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## Green's function calculation of effective nuclear relaxation times in metals

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### ABSTRACT

A two-times Green's function formalism is used together with linear response theory to derive general equations, valid at any temperature, for the effective nuclear relaxation times in metals. The results obtained by selecting the smallest-order pole in the Green's function as the first approximation are in complete correspondence to experimental evidence at high temperatures and exhibit a maximum when the temperature is lowered below the nuclear spin temperature. The results are also compared with those given by Shibata *et al.* and good agreement is obtained in the supposition of a single-exponential spin-lattice relaxation process.

### §1. INTRODUCTION

The theoretical derivation of expressions for the magnetic nuclear relaxation times at very low temperatures, and the description of the behaviour with temperature of such relaxation times, has been of major interest among researchers in the field, especially because of the recent experimental possibility of obtaining measurements of nuclear magnetic properties at such low temperatures. There has been a considerable amount of work in the area of nuclear magnetism (Abragam and Goldman 1982), but a comprehensive theoretical interpretation of nuclear magnetic resonance (NMR) relaxation times at arbitrary temperatures is still lacking. Recently, Shibata and Hamano (1982, 1983) have published a series of papers concerning the theoretical determination of the nuclear spin-lattice relaxation time for a system of nuclear spins interacting with conduction electrons in a metal. Using a theory of nonlinear spin relaxation (Shibata 1980, Shibata and Asou 1980, Asou and Shibata 1981), a multi-exponential spin-lattice relaxation behaviour is predicted.

In the present work, we make use of the two-times Green's function formalism in the regime of the linear response theory to derive the temperature behaviour of nuclear relaxation times (Martin Landrove and Moreno 1986) for nuclei in a metal. The results obtained are in complete agreement both with those derived under the assumption of an effective unique relaxation time (Shibata and Hamano 1983) and with experimental evidence (Brewer, Shirley and Templeton 1968, Bacon, Barclay, Brewer, Shirley and Templeton 1972). The organization of this paper is as follows. In §2, we show very briefly how the formalism is to be used in the calculation of the relaxation time and we work out the Hamiltonian of the system from which the equation for the Green function  $\langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}$ , which contains all the information relevant to the spin-lattice relaxation, is derived. This equation is then solved including terms up to second order in the electron-nucleus interaction. Finally, in §3, we obtain and discuss the relaxation time formulae.

§2. HAMILTONIAN AND EQUATION FOR  $\langle\langle I^0|I^0 \rangle\rangle_\omega^{(-)}$ 

The Fourier transform of the evolution of magnetization subjected to a stepwise external perturbing magnetic field is (Martin Landrove and Moreno 1986, Zubarev 1974)

$$\delta(\mathbf{M} - \langle \mathbf{M} \rangle_0)_\omega = - \frac{i \langle\langle \mathbf{M} | \mathbf{M} \rangle\rangle_\omega^{(-)} (\langle\langle \mathbf{M} | \mathbf{M} \rangle\rangle_0^{(-)})^{-1}}{\omega - i\varepsilon} \cdot \langle \delta \mathbf{M}(t=0) \rangle, \quad \varepsilon \rightarrow 0^+. \quad (1)$$

Its Laplace transform can be obtained through

$$\langle \delta \mathbf{M}(z) \rangle = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \frac{\langle \delta \mathbf{M}(\omega) \rangle}{\omega - iz} d\omega. \quad (2)$$

So we obtain the following expression:

$$\langle \delta \mathbf{M}(z) \rangle = \mathbf{f}(z) \cdot \langle \delta \mathbf{M}(t=0) \rangle, \quad (3)$$

where

$$\mathbf{f}(z) = - \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\omega \frac{\langle\langle \mathbf{M} | \mathbf{M} \rangle\rangle_\omega^{(-)} (\langle\langle \mathbf{M} | \mathbf{M} \rangle\rangle_0^{(-)})^{-1}}{(\omega - i\varepsilon)(\omega - iz)}, \quad \varepsilon \rightarrow 0^+. \quad (4)$$

The relaxation behaviour of the system is usually observed at very long times compared with the microscopic correlation times governing the interaction which causes the relaxation. For this reason we need to consider only the asymptotic representation of the inverse transform of eqn. (3) as  $t \rightarrow \infty$ .

