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Polarization of Nuclei by Macroscopic Rotation

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A theoretical study [1][1]) has been made of the polarization of the nuclei in a crystal by means of a rapid rotation of the crystal [2]. The corresponding polarization of electrons (Barnett effect) has been known for a long time. Assuming that some mechanism for reaching equilibrium inside the crystal exists, one obtains for the equilibrium density matrix describing a spin $\boldsymbol{I}$ in a crystal rotating with angular velocity $\boldsymbol{\omega}$ and acted upon by an external magnetic field $\boldsymbol{H}$

$$\varrho = \frac{\exp\,(-\beta\,\mathfrak{H} - \boldsymbol{\lambda}\cdot\boldsymbol{I})}{\mathrm{Tr}\,\exp\,(-\beta\,\mathfrak{H} - \boldsymbol{\lambda}\cdot\boldsymbol{I})}\;;\;\beta = 1/kT,\;\boldsymbol{\lambda} = \boldsymbol{\omega}/kT \tag{1}$$

where $\mathfrak{H}$ is the Hamiltonian of the spin, and T the temperature of the crystal. The expectation value of the spin is

$$\langle \boldsymbol{I} \rangle = \mathrm{Tr}\,\varrho\,\boldsymbol{I} = \beta\,\hbar\,(\gamma\,\boldsymbol{H} + \boldsymbol{\omega})\,\frac{I(I+1)}{3}\;,\quad \beta\,\hbar\,|\,\gamma\,\boldsymbol{H} + \boldsymbol{\omega}\,| \ll 1\;. \tag{2}$$

From (2) it is seen that the action of the field and the rotation are additive and equivalent:

$$\nu = \frac{\omega}{2\,\pi} \longleftrightarrow g_n\,\frac{eH}{4\,\pi\,Mc} = 762\,g_n\,H\,\frac{rev}{sec}\;,$$

if H is expressed in gauss and g_n is the nuclear g-factor. Some corrections to (2) are obtained by considering the coupling of the single spin with the rest of the crystal. A possible mechanism for bringing about the polarization is the tensor (dipole-dipole) interaction between nuclei. The interaction will depend on time because the relative position vector connecting two nuclei is rotating in space. If $\mathfrak{H}_{12}$ is the dipole coupling for the stationary crystal, then the time-dependent interaction in the rotating crystal may be written $G(t) = U^{-1}(t)\,\mathfrak{H}_{12}U(t)$, with $U(t) = \exp\,(i/\hbar\;\boldsymbol{S}\cdot\boldsymbol{\omega}t)$ where $\boldsymbol{S}$ is the total spin. With this plausible hypothesis

[1]) Numbers in brackets refer to References, page 139.

one may show that the transformed Schroedinger wave function $\psi' = U(t)\psi$ and the energy levels for the rotating crystal in a fixed magnetic field differ from that of a fixed crystal in a rotating magnetic field essentially only through an additional effective field $\boldsymbol{\omega}/\gamma_k$ acting along the axis of rotation at nucleus k. As an explicit example, consider a pair of spins of magnitude 1/2, rigidly connected, each associated with a nucleus lying on the z- axis, and the whole system rotating about the x- axis; by integration of the Schroedinger equation, and averaging over oscillations, one obtains the polarization of the system $\langle S_x \rangle = 9\, E_0\, \hbar\, \omega(1/4 - p)\, [(3\, E_0)^2 + (2\, \hbar\omega)^2]^{-1}$, where $E_0 = (\hbar\gamma)^2/2\, r^3_{12}$ measures the strength of the dipole coupling and p the probability that initially the system was in the state $S = 1$, $m_s = 0$. The spin vector will precess around the x- axis in non-circular orbits for finite initial temperatures. The more general time-dependent behavior of a spin in thermal contact with other spins or a lattice may be treated by adapting the Wangsness-Bloch theory of magnetic resonance to the rotating crystal. The theory then yields the equilibrium density matrix (1). The formal expression for relaxation times are the same as those applying to magnetic field cases; however numerically one will find different values whenever processes involving the coupling of two spins with different gyromagnetic ratios are important. Experimental observation of nuclear polarization by means of macroscopic rotation of a crystal is expected to be possible by modifying some of the nuclear magnetic resonance experiments usually performed with a stationary crystal in an external magnetic field.

I am indebted to Dr. E. T. JAYNES, with whom many of the features of this effect have been discussed.

REFERENCES

[1] S. P. HEIMS, Ph. D. Dissertation, Stanford University (1960).
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