbf{r}| \tag{2.2}$$

r being the distance between the nucleus and the electron. By using the relation

$$\boldsymbol{\mu}=\gamma_n\hbar\mathbf{I}\ , \tag{2.3}$$

Eq. (2.1) can be written in the following form:

$$\begin{aligned}H_{\mathrm{hf}}&=\gamma_n\hbar[I_z(\mathbf{r}_0\times\boldsymbol{\alpha})_z+I_-\tfrac{1}{2}(\mathbf{r}_0\times\boldsymbol{\alpha})_+\\&\quad+I_+\tfrac{1}{2}(\mathbf{r}_0\times\boldsymbol{\alpha})_-]e/r^2\\&=\gamma_n\hbar(I_zH_z^{\mathrm{el}}+I_-H_+^{\mathrm{el}}+I_+H_-^{\mathrm{el}})\ .\end{aligned} \tag{2.4}$$

In Eqs. (2.3) and (2.4), γ_n and $\mathbf{I}$ are the gyromagnetic ratio of the nucleus and the nuclear-spin operator, respectively. The operators $I_\pm$ and $(\mathbf{r}_0\times\boldsymbol{\alpha})_\pm$ in Eq. (2.4) are defined in the usual way as

$$I_\pm = I_x \pm i I_y\ , \quad (\mathbf{r}_0\times\boldsymbol{\alpha})_\pm = (\mathbf{r}_0\times\boldsymbol{\alpha})_x \pm i(\mathbf{r}_0\times\boldsymbol{\alpha})_y\ . \tag{2.5}$$

While the first part of H_{hf} in Eq. (2.4) is responsible for the Knight shift in metals, the last two terms describe the relaxation processes.

To study the relaxation behavior of the nuclear-spin system, one defines for each spin level m the relative deviation of the corresponding population $N_m(t)$ at the time t from the equilibrium population N_m^0 by

$$n_m(t) = [N_m(t) - N_m^0] \Big/ \sum_{m'} N_{m'}^0\ . \tag{2.6}$$

As is shown in the next section, the transition probability $W_{mm'}$ per unit time between two nuclear-spin levels m and m' due to the magnetic interactions between a nucleus and the electronic system is of the form

$$W_{mm'} = W(\,|\langle m'|I_+|m\rangle|^2 + |\langle m'|I_-|m\rangle|^2)\ . \tag{2.7}$$

This leads to the selection rule of $\Delta m = \pm 1$ for the magnetic quantum numbers m and, furthermore, to a linear coupled system of $2I+1$ differential equations for the quantities $n_m(t)$. By introducing the quantity $a_m(t)$, which is proportional to the magnetization of two adjacent spin levels,

$$a_m(t) = n_m(t) - n_{m-1}(t)\ , \tag{2.8}$$

the number of differential equations is reduced to $2I$,

$$\frac{da_m(t)}{dt} = \sum_{m'} A_{mm'} a_{m'}(t)\ . \tag{2.9}$$

As follows from Eq. (2.7), the only nonvanishing elements of the coefficient matrix A are given by

$$\begin{aligned} A_{m,m+1} &= W_{m,m+1} = W[I(I+1) - m(m+1)]\ , \\ A_{m,m} &= -2W_{m,m-1} = -2W[I(I+1) - m(m-1)]\ , \\ A_{m,m-1} &= W_{m-1,m-2} = W[I(I+1) - (m-1)(m-2)]\ . \end{aligned} \tag{2.10}$$

The general solution of the system of differential equations (2.9) is of the form

$$a_m(t) = \sum_n b_n C_{mn} \exp(-\lambda_n t)\ . \tag{2.11}$$

In Eq. (2.11) the λ_n are the eigenvalues of the matrix A and are given by[4]

$$\lambda_n = n(n+1)W\ , \quad n = 1, \ldots, 2I\ . \tag{2.12}$$

The quantity C_{mn} in Eq. (2.11) is the mth component of the nth eigenvector of A. For the special cases $I = \frac{5}{2}$ and $\frac{7}{2}$, C_{mn} is given by Narath[5] and Simmons *et al.*[6] The coefficients b_n, finally, in Eq. (2.11), are determined by the initial conditions and the inverse of the matrix C_{mn},

$$b_n = \sum_{m'} (C^{-1})_{nm'} a_{m'}(0)\ . \tag{2.13}$$

The initial conditions produced in a standard T_1 experiment can be expressed by

$$a_m(0) = \gamma_n \hbar B / k_B T\ , \tag{2.14}$$

with B the external field, k_B the Boltzmann constant, and T the temperature. For cubic lattices there is only one contribution to the sum in Eq. (2.11) with $\lambda_n = 2W$. This leads to a spin-lattice relaxation time $T_1 = 1/2W$, which is independent of I. However, as can be seen from Eq. (2.11), T_1 describes the time dependence of the relaxation process also for noncubic lattices.[4]

