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1976 J. Phys. A: Math. Gen. 9 1947

(http://iopscience.iop.org/0305-4470/9/11/019)

J. Phys. A: Math. Gen., Vol. 9, No. 11, 1976. Printed in Great Britain. © 1976

An analogue of Shirley's equation for a spin-1 system

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Received 7 June 1976

Abstract. An analogue of Shirley's equation for a spin-1 system subjected to a periodic perturbation is derived, and shown to be consistent with the results of Brossel and Bitter.

In a well known paper, Shirley (1965) obtained the following equation for the time-averaged probability, $\bar{P}_{\alpha\beta}^{(1/2)}$ for transitions between the two states $|\alpha\rangle$ and $|\beta\rangle$ of a spin-$\frac{1}{2}$ system under the influence of a periodic classical field coupled to the spin system:

$$\bar{P}_{\alpha\beta}^{(1/2)} = \frac{1}{2}\left[1 - 4\left(\frac{\partial q}{\partial \omega_0}\right)^2\right], \tag{1}$$

where ω_0 is the difference in energy between $|\alpha\rangle$ and $|\beta\rangle$ and q is the so called Floquet, or characteristic exponent. This remarkable result enables one to sketch the time-averaged transition probability directly from a plot of the characteristic exponent, and has been used as the starting point in many papers which calculate the Bloch–Siegert shift and multiple quantum resonances in strong oscillating fields (see for example the references cited in Swain 1974, and Bialynicka-Birula and Bialynicka-Birula 1976).

In this paper we obtain a generalization of (1) which applies to a *symmetric* three-level system (for brevity we will refer to such a system as a spin-1 system) which has a Hamiltonian periodic in time with frequency ω. An example of such a system is provided by the 6^3P_1 excited state of the mercury atom, which was investigated by Brossel and Bitter (1952) in their double resonance experiments. In their theory of these experiments the rotating wave approximation (RWA) was assumed, so that the Hamiltonian may be written in the form

$$H = \sum_{i=\alpha,\beta,\gamma} |i\rangle E_i \langle i| + V(|\alpha\rangle\langle\beta|\, e^{-i\omega t} + |\gamma\rangle\langle\beta|\, e^{i\omega t} + \text{HC}) \tag{2}$$

where β now denotes the middle level, α and γ the extreme levels; HC stands for Hermitian conjugate. For the system to be symmetric the energy levels must be equally spaced, i.e. $E_\alpha - E_\beta = E_\beta - E_\gamma = \omega_0$, say. The coupling constant V is proportional to the applied RF magnetic field (for simplicity we have taken V to be real) and ω_0 is proportional to the DC magnetic field. It is clear that (2) describes a situation in which the middle level is connected to the two outer levels by the RF field, but the two outer levels are not connected directly. Before giving this system further consideration we will first obtain our general result.

According to Shirley (1965) (see also Stey and Gusman 1974) the time-averaged transition probability between any two levels k and l of a three-level system is given by the expression

$$\bar{P}^{(1)}_{kl} = \sum_{i=\alpha,\beta,\gamma} \frac{\partial q_i}{\partial E_k} \frac{\partial q_i}{\partial E_l} \tag{3}$$

where q_α, q_β and q_γ, the Floquet exponents, satisfy the condition

$$q_\alpha + q_\beta + q_\gamma = E_\alpha + E_\beta + E_\gamma. \tag{4}$$

In particular, for $k = l = \beta$, we have

$$\bar{P}^{(1)}_{\beta\beta} = \left(\frac{\partial q_\alpha}{\partial E_\beta}\right)^2 + \left(\frac{\partial q_\beta}{\partial E_\beta}\right)^2 + \left(\frac{\partial q_\gamma}{\partial E_\beta}\right)^2. \tag{5}$$

For the special case of a spin-1 atom we have the symmetry relation

$$\partial q_\gamma/\partial E_\beta = \partial q_\alpha/\partial E_\beta, \tag{6}$$

so that expression (5) reduces to

$$\bar{P}^{(1)}_{\beta\beta} = \left(\frac{\partial q_\beta}{\partial E_\beta}\right)^2 + 2\left(\frac{\partial q_\alpha}{\partial E_\beta}\right)^2. \tag{7}$$

However, by differentiating expression (4) with respect to E_β, and using expression (6), we obtain

$$\frac{\partial q_\alpha}{\partial E_\beta} = \frac{1}{2}\left(1 - \frac{\partial q_\beta}{\partial E_\beta}\right) \tag{8}$$

so that $\bar{P}^{(1)}_{\beta\beta}$ may be expressed in terms of $\partial q_\beta/\partial E_\beta$ alone as

$$\bar{P}^{(1)}_{\beta\beta} = \frac{1}{2}\left[1 - 2\frac{\partial q_\beta}{\partial E_\beta} + 3\left(\frac{\partial q_\beta}{\partial E_\beta}\right)^2\right]. \tag{9}$$