The asymptotic behaviour of the  $\mathbf{f}(t)$  function can be derived by using Tauber's theorem (Paley and Wiener 1934, Berg 1967) which expresses the fact that, as  $t \rightarrow \infty$ ,

$$\mathbf{f}(t) = \sum_v \exp(z_v t) \sum_{k=0}^{+\infty} \mathbf{C}_k^{(v)} [\Gamma(-n_k^{(v)})]^{-1} t^{-(1+n_k^{(v)})}, \quad (5)$$

where  $z_v$  denotes the singular points of  $\mathbf{f}(z)$ ,  $\mathbf{C}_k^{(v)}$  are the coefficients of a Laurent expansion near  $z_v$  and  $n_k^{(v)}$  is related to the order of the singularity; for a first-order pole,  $n_k^{(v)} = -1$ .

As is often the case, the solution of the Green's function equation for the  $\alpha$  components of the magnetization ( $\alpha=0, \pm 1$ ) assumes the following form:

$$\langle\langle M_\alpha | M_{-\alpha} \rangle\rangle^{(-)} = \sigma_\alpha(\omega) / [\omega - \alpha\omega_0 - W_\alpha(\omega)]. \quad (6)$$

Since our goal is to determine the nuclear spin relaxation times, defined only in the case of exponential relaxation, we shall be concerned with finding the first-order poles of eqn. (6) in the neighbourhood of  $\alpha\omega_0$ .

When the complex functions  $\sigma_\alpha$  and  $W_\alpha$  are slowly varying around  $\alpha\omega_0$ , we obtain

$$f_\alpha(t) = \exp \{ -i\{\alpha\omega_0 + \text{Re} [W_\alpha(\alpha\omega_0)t]\} \exp \{ \text{Im} [W_\alpha(\alpha\omega_0)t]\} \}, \quad (7)$$

resulting in the characteristic exponential relaxation form usually assumed in nuclear magnetic resonance work. In these circumstances, it can be stated that the relaxation times are given by

$$\left. \begin{aligned} 1/T_1 &= -\text{Im} [W_0(0)], \\ 1/T_2 &= -\text{Im} [W_+(+\omega_0)] = -\text{Im} [W_-(-\omega_0)]. \end{aligned} \right\} \quad (8)$$

The procedure for calculating the nuclear relaxation times can then be stated as follows. First the relevant Green function equation is derived and solved, usually by making some appropriate decoupling approximations. From this solution, which is typically of the form of eqn. (6), an analysis of the singularities of the function  $\mathbf{f}(z)$  is performed and the relaxation parameters are obtained. When we are solely interested in exponential relaxation, only the first-order poles need to be considered. This procedure can, in some circumstances, result in a superposition of relaxation times for the relaxation form.

The total Hamiltonian for the system can be written in the following way:

$$H = H_z + H_{n-e} + H_e, \quad (9)$$

where

$$\left. \begin{aligned} H_z &= -\gamma\hbar H_0 I^0 = -\hbar\omega_0 I^0, \\ H_e &= \sum_{\mathbf{k}, s, v} E_v(\mathbf{k}s) a_{v\mathbf{k}s}^+ a_{v\mathbf{k}s}, \end{aligned} \right\} \quad (10)$$

where  $v$  represents the band index for the conduction electrons,  $s$  the spin component and  $\mathbf{k}$  the wave-vector. The interaction between the nuclear spins and the conduction electrons will correspond to the Fermi contact interaction, and can be written as

$$\begin{aligned} H_{n-e} = C \sum_{\substack{v, v' \\ \mathbf{k}, \mathbf{k}'}} \psi_{v'\mathbf{k}'}^*(\mathbf{R}) \psi_{v\mathbf{k}}(\mathbf{R}) & \left( \frac{1}{2} I^0 (a_{v'\mathbf{k}'}^+ + a_{v\mathbf{k}} - a_{v'\mathbf{k}}^+ - a_{v\mathbf{k}'}) \right. \\ & \left. + \frac{1}{2} I^+ a_{v'\mathbf{k}'}^+ - a_{v\mathbf{k}} + \frac{1}{2} I^- a_{v'\mathbf{k}'} - a_{v\mathbf{k}'} \right), \end{aligned} \quad (11)$$

where  $C = (8\pi/3) \gamma_e \gamma \hbar^2$ .