III. FORMULA FOR THE NUCLEAR-SPIN-LATTICE RELAXATION RATE

The total transition probability per unit time for a transition from a nuclear state $|m\rangle$ to state $|m'\rangle$ is given by the sum over all transitions of the total system from a state $|n,m\rangle = |n\rangle|m\rangle$ to a state $|n'\rangle|m'\rangle$, where $|n\rangle$ and $|n'\rangle$ are occupied and unoccupied electronic states, respectively,

$$W_{mm'} = (2\pi/\hbar) \sum_{n,n'} |\langle n',m'|H_{\text{hf}}|n,m\rangle|^2 \times \delta(E_{n'} - E_n + \hbar\omega_I) f(E_n)[1 - f(E_{n'})]\ . \tag{3.1}$$

Here, $\hbar\omega_I = E_{m'} - E_m$ is the difference in energy for the states $|m\rangle$ and $|m'\rangle$ of the nucleus, and $f(E)$ is the Fermi function. By approximating the energy conservation as follows,[7]

$$\delta(E_{n'} - E_n + \hbar\omega_I) f(E_n)[1 - f(E_{n'})] \sim k_B T \delta(E_{n'} - E_F)\delta(E_n - E_F)\ , \tag{3.2}$$

and separating the hyperfine-interaction operator according to Eq. (2.4) for the case $m' = m+1$, $W_{mm'}$ can be written as

$$W_{mm'} = 2\pi k_B T \hbar \gamma_n^2 |\langle m'|I_+|m\rangle|^2 \times \sum_{n,n'} |\langle n'|H_-^{\text{el}}|n\rangle|^2 \delta(E_n - E_F)\delta(E_{n'} - E_F)\ , \tag{3.3}$$

and in an analogous way for the other possible transition, $m' = m-1$. From Eq. (3.3) one can see that the quantity W in Eq. (2.7) is given by

$$W = 2\pi k_B T \hbar \gamma_n^2 \sum_{n,n'} |\langle n'|H_-^{\text{el}}|n\rangle|^2 \times \delta(E_n - E_F)\delta(E_{n'} - E_F)\ . \tag{3.4}$$

By using a configuration-space representation for the matrix elements $\langle n'|H_-^{\text{el}}|n\rangle$ and the corresponding spectral representation for the one-particle Green's function, Eq. (3.4) can be written as

$$W=2\pi k_{\mathrm{B}}T\hbar\gamma_n^2\frac{1}{\pi^2}\int\int H_{-}^{\mathrm{el}}(\mathbf{r})\,\mathrm{Im}G(\mathbf{r},\mathbf{r}',E_F)\,\mathrm{Im}G(\mathbf{r}',\mathbf{r},E_F)H_{-}^{\mathrm{el}}(\mathbf{r}')d\mathbf{r}\,d\mathbf{r}' \ . \tag{3.5}$$

This formulation does not only apply to pure metals, but also to random alloys. In that case, $G(\mathbf{r},\mathbf{r}',E_F)$ has to be replaced by the configurationally averaged Green's function $G^{\alpha}(\mathbf{r},\mathbf{r}',E_F)$, where the considered nucleus α is placed on the central site. Because of the short range of the hyperfine-interaction operator [see Eq. (2.4)], the integrations in Eq. (3.5) can be restricted to the volume of the central cell (see Sec. IV). In terms of the site-diagonal scattering-path operator $\tau_{\Lambda\Lambda'}^{00,\alpha}(E)$ $(\Lambda=\kappa,\mu)$ (e.g., Ref. 8) generally used within the KKR-CPA framework, $\mathrm{Im}G^{\alpha}(\mathbf{r},\mathbf{r}',E)$ is given by

