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BRIEF REPORT

Joint probabilities for an aligned spin-1 system

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Abstract. Following Margenau and Hill we adduce arguments to show that an aligned spin-1 system (for e.g. ^{2}H or ^{14}N nuclei in external electric quadrupole fields) can be viewed in terms of bivariate probability distributions obtained by identifying the associated characteristic function.

It is well known that spin-1 nuclei with non-zero electric quadrupole moments are polarized in the presence of external electric quadrupole fields such that their vector polarization is zero whereas their tensor polarization is non-zero, i.e. the spin-1 system is aligned. The state of polarization can either be defined in terms of a Cartesian tensor $P_{\alpha\beta}$ or equivalently in terms of an irreducible tensor t^2_q which are defined following the Madison convention (Satchler *et al* 1970). It was pointed out (Ramachandran *et al* 1987) that such an aligned spin-1 system is characterized by two axes Q_1 and Q_2 which lie in one of the planes ZX, XY or YZ in the principal axes of alignment frame (PAAF) such that one of the coordinate axes bisects the angles formed by Q_1 and Q_2. Moreover, it was remarked that only in the special case when the asymmetry parameter η of the electric field is zero, the aligned system considered is oriented (Blin-Stoyle and Grace 1959), i.e. probabilities W_m can be assigned to the three magnetic substates $|1m\rangle$, $m = 1, 0, -1$. Remarking that such a probability distribution has only one of the components J_z as a variate in the statistical sense, the purpose of the present paper is to point out that in the more general case where $\eta \neq 0$, the aligned system can be characterized in terms of a bivariate distribution with J_x, J_y or J_y, J_z or J_x, J_z as variates. In this context, we recall that Margenau and Hill (1961) have considered the criteria for defining joint probability distributions with respect to two variates which in the case of quantum system are represented in general by non-commuting observables. In fact they have considered the case of a spin-1 system as one of the examples although the discussion was confined only to pure states, i.e. the density matrix for such a system satisfies the condition $\rho^2 = \rho$. On the other hand, we have here density matrices which represent mixed states of polarization of the system. This more general situation can still be handled, provided we observe that the expectation values $E(XY) = \langle\psi, ((XY + YX)/2)\psi\rangle$ of Margenau and Hill are replaced by the average expectation values given by $\mathrm{Tr}[\rho(XY + YX)/2]$. The considerations of Margenau

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and Hill could be interpreted in a wider sense (Cohen 1966) by associating the correspondence rule

$$x^n y^m \to \tfrac{1}{2}(X^n Y^m + Y^m X^n)$$

and

$$\exp(ixI_x)\exp(iyI_y) \to \tfrac{1}{2}[\exp(iXI_x)\exp(iYI_y) + \exp(iYI_y)\exp(iXI_x)].$$

This immediately leads to the characteristic function

$$\varphi(I_x, I_y) = \tfrac{1}{2}\,\mathrm{Tr}\{\rho[\exp(iXI_x)\exp(iYI_y) + \exp(iYI_y)\exp(iXI_x)]\}. \tag{1}$$

Identifying the operators X, Y as the spin components J_x, J_y of the spin-1 system, we may express the characteristic function in terms of the bivariate probability distribution $P(m_x, m_y)$ as

$$\varphi(I_x, I_y) = \sum_{m_x, m_y = 1, 0, -1} \exp[\mathrm{i}(m_x I_x + m_y I_y)] P(m_x, m_y) \tag{2}$$

where

$$P(m_x, m_y) = \mathrm{Re}(U_y \rho U_x^\dagger)_{m_y m_x} (U_x U_y^\dagger)_{m_x m_y}. \tag{3}$$