Since we are interested in the calculation of the spin-lattice relaxation time  $T_1$ , it is necessary to derive the equation for the commutator Green's function  $\langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}$ , which assumes the form

$$\hbar\omega \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)} = \frac{C}{2} \sum_{\mathbf{k}, \mathbf{k}'} \psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} \{ \langle\langle I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} - \langle\langle I^- a_{\mathbf{k}'}^+ + a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} \}. \quad (12)$$

The equations for the newly generated Green functions are the following:

$$\begin{aligned} [\hbar(\omega - \omega_0) + E(\mathbf{k}') - E(\mathbf{k})] \langle\langle I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} &= \langle [I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}}, I^0] \rangle_0 \\ &- \frac{C}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_2} \langle\langle I^+ (a_{\mathbf{k}_1}^+ - a_{\mathbf{k}_2}^+) a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} \\ &+ \frac{C}{2} \sum_{\mathbf{k}_1} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}} \{ \langle\langle I^+ I^0 a_{\mathbf{k}_1}^+ - a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} + \langle\langle I^- I^0 a_{\mathbf{k}_1}^+ - a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} \} \\ &+ \frac{C}{2} \sum_{\mathbf{k}_1} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}'} \{ \langle\langle I^+ I^0 a_{\mathbf{k}_1}^+ - a_{\mathbf{k}'} | I^0 \rangle\rangle_{\omega}^{(-)} - \langle\langle I^- I^0 a_{\mathbf{k}_1}^+ - a_{\mathbf{k}'} | I^0 \rangle\rangle_{\omega}^{(-)} \} \\ &- C \sum_{\mathbf{k}_1, \mathbf{k}_2} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_2} \langle\langle I^0 a_{\mathbf{k}_1}^+ - a_{\mathbf{k}_2}^+ a_{\mathbf{k}} | I^0 \rangle\rangle_{\omega}^{(-)} \end{aligned} \quad (13)$$

and

$$\begin{aligned}
& [\hbar(\omega + \omega_0) + E(\mathbf{k}^+) - E(\mathbf{k}^-)] \langle\langle I^0 a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)} = \langle [I^- a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-}, I^0] \rangle_0 \\
& + \frac{C}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_2} \langle\langle I^- (a_{\mathbf{k}_1^+}^+ a_{\mathbf{k}_2^+} - a_{\mathbf{k}_1^-}^+ a_{\mathbf{k}_2^-}) a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)} \\
& - \frac{C}{2} \sum_{\mathbf{k}_1} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_1} (\langle\langle I^- I^0 a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_1^-} | I^0 \rangle\rangle_{\omega}^{(-)} - \langle\langle I^- I^+ a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^+} | I^0 \rangle\rangle_{\omega}^{(-)}) \\
& - \frac{C}{2} \sum_{\mathbf{k}_1} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_1} (\langle\langle I^- I^0 a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_1^-} | I^0 \rangle\rangle_{\omega}^{(-)} + \langle\langle I^+ I^- a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^+} | I^0 \rangle\rangle_{\omega}^{(-)}) \\
& + C \sum_{\mathbf{k}_1, \mathbf{k}_2} \psi_{\mathbf{k}_1}^* \psi_{\mathbf{k}_2} \langle\langle I^0 a_{\mathbf{k}^+}^+ + a_{\mathbf{k}_2^-} a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)}. \tag{14}
\end{aligned}$$