$$\mathrm{Im}G^{\alpha}(\mathbf{r},\mathbf{r}',E)=\sum_{\Lambda,\Lambda'}Z_{\Lambda}^{\alpha}(\mathbf{r},E)\,\mathrm{Im}\tau_{\Lambda\Lambda'}^{00,\alpha}(E)[Z_{\Lambda'}^{\alpha}(\mathbf{r}',E)]^* \ , \tag{3.6}$$

and hence W_α by

$$W_\alpha=2\pi k_{\mathrm{B}}T\hbar\left[\gamma_n\frac{1}{\pi}\right]^2\sum_{\substack{\Lambda,\Lambda'\\ \Lambda'',\Lambda'''}}\mathrm{Im}\tau_{\Lambda\Lambda'}^{00,\alpha}(E_F)\,\mathrm{Im}\tau_{\Lambda''\Lambda'''}^{00,\alpha}(E_F)I_{\Lambda'''\Lambda}^{\alpha}(E_F)[I_{\Lambda''\Lambda'}^{\alpha}(E_F)]^* \ , \tag{3.7}$$

where

$$I_{\Lambda\Lambda'}^{\alpha}(E)=\int[Z_{\Lambda}^{\alpha}(\mathbf{r},E)]^*H_{-}^{\mathrm{el}}(\mathbf{r})Z_{\Lambda'}^{\alpha}(\mathbf{r},E)d\mathbf{r} \ . \tag{3.8}$$

In Eqs. (3.6) and (3.8), $Z_{\Lambda}^{\alpha}(\mathbf{r},E)$ is a radial bispinor of the type

$$Z_{\Lambda}^{\alpha}(\mathbf{r},E)=\begin{bmatrix} g_{\kappa}^{\alpha}(r,E)\chi_{\kappa}^{\mu}(\mathbf{r}_0) \\ if_{\kappa}^{\alpha}(r,E)\chi_{-\kappa}^{\mu}(\mathbf{r}_0)\end{bmatrix} \tag{3.9}$$

normalized according to single-site scattering.[9,10]

The matrix elements $I_{\Lambda\Lambda'}^{\alpha}(E)$ are evaluated in a manner similar to that of Rose,[3]

$$I_{\Lambda\Lambda'}^{\alpha}(E)=-i\frac{e}{2}R_{\kappa\kappa'}^{\alpha}(E)A_{\kappa\kappa'}^{\mu\mu'} \ , \tag{3.10}$$

with

$$R_{\kappa\kappa'}^{\alpha}(E)=\int[g_{\kappa}^{\alpha}(r,E)f_{\kappa'}^{\alpha}(r,E)+g_{\kappa'}^{\alpha}(r,E)f_{\kappa}^{\alpha}(r,E)]dr \tag{3.11}$$

and

$$\begin{aligned}A_{\kappa\kappa'}^{\mu\mu'}=\;&i[2(2\bar{l}'+1)/(2l+1)]^{1/2}C(\bar{l}'1l;00)\\ &\times[2^{1/2}C(l\tfrac{1}{2}j;(\mu+\tfrac{1}{2})-\tfrac{1}{2})C(\bar{l}'\tfrac{1}{2}j';(\mu'-\tfrac{1}{2})+\tfrac{1}{2})C(\bar{l}'1l;(\mu+\tfrac{1}{2})0)\\ &\quad-C(l\tfrac{1}{2}j;(\mu-\tfrac{1}{2})+\tfrac{1}{2})C(\bar{l}'\tfrac{1}{2}j';(\mu'-\tfrac{1}{2})+\tfrac{1}{2})C(\bar{l}'1l;(\mu+\tfrac{1}{2})-1)\\ &\quad+C(l\tfrac{1}{2}j;(\mu+\tfrac{1}{2})-\tfrac{1}{2})C(\bar{l}'\tfrac{1}{2}j';(\mu'+\tfrac{1}{2})-\tfrac{1}{2})C(\bar{l}'1l;(\mu+\tfrac{3}{2})-1)] \ .\end{aligned} \tag{3.12}$$

