SPIN RESONANCE LINE SHAPES

A. M. STONEHAM
Theoretical Physics Division, A.E.R.E.Harwell, Didcot, Berks.

Received 19 January 1965

Spin resonance is observed using microwave electromagnetic and acoustic fields as probes. Interactions between the spins broaden the resonance, whose line shape has been defined elsewhere [1]. The shape may depend on the probe used, and for ions with an effective spin $S' > \frac{1}{2}$ different line shapes result in general [2]. It is proposed to show that the line shape does not depend on the probe for $S' = \frac{1}{2}$; this follows from the possibility of writing any moment of the line shape in a form which does not depend on the details of the probe.

The Hamiltonian for the system of spins is

$$\mathcal{H} = \mathcal{H}_z + \mathcal{H}_{ss} + \mathcal{H}_I ,$$

where $\mathcal{H}_2$ is the Zeeman energy for a magnetic field parallel to the z axis, and $\mathcal{H}_I$ describes the effect of the probe. $\mathcal{H}_I$ will be considered small. $\mathcal{H}_{ss}$ is the spin-spin interaction:

$$\mathcal{H}_{ss} = h_{ss} + h'_{ss} ,$$

where h_{ss} commutes with $\mathcal{H}_z$. The spin-spin interaction is truncated by dropping h'_{ss}, which gives subsidiary lines to the main resonance line [3]. If

$$(\mathcal{H}_z + h_{ss})|n\rangle = E_n|n\rangle$$

the moments of the line shape for the interaction $\mathcal{H}_I$ are:

$$\langle\omega^N\rangle_I = K \sum_{n,n'} \omega^N_{nn'} |\langle n|\mathcal{H}_I|n'\rangle|^2 ,$$

where

$$\hbar\omega_{nn'} = E_n - E_{n'}$$

and K is a normalising factor.

It follows from the definition of an effective spin of $\frac{1}{2}$ that it is always possible to write the probe interaction, $\mathcal{H}_I$, with such spins as:

$$\mathcal{H}_I = \sum_i (a_i S^i_x + b_i S^i_y + c_i S^i_x + d_i I^i), \qquad (1)$$

i labelling the spins.

In some cases this can be written

$$\begin{aligned} \mathcal{H}_I &= (A\, S_x + B\, S_y) + (C\, S_z + D\, I) \\ &= h_I + h'_I \end{aligned} \qquad (2)$$

where

$$S_\alpha = \sum_i S^i_\alpha$$

and

$$[\mathcal{H}_z + h_{ss}, h'_I] = 0 .$$

h'_I can only connect $|n\rangle$ and $|n'\rangle$ if $\omega_{nn'}$ is zero, and so does not contribute to the moments.

The important terms in the Hamiltonian are:

$$\mathcal{H}_z = E\, S_z$$

$$h_{ss} = \sum_{k>j} [F_{jk} S^j_z S^k_z + G_{jk}(S^j_+ S^k_- + S^j_- S^k_+)]$$

$$h_I = A\, S_x + B\, S_y .$$

h_{ss} is a very general form of truncated two-body interaction between effective spins of $\frac{1}{2}$. The sum over j and k may include spins which do not contribute to the resonance line.

Under the transformation

$$S_x \to \sigma_x = S_x c + S_y s$$

$$S_y \to \sigma_y = S_x(-s) + S_y c$$

$$S_z \to \sigma_z = S_z ,$$

where

$$c^2 + s^2 = 1$$

the commutation relations and the form of $\mathcal{H}_z$ and h_{ss} are unaltered apart from the replacement of S_α by σ_α. The transformation is equivalent to a virtual rotation about the z axis. The probe interaction becomes

$$h_I = (Ac + Bs)\sigma_x + (Bc - As)\sigma_y .$$

Choosing $Bc = As$ and writing

$$K = \{\sum_{n,n'} |\langle n|h_I|n'\rangle|^2\}^{-1}$$

the Nth moment is

$$\langle\omega_I^N\rangle = \frac{\sum_{n,n'} \omega_{nn'}^N |\langle n|\sigma_x|n'\rangle|^2}{\sum_{n,n'} |\langle n|\sigma_x|n'\rangle|^2} \qquad (3)$$

and does not depend on A, B, C, D which characterise the probe. The moments (and therefore the line shape) are the same for any probe for which (1) and (2) are equivalent. They are certainly equivalent if the probe interaction does not vary from spin to spin, i.e. if a_i, b_i, c_i and d_i are independent of i. In practice there is a complication in that the probe is often a system of standing waves which interact less strongly with spins near nodes than with those near antinodes. Microwave acoustic and electromagnetic fields correspond to wavelengths which are large compared with the spin separations; the a_i, b_i, c_i and d_i are constant over regions containing many spins and (3) holds for each region.

The proof cannot be extended to include spin systems with more complex groups of low lying levels, for their interaction with the probe need not be linear in the spin components. The linearity in spin components was used at several points in this discussion.

This work was performed at Bristol University while the author was in receipt of a D.S.I.R. Research Studentship.

References

1. A. Abragam, The principles of nuclear magnetism, (Oxford University Press: London, 1961) p.98.
2. R. Loudon, Phys.Rev. 119 (1960) 919.
3. J.H. Van Vleck, Phys.Rev. 74 (1948) 1168.

* * * * *

A NOTE ON A PARTIAL SUMMATION OF GRAPHS IN MANY BODY THEORY

K. KURKI-SUONIO
Department of Physics, University of Helsinki, Finland

Received 18 January 1965

The relation of the Hartree-Fock theory to the graphical perturbation theory of many partial systems was shown by Goldstone [1]. Thouless [2] noted that starting from free particles one can formally do a partial summation of graphs which leads to the replacement of the kinetic energies with the Hartree-Fock energies. In this summation there is a geometrical series and as emphasized several times [2-4] it does not converge in general and the result is therefore only formal.

Attention should be paid, however, to the fact that the rules for graphs are derived by a limiting process and one must always be careful in changing the order of an infinite summation and a limiting process. In this case it proves that doing the partial summation before going to the limit the result will come out quite correctly. The calculation goes then as follows:

Take an arbitrary "naked" graph, fig. 1, and consider especially the contribution in it of a particle line j which starts at the time t_μ and ends at t_ν. The value of the graph can be written

$$\ldots \sum_{\ldots j \ldots} \ldots \exp\{-\mathrm{i}T_j (t_\nu - t_\mu)\} \ldots .$$

Next, "dress" this particular line of the graph as shown in fig. 2 with the additional interaction lines at the times $t_1', \ldots, t_k'$. Now, the sum of all graphs with fixed n_1, n_2, n_3, n_4 wil be

$$\ldots \sum_{\ldots j \ldots} \ldots \frac{\exp\{\mathrm{i}T_j (t_\nu - t_\mu)\}}{n_1! n_2! n_3! n_4!} \{\int_{t_\mu}^{t_\nu} \Sigma_1 \mathrm{d}t'\}^{n_1} \times$$

$$\times \{\int_{t_\mu}^{t_\nu} \Sigma_2 \mathrm{d}t'\}^{n_2} \{\int_{t_\mu}^{t_\nu} \Sigma_3 \mathrm{d}t'\}^{n_3} \{\int_{t_\mu}^{t_\nu} \Sigma_4 \mathrm{d}t'\}^{n_4} \ldots$$

where

$$\Sigma_1 = \Sigma_2 = \sum_{r \leq k_F} \tfrac{1}{2} V_{jrjr}; \quad \Sigma_3 = \Sigma_4 = \sum_{r \leq k_F} \tfrac{1}{2} V_{jrrj}$$

yielding