At this point, it is necessary to introduce some decoupling scheme of approximations in order to solve this increasingly complicated system of algebraic equations. Usually this can be done by approximating some of the operators present in the Green's function by their mean values, assuming that there is no correlation between these operators and those remaining in the Green's function, which is the so-called random-phase approximation. In our case, we approximate

$$\begin{aligned}
\langle\langle I^{+-} (a_{\mathbf{k}_1^+}^+ a_{\mathbf{k}_1^+} - a_{\mathbf{k}_1^-}^+ a_{\mathbf{k}_1^-}) a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)} \\
= [n(\mathbf{k}_1^+) - n(\mathbf{k}_1^-)] \langle\langle I^{+-} a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)}, \tag{15}
\end{aligned}$$

$$\langle\langle I^{+-} I^{-+} a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_1^-} | I^0 \rangle\rangle_{\omega}^{(-)} = n(\mathbf{k}_1^+) \langle\langle I^{+-} I^{-+} | I^0 \rangle\rangle_{\omega}^{(-)}, \tag{16}$$

$$\langle\langle I^0 a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_1^-} + a_{\mathbf{k}_2^+}^+ - a_{\mathbf{k}_2^-} | I^0 \rangle\rangle_{\omega}^{(-)} = n(\mathbf{k}_1^+) n(\mathbf{k}_2^+) \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}, \tag{17}$$

$$\langle\langle I^{+-} I^0 a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_2^-} + | I^0 \rangle\rangle_{\omega}^{(-)} = \langle I^{+-} a_{\mathbf{k}_1^+}^+ + a_{\mathbf{k}_2^-} + a_{\mathbf{k}_2^+} \rangle_0 \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}. \tag{18}$$

The first three equations assume that there is no correlation between the electronic occupation number and the  $z$  component of the nuclear spin, or equivalently the nuclear Zeeman energy, because the interaction energy between both systems is very weak. The last equation involves the equilibrium transition probability between both systems and depends on the coupling constant  $C$  in a higher order; so it can be discarded if an expansion of the solutions with respect to that constant is performed. Finally, if we discard in eqns. (13) and (14) all the Green's functions related to two-electron processes and keep only terms linear in the coupling constant  $C$ , we find that

$$\begin{aligned}
[\hbar(\omega - \omega_0) + E(\mathbf{k}^-) - E(\mathbf{k}^+) + \Gamma] \langle\langle I^+ a_{\mathbf{k}^+}^+ - a_{\mathbf{k}^+} | I^0 \rangle\rangle_{\omega}^{(-)} = -\langle I^+ a_{\mathbf{k}^+}^+ - a_{\mathbf{k}^+} \rangle_0 \\
+ (C/2) \psi_{\mathbf{k}}^* \psi_{\mathbf{k}} \{ n(\mathbf{k}^-) [1 - n(\mathbf{k}^+)] + n(\mathbf{k}^+) [1 - n(\mathbf{k}^-)] \} \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}, \tag{19}
\end{aligned}$$

where  $\Gamma$  corresponds to the Knight shift and

$$\begin{aligned}
[\hbar(\omega + \omega_0) + E(\mathbf{k}^+) - E(\mathbf{k}^-) - \Gamma] \langle\langle I^- a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} | I^0 \rangle\rangle_{\omega}^{(-)} = \langle I^- a_{\mathbf{k}^+}^+ + a_{\mathbf{k}^-} \rangle_0 \\
- (C/2) \psi_{\mathbf{k}}^* \psi_{\mathbf{k}} \{ n(\mathbf{k}^+) [1 - n(\mathbf{k}^-)] + n(\mathbf{k}^-) [1 - n(\mathbf{k}^+)] \} \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}. \tag{20}
\end{aligned}$$

By substituting these equations in eqn. (12) we obtain an approximate equation for  $\langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)}$ , which can be written as

$$[\hbar\omega - W(\omega)] \langle\langle I^0 | I^0 \rangle\rangle_{\omega}^{(-)} = \sigma(\omega), \quad (21)$$

where

$$\sigma(\omega) = -\frac{C}{2} \sum_{\mathbf{k}, \mathbf{k}'} \psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} \left( \frac{\langle I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}+} \rangle_0}{\hbar(\omega - \omega_{\mathbf{k}\mathbf{k}'})} + \frac{\langle I^- a_{\mathbf{k}'}^+ + a_{\mathbf{k}-} \rangle_0}{\hbar(\omega + \omega_{\mathbf{k}\mathbf{k}'})} \right) \quad (22)$$