For the angle-dependent part of the matrix element [see Eq. (3.10)], $A_{\kappa\kappa'}^{\mu\mu'}$, the following selection rules apply:

$$\mu'-\mu=1 \ , \ j'-j=0,\pm 1 \ , \ l'-l=0,\pm 2 \ . \tag{3.13}$$

Performing the triple products of Clebsch-Gordan coefficients in Eq. (3.12), the nonvanishing terms of $A_{\kappa\kappa'}^{\mu\mu}$ can be written in the following compact form:

$$A_{\kappa\kappa'}^{\mu\mu'}=\begin{cases}[4i\kappa/(4\kappa^2-1)][\kappa^2-(\mu+\tfrac{1}{2})^2]^{1/2}, & \kappa'=\kappa\\ -[i/(2\kappa-s)]\{[\kappa-s(\mu+\tfrac{1}{2})][\kappa-s(\mu+\tfrac{3}{2})]\}^{1/2}, & \kappa'=-\kappa+s, \ \ s=\pm 1\end{cases} \ . \tag{3.14}$$

This leads, finally, to the following expression for the spin-lattice relaxation rate $(T_1T)_{\alpha}^{-1}$:

$$(T_1T)_{\alpha}^{-1}=4\pi k_{\mathrm{B}}\hbar\left[\gamma_n\frac{e}{2\pi}\right]^2\sum_{\substack{\Lambda,\Lambda'\\ \Lambda'',\Lambda'''}}[\mathrm{Im}\tau_{\Lambda\Lambda'}^{00,\alpha}(E_F)\,\mathrm{Im}\tau_{\Lambda''\Lambda'''}^{00,\alpha}(E_F)R_{\kappa'''\kappa}^{\alpha}(E_F)R_{\kappa''\kappa'}^{\alpha}(E_F)A_{\kappa'''\kappa}^{\mu'''\mu}(A_{\kappa''\kappa'}^{\mu''\mu'})^*] \ . \tag{3.15}$$

This result can be further simplified by restricting the selection rule for l [Eq. (3.13)] to $\Delta l=0$ (see Sec. IV) and assuming that the scattering-path operator is diagonal in κ and μ,

$$(T_1T)_\alpha^{-1}=4\pi k_B\hbar\left[\gamma_n\frac{e}{2\pi}\right]^2\left[\sum_\kappa\frac{(2j+1)^3}{6j(j+1)}[\mathrm{Im}\bar{\tau}_\kappa^\alpha(E_F)R_{\kappa\kappa}^\alpha(E_F)]^2\right.$$
$$\left.+\sum_{\kappa>0}\frac{(2j+1)(2j+3)}{3(j+1)}\mathrm{Im}\bar{\tau}_\kappa^\alpha(E_F)\mathrm{Im}\bar{\tau}_{-\kappa-1}^\alpha(E_F)[R_{\kappa,-\kappa-1}^\alpha(E_F)]^2\right], \tag{3.16}$$

with

$$\bar{\tau}_\kappa^\alpha(E_F)=[1/(2j+1)]\sum_\mu\tau_{\Lambda\Lambda}^{00,\alpha}(E_F)\ . \tag{3.17}$$

Identifying $-[(2j+1)/\pi]\mathrm{Im}\bar{\tau}_\kappa^\alpha(E_F)N_\kappa^\alpha(E_F)$ with the κ-like density of states at the Fermi level, $n_\kappa(E_F)$, and redefining the matrix element by

$$\bar{R}_{\kappa\kappa'}^\alpha(E)=R_{\kappa\kappa'}^\alpha(E)/[N_\kappa^\alpha(E)N_{\kappa'}^\alpha(E)]^{1/2}\ , \tag{3.18}$$

where

$$N_\kappa^\alpha(E)=\int\{[g_\kappa^\alpha(r,E)]^2+[f_\kappa^\alpha(r,E)]^2\}r^2\,dr\ , \tag{3.19}$$

one gets

$$(T_1T)_\alpha^{-1}=4\pi k_B\hbar\left[\gamma_n\frac{e}{2}\right]^2\left[\sum_\kappa\frac{(2j+1)}{6j(j+1)}[n_\kappa^\alpha(E_F)\bar{R}_{\kappa\kappa}^\alpha(E_F)]^2+\sum_{\kappa>0}\frac{1}{3(j+1)}n_\kappa^\alpha(E_F)n_{-\kappa-1}^\alpha(E_F)[\bar{R}_{\kappa,-\kappa-1}^\alpha(E_F)]^2\right]\ . \tag{3.20}$$

Equation (3.20) is, apart from a constant prefactor in the second sum, identical with the expression for $(T_1T)^{-1}$ given by John *et al.*[11]