Also by symmetry we have

$$\bar{P}^{(1)}_{\alpha\beta} = \bar{P}^{(1)}_{\gamma\beta} \tag{10}$$

and conservation of probability implies

$$\bar{P}^{(1)}_{\alpha\beta} + \bar{P}^{(1)}_{\beta\beta} + \bar{P}^{(1)}_{\beta\gamma} = 1. \tag{11}$$

Hence

$$\bar{P}^{(1)}_{\alpha\beta} = \bar{P}^{(1)}_{\beta\gamma} = \tfrac{1}{2}(1 - \bar{P}^{(1)}_{\beta\beta}) = \frac{1}{4}\left(1 - \frac{\partial q_\beta}{\partial E_\beta}\right)\left(1 + 3\frac{\partial q_\beta}{\partial E_\beta}\right). \tag{12}$$

Expression (12) is the desired result: an analogue of Shirley's equation applicable to a spin-1 system. The transition probability is expressed in terms of a derivative of just one of the Floquet exponents.

In the Brossel–Bitter experiments the measured quantity is essentially $\bar{P}^{(1)}_{\alpha\beta}$ as a function of ω_0. The most obvious features of the spectrum are its maxima and minima. It is easily seen from (12) that the maxima of $\bar{P}^{(1)}_{\alpha\beta}$ occur when the condition

$$\partial q_\beta/\partial E_\beta = \tfrac{1}{3} \tag{13}$$

is satisfied, and that the minima with respect to a parameter z (such as ω or ω_0) occur when

$$\frac{\partial}{\partial z}\left(\frac{\partial q_\beta}{\partial E_\beta}\right)=0. \tag{14}$$

Expressions (13) and (14) can be used to investigate the resonances of any spin-1 system from a knowledge of q_β alone.

We conclude by showing that expression (12) is consistent with that obtained by Brossel and Bitter (1952) when the natural lifetime of the atomic levels may be neglected. Adopting the Hamiltonian (2) and substituting the following *ansatz* for the wavefunction in the time-dependent Schrödinger equation;

$$|\psi(t)\rangle = e^{-iqt}\sum_{n=-\infty}^{\infty}\{a_n|\alpha\rangle + b_n|\beta\rangle + c_n|\gamma\rangle\}\,e^{in\omega t} \tag{15}$$

one readily obtains the following equations for the coefficients a_n, b_n and c_n:

$$(q-n\omega-E_\alpha)a_n = Vb_{n+1} \tag{16a}$$

$$(q-n\omega-E_\beta)b_n = V(a_{n-1}+c_{n+1}) \tag{16b}$$

$$(q-n\omega-E_\gamma)c_n = Vb_{n-1}. \tag{16c}$$

The condition for consistent solutions leads to the cubic eigenvalue equation (with $n=0$)

$$(q-E_\beta)(q-E_\alpha+\omega)(q-E_\gamma-\omega)-V^2(2q-E_\alpha-E_\gamma)=0, \tag{17}$$

the solutions of which are $q_\alpha-\omega$, q_β and $q_\gamma+\omega$.

In a spin-1 system the energy levels are equally spaced. If we choose the particularly simple scheme

$$E_\alpha=-E_\gamma=\omega_0, \qquad E_\beta=0 \tag{18}$$

then the solutions of (17) are

$$q_\beta=0, \qquad q_\alpha=-q_\gamma=[(\omega-\omega_0)^2+2V^2]^{1/2}. \tag{19}$$

However, to obtain $\partial q_\beta/\partial E_\beta$ we must differentiate (17) with respect to E_β *before* adopting the scheme (18). We thus obtain

$$\frac{\partial q_\beta}{\partial E_\beta}=\frac{(\omega-\omega_0)^2}{(\omega-\omega_0)^2+2V^2}. \tag{20}$$

Using the criteria (13) and (14) we find that maxima and the minimum of $\bar{P}^{(1)}_{\alpha\beta}$ occur at

$$\omega=\omega_0\pm V, \qquad \omega=\omega_0 \tag{21}$$

respectively. Substituting (20) into (12) we obtain

$$\bar{P}^{(1)}_{\alpha\beta}=\frac{V^2[2(\omega-\omega_0)^2+V^2]}{[(\omega-\omega_0)^2+2V^2]^2} \tag{22}$$

which is identical to the expression obtained by Brossel and Bitter (1952) in the absence of natural damping (in their notation, $1/T_e=0$).

Acknowledgments

One of us (JH) wishes to acknowledge financial support in the form of a grant awarded by the Academic Council of The Queen's University of Belfast. The research reported was accomplished with the support of the US Office of Naval Research under Contract No. N00014-69-C-0035.

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