and

$$W(\omega) = \left(\frac{C}{2}\right)^2 \sum_{\mathbf{k}, \mathbf{k}'} |\psi_{\mathbf{k}'}|^2 |\psi_{\mathbf{k}}|^2 \{n(\mathbf{k}^+) [1 - n(\mathbf{k}'^-)] + n(\mathbf{k}'^-) [1 - n(\mathbf{k}^+)]\} \left( \frac{1}{\hbar(\omega - \omega_{\mathbf{k}\mathbf{k}'})} + \frac{1}{\hbar(\omega + \omega_{\mathbf{k}\mathbf{k}'})} \right), \quad (23)$$

where  $\hbar\omega_{\mathbf{k}\mathbf{k}'} = \hbar\omega_0 - \Gamma + E(\mathbf{k}^+) - E(\mathbf{k}'^-)$ .

The functions  $\sigma(\omega)$  and  $W(\omega)$  are in general complex functions but in this case it is straightforward to show that

$$\left. \begin{aligned} \operatorname{Re} [\sigma(0)] &= 0, \\ \operatorname{Re} [W(0)] &= 0, \end{aligned} \right\} \quad (24)$$

and that

$$\operatorname{Im} [\sigma(0)] = CP \sum_{\mathbf{k}, \mathbf{k}'} \frac{\operatorname{Im} [\psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} \langle I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}+} \rangle_0]}{\hbar\omega_{\mathbf{k}\mathbf{k}'}} + C\pi \sum_{\mathbf{k}, \mathbf{k}'} \operatorname{Re} [\psi_{\mathbf{k}'}^* \psi_{\mathbf{k}} \langle I^+ a_{\mathbf{k}'}^+ - a_{\mathbf{k}+} \rangle_0] \delta(\omega_{\mathbf{k}\mathbf{k}'}), \quad (25)$$

$$\operatorname{Im} [W(0)] = -2\pi \left(\frac{C}{2}\right)^2 \sum_{\mathbf{k}, \mathbf{k}'} |\psi_{\mathbf{k}'}|^2 |\psi_{\mathbf{k}}|^2 \{n(\mathbf{k}^+) [1 - n(\mathbf{k}'^-)] + n(\mathbf{k}'^-) [1 - n(\mathbf{k}^+)]\} \delta(\omega_{\mathbf{k}\mathbf{k}'}). \quad (26)$$

As was mentioned earlier in this section, by studying the pole composition of eqn. (21), it is possible to derive an expression for the spin-lattice relaxation time. In this case, it results in a unique effective relaxation time, which can be expressed as

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} \left(\frac{C}{2}\right)^2 \sum_{\mathbf{k}, \mathbf{k}'} |\psi_{\mathbf{k}'}|^2 |\psi_{\mathbf{k}}|^2 \{n(\mathbf{k}^+) [1 - n(\mathbf{k}'^-)] + n(\mathbf{k}'^-) [1 - n(\mathbf{k}^+)]\} \delta(\omega_{\mathbf{k}\mathbf{k}'}). \quad (27)$$

### § 3. CALCULATION OF THE SPIN-LATTICE RELAXATION TIME IN A SIMPLIFIED MODEL

We shall apply eqn. (27) to the case of a very simple model for the conduction electrons. We shall suppose a nearly-free-electron gas system, characterized by some density of states  $g(E)$  and with single-particle wavefunctions very close to a plane-wave

form, such that it is possible to replace the sums in eqn. (27) by integrals over the energy spectrum; thus,

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} \left(\frac{C}{2}\right)^2 \left( \int_0^\infty dE g(E) |\psi(E)|^2 \int_0^\infty dE' g(E') |\psi(E')|^2 \right. \\ \left. \times \{n(E'_-)[1 - n(E_+)] + n(E_+)[1 - n(E'_-)]\} \delta(E_+ + \hbar\omega_0 - \Gamma - E'_-) \right) \quad (28)$$

where use has been made of the small dependence of  $|\psi(E)|^2$  on energy under the assumptions already given. In the high-temperature limit, where the thermal energy is larger than the nuclear spin energy, eqn. (28) becomes