In our derivation for the spin-lattice relaxation rate, we have ignored the possible dependence of $(T_1T)^{-1}$ on the orientation of the external field because it has been shown, for the nonrelativistic case, that $(T_1T)^{-1}$ in cubic metals is isotropic.[12] This approximation is also justified by the fact that the anisotropic part of the Knight shift in the cubic metals Pt and Pb is much smaller than the isotropic part.[13,14]

Furthermore, we have inserted in Eq. (3.5) the Green's function for the case of vanishing external field. Inserting a perturbation series for $G(\mathbf{r},\mathbf{r}',E)$ in Eq. (3.5) would instead lead to additional field-dependent terms in Eq. (3.7) that would be very small compared to the field-independent term. These terms can therefore be neglected in full agreement with experimental experience.

IV. APPLICATIONS TO $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$

The results of fully relativistic KKR-CPA calculations for $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$ (Ref. 15) are used to calculate the spin-lattice relaxation rates $(T_1T)^{-1}$ of the isotopes ^{109}Ag and ^{195}Pt in this alloy system. Figures 1 and 2 show the theoretically calculated rates of Ag and Pt, respectively, together with the corresponding experimental values[16–18] as a function of the Pt concentration. In Figs. 3 and 4 the theoretical values for $(T_1T)^{-1}$ are broken down into their angular-momentum contributions corresponding to Eq. (3.16), i.e., reflecting only a selection rule of $\Delta l=0$ for the angular-momentum quantum number l. Also shown in Figs. 3 and 4 are the total relaxation rates according to Eqs. (3.15) and (3.16), respectively.

For Ag as well as Pt the calculated rates agree fairly well with the experimental results. From Fig. 1 one can see that the relaxation rate for Ag decreases rapidly with increasing Pt concentration and shows a minimum at about 70 at. % Pt. As evident from Fig. 3, the concentration dependence for the Ag rate is caused by a steady decrease of the s-like contribution and a rapid increase of d-like contributions for Pt concentrations larger than 70 at. % Pt.

A similar behavior exists for the s- and d-like contribu-

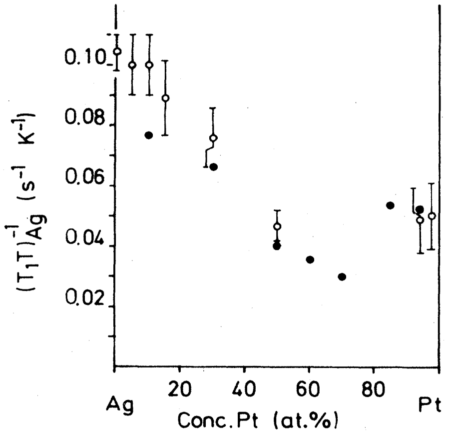

FIG. 1. Nuclear-spin-lattice relaxation rate for ^{109}Ag in $\mathrm{Ag}_x\mathrm{Pt}_{1-x}$. Open circles denote the experimental values (Ref. 16). Solid circles the theoretical ones. For the experimental values the error bars are shown.

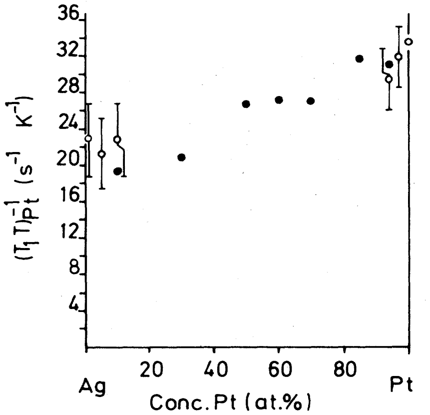

FIG. 2. Nuclear-spin-lattice relaxation rate for ^{195}Pt in Ag_xPt_{1-x}. Open circles denote the experimental values (Refs. 17 and 18). Solid circles the theoretical ones. For the experimental values the error bars are shown.

tions to $(T_1T)^{-1}$ of Pt. For Pt, however, the rapid increase for the d-like contributions is seen already at small concentrations of about 20—40 at. % Pt and this therefore leads to a continuous increase for the total relaxation rate. For both components, the p-like contributions to $(T_1T)^{-1}$ are rather small and decrease continuously with increasing Pt concentration.

