Nuclear Spin Relaxation by Translational Diffusion. II. Diffusion in a B.C.C. Lattice

H. C. TORREY

Department of Physics, Rutgers University, New Brunswick, New Jersey

(Received July 30, 1954)

The calculations previously reported of nuclear spin relaxation time when relaxation is influenced by random-walk processes have been extended to the case of random walk to nearest neighbor positions in a body-centered cubic lattice. Some corrigenda of the previous work are noted.

IN a previous article with the above major title[1] (hereinafter referred to as I) the general problem of nuclear spin relaxation by diffusion was discussed. Quantitative results were obtained for the relaxation time T_1 for lattice diffusion describable by a random walk to nearest neighbor positions in a f.c.c. lattice. In the present article the calculations have been extended to a b.c.c. lattice. The new results should apply to self-diffusion in metallic lithium provided that the mechanism in this case is vacancy diffusion as appears to be so from the recent studies by Norberg.[2]

In I, it was shown that the spin-lattice relaxation time T_1 may be obtained to a good approximation, if

TABLE I. Table of the function $\psi(k_b,y)$ and of $\delta\psi = \psi(k_f,y)$ $-\psi(0.74335,y)$; $(k_b = 0.76293,\ k_f = 0.74280)$.

y	$\psi(k_b,y)$	$\delta\psi \times 10^5$
0	0	0
0.025	0.04043	-4
0.05	0.07394	-6
0.10	0.12866	-6
0.15	0.17172	-6
0.20	0.20542	-6
0.25	0.23137	-5
0.30	0.25094	-4
0.35	0.26543	-2
0.40	0.27571	-1
0.45	0.28264	0
0.50	0.28693	$+1$
0.55	0.28907	2
0.5922	0.28955 (max)	
0.60	0.28953	3
0.65	0.28864	4
0.70	0.28681	4
0.80	0.28086	6
0.90	0.27304	6
1.00	0.26417	7
1.20	0.24535	7
1.40	0.22686	8
1.60	0.20967	8
1.80	0.19415	8
2.00	0.18024	7
2.25	0.16497	7
2.5	0.15174	6
3.0	0.13029	6
3.5	0.11380	5
4.0	0.10083	5
5.0	0.08189	4
6.0	0.06883	3
7.0	0.05930	3
10.0	0.04181	2
20.0	0.02102	1
30.0	0.01403	1
40.0	0.01052	1

one assumes relaxation to be due to dipolar coupling rendered time-dependent by lattice diffusion of the above type, from the equation

$$T_1^{-1} = (8\pi/5)\gamma^4\hbar^2 I(I+1)(n/k^3 l^3\omega)\psi(k,\tfrac{1}{2}\omega\tau),$$

where

$$\psi(k,y) = yG(k,y) + 2yG(k,2y)$$

and

$$G(k,y) = \int_0^\infty J_{\frac{3}{2}}^2(kx)\frac{1-\sin x/x}{(1-\sin x/x)^2+y^2}\frac{dx}{x}.$$

In these equations the parameter k depends on the lattice structure and is given by

$$k^3 = (4\pi/3)n_0 b^{-3}l^{-3}/\sum_k r_k^{-6},$$

where n_0 is the number of sites in a unit cell, b is the lattice parameter, and l is the distance between nearest neighbor sites.

For a b.c.c. lattice $n_0 = 2$, $l = \tfrac{1}{2}\sqrt{3}b$, and[3] $\sum_k r_k^{-6} = 29.045/b^6$. From these data we obtain for a b.c.c. lattice $k = k_b = 0.76293$.

With this value of k we have computed the function $\psi(k_b,y)$ by numerical methods. Its values are given in Table I.

In I we stated a value of $\sum_k r_k^{-6}$ for a f.c.c. lattice. We had obtained this value by summing directly over a large number of lattice sites and by integration over the remainder. It has since come to our attention that this sum has been computed by more accurate methods[3] and that the correct value is $115.631b^{-6}$. This value is 0.2 percent larger than that used in I and leads to the value $k = k_f = 0.74280$ for a f.c.c. lattice. This new value of k results in small changes in the function $\psi(k_f,y)$ reported in I. Although these changes are not significant experimentally, we reproduce them for completeness in the third column of Table I. The numbers in this column should be added to the tabulated values of $\psi(k,y)$ in Table II of article I in order to obtain $\psi(0.74280,y)$. Also the value of y at maximum ψ is changed to 0.6027 for the new value of k. The corresponding value of ψ_{max} is 0.29063. These corrections were obtained by linear extrapolation from the previous results for $k = 0.74335$ and the present results for $k = 0.76293$. Incidently, Eq. (84) of I was incorrectly reproduced and should contain a factor k^{-1} on the right.

The author is indebted to Mr. James Simpson for help in computational work.

[1] H. C. Torrey, Phys. Rev. **92**, 962 (1953).
[2] R. E. Norberg, University of Illinois (private communication).
[3] J. E. Jones and A. E. Ingham, Proc. Roy. Soc. (London) **A107**, 636 (1925).