$$1/T_1 = (4\pi/\hbar)(C/2)^2 |\psi(E_F)|^4 g^2(E_F) k_B T. \quad (29)$$

In contrast, the Knight shift in the same limit can be written

$$\Gamma = -(C/2) |\psi(E_F)|^2 g(E_F) \hbar\omega_e; \quad (30)$$

so we obtain

$$T_1 T k_B (\Gamma/\hbar\omega_e)^2 = \hbar/4\pi, \quad (31)$$

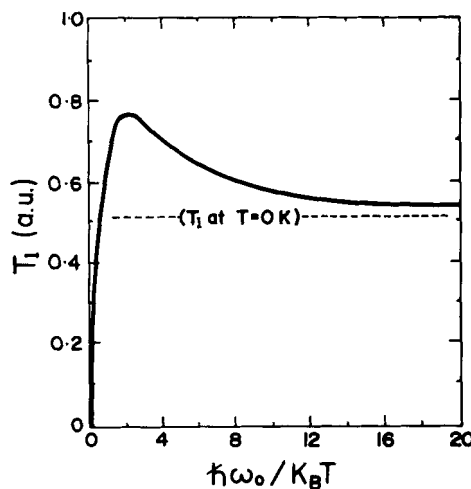
which corresponds to the well known Korringa temperature behaviour. At extremely low temperatures, eqn. (28) can be approximated differently and

$$1/T_1 = (2\pi/\hbar)(C/2)^2 |\psi(E_F)|^4 g^2(E_F) \hbar\omega_1, \quad (32)$$

where  $\hbar\omega_1$  is the nuclear energy corrected by the Knight shift. We thus obtain a temperature-independent value for the spin-lattice relaxation rate, which can be rewritten as

$$1/T_1 = (2\pi/\hbar)(\Gamma/\hbar\omega_e)^2 \hbar\omega_1. \quad (33)$$

In the whole temperature range, eqn. (28) can be calculated numerically, and the result is shown in the figure.  $T_1$  shows a maximum at a temperature that is approximately one-half the nuclear spin temperature; this is consistent with the result



Numerical calculations of effective longitudinal relaxation time  $T_1$  for the nearly-free-electron model. The curve exhibits a maximum at nearly one-half the nuclear spin energy.

obtained by Shibata and co-workers under the supposition that the relaxation process can be described by a unique effective relaxation time  $T_1$ , as observed experimentally. Also there is a correspondence between both results in the low-temperature limit, leading us to think that our calculation, even in its simpler approximation, is quantitatively correct. From the experimental point of view, there are insufficient data to decide whether a single-exponential or a multi-exponential relaxation takes place, but the general tendency is to believe that, even though the process seems actually to be multiexponential, it could be described by an effective relaxation time  $T'_1$ , which is the time that characterizes the evolution of observable parameters and, in particular, the longitudinal magnetization (Brewer *et al.* 1968, Bacon *et al.* 1972). The temperature dependence shown experimentally by this time  $T'_1$ , agrees completely with the behaviour shown in the figure. We recall that the expressions presented here are the zero-order approximation of the pole structure of the Green function, eqn. (21), which was performed by taking  $\omega = 0$  in the functions  $\sigma(\omega)$  and  $W(\omega)$ . This approximation was justified by assuming that both  $\sigma(\omega)$  and  $W(\omega)$  were slowly varying functions of frequency. In a rigorous way, this assignment is somewhat risky, because there is the possibility that part of the pole structure could be missed, even branch points; so a detailed study of the Green function pole structure should be made. In particular, our results show no spin dependence, i.e.  $\sigma(0)$  and  $W(0)$  do not depend on  $I$ , which is contrary to what is to be expected, since the transition probabilities between Zeeman levels, induced by the lattice, should be spin dependent. The difference comes from the zero-order expansion of the function  $\sigma(\omega)$ , since this function contains information related to the population dependence of nuclear–electronic transition probabilities and strongly depends on nuclear spin. It is possible that a higher-order expansion of  $\sigma(\omega)$  and  $W(\omega)$  could take account of the spin dependence of the spin–lattice relaxation time. We have already performed a second-order expansion of the function  $W(\omega)$  and obtained again a single pole for the Green function, corresponding to a small correction to eqn. (27). Nevertheless the approximation assumed in this work, besides its simplicity, takes into account the main features present in the temperature behaviour of relaxation times, within the limits of linear response theory, and can be extended to consider more realistic models or systems.

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