As can be seen from Figs. 3 and 4, the use of Eq. (3.16), or, equivalently, Eq. (3.20), is indeed an excellent approximation to Eq. (3.15), where no assumptions are made. Only in the case of Pt-rich alloys do small differences between the rates corresponding to Eqs. (3.15) and (3.16), respectively, occur. These differences are mainly due to the off-diagonal terms in the site-diagonal scattering-path operator, the so-called spin-flip components.[8]

The short-range property of the hyperfine interaction mentioned in Sec. III can easily be checked by extending the volume for the radial integrations in Eq. (3.11) to the volume of the Wigner-Seitz sphere. For the present results there were virtually no differences.

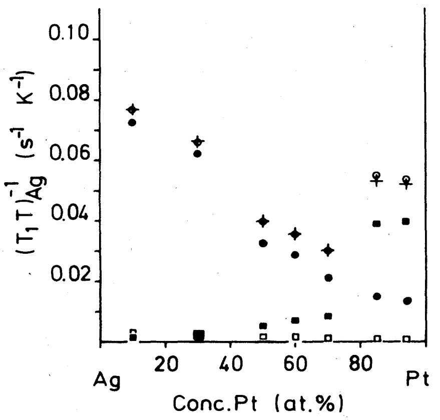

FIG. 3. l-like contributions to the nuclear-spin-lattice relaxation rate for ^{109}Ag in Ag_xPt_{1-x}. Solid circles correspond to the s-like, open squares to the p-like, and solid squares to the d-like contributions. The open circles and crosses correspond to the total rate according to Eqs. (3.16) and (3.15), respectively.

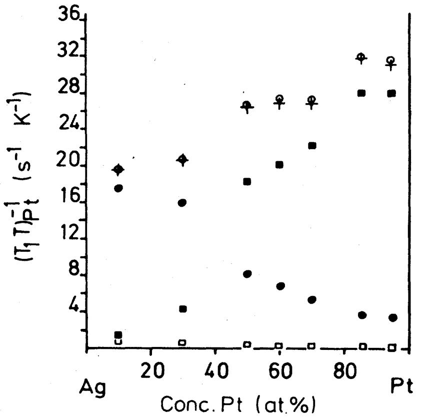

FIG. 4. l-like contributions to the nuclear-spin-lattice relaxation rate for ^{195}Pt in Ag_xPt_{1-x}. Solid circles correspond to the s-like, open squares to the p-like, and solid squares to the d-like contributions. The open circles and crosses correspond to the total rate according to Eqs. (3.16) and (3.15), respectively.

V. CONCLUSIONS

Nuclear-spin-lattice relaxation rates probe the local, angular-momentum-dependent densities of states at the Fermi energy and can be used to describe characteristic changes in the electronic structure of disordered alloys. As compared to the unenhanced total density of states at E_F, $n(E_F)$, and its relation to the linear coefficient of the electronic specific heat, γ, the spin-lattice relaxation rates allow us to investigate the components separately. In particular, for systems where spin fluctuations form a major contribution to γ, the theoretical spin-lattice relaxation rates are a useful tool in the discussion of the quality of calculated spectral functions. The results shown in Figs. 1 and 2 prove that the fully relativistic KKR-CPA method is capable of describing the concentration dependence of the spin-lattice relaxation rates properly. It should be noted that, as compared to soft-x-ray—emission spectra, where also partial densities of states are mapped, the spin-lattice relaxation rates allow a comparison of absolute numbers and are therefore a much more rigorous test of the quality of a theoretical calculation.

The present paper is based on data from KKR-CPA calculations that are non-self-consistent with respect to the potential field. Inherent in the CPA method used, the alloys are assumed to be statistically disordered.

The deviation of the calculated $(T_1T)^{-1}$ rates for Ag in Ag-rich alloys from the experimental ones might be an indication that, for these alloys, charge transfer is not negligible. However, it is also well known that different spin-density functionals give slightly different s-d interactions. To exclude charge-transfer effects implies performing fully relativistic KKR-CPA calculations self-consistently, which at least at the moment is still a major practical task. However, by comparing the present results with similar calculations on Ag_xPd_{1-x},[1] where the self-consistent nonrelativistic KKR-CPA method was used, it seems that most of the theoretical worries about charge transfer seem to be superfluous in the case of Ag_xPt_{1-x}.

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