Here

$$U_x = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix} \qquad U_y = \frac{1}{2}\begin{pmatrix} 1 & -\mathrm{i}\sqrt{2} & -1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & \mathrm{i}\sqrt{2} & -1 \end{pmatrix} \tag{4}$$

transform J_x, J_y respectively to their diagonal form and m_x, m_y take values $1, 0, -1$. Considering the physical example of a spin-1 system like ^{2}H or ^{14}N, exposed to an external electric quadrupole field, where the density matrix ρ in the PAAF is given in terms of the populations Π_x, Π_y, Π_z by (Ramachandran *et al* 1987)

$$\rho = \frac{1}{2}\begin{pmatrix} \Pi_x + \Pi_y & 0 & \Pi_y - \Pi_x \\ 0 & 2\Pi_z & 0 \\ \Pi_y - \Pi_x & 0 & \Pi_x + \Pi_y \end{pmatrix} \tag{5}$$

the bivariate probability distribution is given explicitly by

$$P(m_x, m_y) = \frac{1}{4}\begin{pmatrix} \Pi_z & 2\Pi_y & \Pi_z \\ 2\Pi_x & 0 & 2\Pi_x \\ \Pi_z & 2\Pi_y & \Pi_z \end{pmatrix} \tag{6}$$

which is positive definite. It is clear that

$$\sum_{m_x, m_y} P(m_x, m_y) = \Pi_x + \Pi_y + \Pi_z = 1 \tag{7}$$

and the marginal distributions $P(m_x)$, $P(m_y)$ are readily obtained through

$$P(m_y) = \sum_{m_x} P(m_x, m_y) = \tfrac{1}{2}(\Pi_z + \Pi_x, 2\Pi_y, \Pi_z + \Pi_x) \tag{8}$$

$$P(m_x) = \sum_{m_y} P(m_x, m_y) = \frac{1}{2}\begin{pmatrix} \Pi_z + \Pi_y \\ 2\Pi_x \\ \Pi_z + \Pi_y \end{pmatrix}. \tag{9}$$

Conversely, the populations Π_x, Π_y, Π_z could, in general, be expressed in terms of the joint probabilities $P(m_x, m_y)$ as follows:

$$\begin{aligned}
\Pi_x &= P(0,1) + P(0,-1) \\
\Pi_y &= P(1,0) + P(-1,0) \\
\Pi_z &= P(1,1) + P(1,-1) + P(-1,1) + P(-1,-1).
\end{aligned} \tag{10}$$

It may also be pointed out that the joint probability distribution discussed above need not be with respect to the J_x, J_y components only. One can as well take the two variates to be J_y, J_z or equally well the J_z, J_x components, in which case the joint probabilities $P(m_y, m_z)$, $P(m_z, m_x)$ are readily obtained as

$$P(m_y, m_z) = \mathrm{Re}(U_y\rho)_{m_y m_z}(U_y^\dagger)_{m_z m_y} = \frac{1}{4}\begin{pmatrix} \Pi_x & 2\Pi_z & \Pi_x \\ 2\Pi_y & 0 & 2\Pi_y \\ \Pi_x & 2\Pi_z & \Pi_x \end{pmatrix} \tag{11}$$

and

$$P(m_z, m_x) = \mathrm{Re}(U_x\rho)_{m_x m_z}(U_x^\dagger)_{m_z m_x} = \frac{1}{4}\begin{pmatrix} \Pi_y & 2\Pi_x & \Pi_y \\ 2\Pi_z & 0 & 2\Pi_z \\ \Pi_y & 2\Pi_x & \Pi_y \end{pmatrix}. \tag{12}$$

It is pertinent to point out that the W_{m_z}, $m_z = 1, 0, -1$ is realized as the marginal distribution $P(m_z) = \sum_{m_x} P(m_z, m_x) = \sum_{m_y} P(m_y, m_z)$ of J_z in the special case $\eta = 0$, i.e. when the system is oriented. However, when $\eta \neq 0$, the system can only be described in terms of bivariate distributions $P(m_x, m_y)$ or $P(m_y, m_z)$ or $P(m_x, m_z)$. If in addition to the external electric quadrupole field, an external magnetic field in an arbitrary direction is switched on, the expectation values $\langle J_i \rangle$, $\frac{1}{2}\langle J_i J_j + J_j J_i \rangle$, $i \neq j$ which were zero in the absence of a magnetic field will then turn out to be non-zero, and the bivariate description becomes inadequate in such a case. The nature of the more general trivariate distribution is taken up elsewhere.

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