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COMMENTS AND ADDENDA

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Nuclear quadrupolar relaxation in liquid ^{69}Ga

C. A. Sholl
Physics Department, University of New England, Armidale, N.S.W., Australia
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Halder has recently calculated the quadrupolar relaxation rate in liquid Ga and has obtained results which are not consistent with the original calculations of Sholl. It is pointed out that the disagreement is not due to algebraic or arithmetical errors in the original work as suggested Halder, but that Halder's results may be in error.

The nuclear spin-lattice relaxation rate in liquid Ga has recently been calculated by Halder.[1] The important contributions to the relaxation are the magnetic hyperfine interaction between a nuclear spin and the conduction electrons, and the electric quadrupolar interaction between the quadrupole moment of a nucleus and the time-dependent field gradient at the nuclear site. The theory Halder used to calculate the quadrupolar contribution to the relaxation rate was that developed by Sholl[2] which relates the relaxation rate to the diffusive motion of the ions. Halder has, therefore, repeated the calculations of Sholl for Ga with different choices of the parameters involved.

The expression for the quadrupolar relaxation rate[2] depends on a term $I_1 + 2\pi\rho I_2$, where ρ is the number density of the liquid and I_1 and I_2 are complicated integrals depending respectively on two-particle and three-particle distribution functions. In the original calculations[2] I_1 and I_2 were found to be of comparable magnitudes but to have opposite signs. Halder on the other hand found both I_1 and I_2 positive and attributes the difference to computational and algebraic errors in the original calculations.

There were two printing errors in the paper of Sholl. Firstly, as noted by Halder, the expression (3.6) should be

$$v_2(r) = A(2k_F^2)[7x\sin x + (15 - x^2)\cos x]/x^5 ,$$

$$x = 2k_F r$$

[see also expression (4.27)]. Secondly, the analytic result of evaluating the inner integral in I_2 given in the Appendix is in error by a factor of 2 and should read

$$\int_{-1}^{1} g(\rho)P_2(z)dz = \frac{1}{8r_0^3 r_2^3}\,[(3a^2 - b^2)F_1 - 6aF_3 + 3F_5] ,$$

$$a = r_0^2 + r_2^2, \qquad b = 2r_0 r_2 ,$$

$$F_p = \int_{|r_0 - r_2|}^{r_0 + r_2} [g(\rho) - 1]\rho^p d\rho .$$

Neither of these errors was included in the computations and particular care was taken with the accuracy of the integrations so the calculations of Sholl for Ga are not in error for the reasons suggested by Halder.

The first of these printing errors was corrected by Halder but the second was not and so his results for I_2 are too large by a factor of 2. The difference of sign of I_2 cannot however be explained in this way. The only other difference between the calculations, apart from a constant multiplying both I_1 and I_2, is the choice of the pair distribution function and it is most unlikely this would lead to a difference in sign of I_2. In fact with the factor of 2 corrected in Halder's calculations his value of I_2/I_1 is 0.75 at 20 °C which is comparable in magnitude to -0.69 from the calculation of Sholl which suggests an error only in the sign of I_2.

The sign of I_2 is of some importance in the theory since a negative sign means the effect of the three-particle correlations is to partly cancel the effect of the two-particle correlations and can make accurate calculations difficult. There is evidence apart from the results discussed above that the sign of I_2 is negative. Titman and Jolly[3] have given a physical interpretation of the cancellation between I_1 and I_2, and an analytic reason has been given by Sholl.[4] Also the behavior of the quadrupolar relaxation rates as a function of concentration in liquid metal alloys can be explained[5-7] if $I_1/I_2 \sim -1$.

For the above reasons the quadrupolar relaxation rates calculated by Halder should be treated with caution and the 2% agreement with experiment at 50 °C regarded as fortuitous even apart from the uncertainties in the form of the ion-ion potential, the antishielding factor, the pair distribution function and the experimental relaxation times.

Recently, Sholl[4] and Warren[7] have discussed the quadrupolar relaxation theory without the assumption made in the above calculations of describing the ion motions by classical diffusion theory.

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[1] N. C. Halder, Phys. Rev. B 10, 2333 (1974).

[2] C. A. Sholl, Proc. Phys. Soc. Lond. 91, 130 (1967).

[3] J. M. Titman and R. I. Jolly, Phys. Lett. A 39, 213 (1974).

[4] C. A. Sholl, J. Phys. F 4, 1556 (1974).

[5] R. I. Jolly and J. M. Titman, J. Phys. C 5, 1284 (1972); J. Phys. F 3, 1071 (1973).

[6] E. Claridge, D. S. Moore, E. F. W. Seymour, and C. A. Sholl, J. Phys. F 2, 1162 (1972).

[7] W. W. Warren, Jr., Phys. Rev. A 10, 657 (1974).