Geometrical Representation of the Schrödinger Equation for Solving Maser Problems

RICHARD P. FEYNMAN AND FRANK L. VERNON, JR., *California Institute of Technology, Pasadena, California*

AND

ROBERT W. HELLWARTH, *Microwave Laboratory, Hughes Aircraft Company, Culver City, California*

(Received September 18, 1956)

A simple, rigorous geometrical representation for the Schrödinger equation is developed to describe the behavior of an ensemble of two quantum-level, noninteracting systems which are under the influence of a perturbation. In this case the Schrödinger equation may be written, after a suitable transformation, in the form of the real three-dimensional vector equation $d\mathbf{r}/dt=\boldsymbol{\omega}\times\mathbf{r}$, where the components of the vector $\mathbf{r}$ uniquely determine ψ of a given system and the components of $\boldsymbol{\omega}$ represent the perturbation. When magnetic interaction with a spin $\frac{1}{2}$ system is under consideration, "$\mathbf{r}$" space reduces to physical space. By analogy the techniques developed for analyzing the magnetic resonance precession model can be adapted for use in any two-level problems. The quantum-mechanical behavior of the state of a system under various different conditions is easily visualized by simply observing how $\mathbf{r}$ varies under the action of different types of $\boldsymbol{\omega}$. Such a picture can be used to advantage in analyzing various MASER-type devices such as amplifiers and oscillators. In the two illustrative examples given (the beam-type MASER and radiation damping) the application of the picture in determining the effect of the perturbing field on the molecules is shown and its interpretation for use in the complex Maxwell's equations to determine the reaction of the molecules back on the field is given.

INTRODUCTION

ELECTROMAGNETIC resonances in matter have become a fundamental tool for studying the structure of matter. Moreover, recently it has become of interest to use such resonances for radio and microwave frequency circuit components, such as highly stable oscillators, high Q filters, isolators, and amplifiers. The purpose of this paper will be to aid in the understanding of simple resonances and especially in the conception and design of microwave "atomic" devices (now commonly called MASER-type devices) which involve these simple resonances. In this paper we propose to do the following things: (a) To develop a simple but rigorous and complete geometrical picture of the Schrödinger equation describing the resonance behavior of a quantum system when only a pair of energy levels is involved (the resulting picture has the same form as the well-known three-dimensional classical precession of a gyromagnet in a magnetic field); (b) To note further properties of the model which permit its direct interpretation in terms of the physical properties which couple the quantum systems to the electromagnetic fields, and to state these explicitly for dipole transitions; (c) To illustrate the use of the picture by solving the particular cases of the beam MASER oscillator characteristics and "radiation damping."

Although the approach does not obtain results inaccessible to straight-forward calculation, the simplicity of the pictorial representation enables one to gain physical insight and to obtain results quickly which display the main features of interest.

FORMULATION

We will be concerned with an ensemble of spacially non-overlapping systems, e.g., molecules in a molecular beam, such that the wave function for any one individual system may be written

$$\psi(t)=a(t)\psi_a+b(t)\psi_b \tag{1}$$

during some time of interest. ψ_a and ψ_b are the two eigenstates of interest of the Hamiltonian for the single system corresponding to the energies $W+\hbar\omega_0/2$ and $W-\hbar\omega_0/2$ respectively. W is the mean energy of the two levels determined by velocities and internal interactions which remain unchanged. W will be taken as the zero of energy for each system. ω_0 is the resonant angular frequency associated with a transition between the two levels and is always taken positive.

It is usual to solve Schrödinger's equation with some perturbation V for the complex coefficients $a(t)$ and $b(t)$, and from them calculate the physical properties of the system. However, the mathematics is not always transparent and the complex coefficients do not give directly the values of real physical observables. Neither is it sufficient to know only the real magnitudes of a and b, i.e., the level populations and transition probabilities, when coherent processes are involved. We propose instead to take advantage of the fact that the phase of $\psi(t)$ has no influence so that only three real numbers are needed to completely specify $\psi(t)$. We construct three real functions (r_1,r_2,r_3) of a and b which have direct physical meaning and which define a 3-vector $\mathbf{r}$ whose time dependance is easily pictured:

$$\begin{aligned} r_1&\equiv ab^*+ba^* \\ r_2&\equiv i(ab^*-ba^*) \\ r_3&\equiv aa^*-bb^*. \end{aligned} \tag{2}$$

(*) always indicates complex conjugate. The time dependence of $\mathbf{r}$ can be obtained from Schrödinger's

equation which gives

$$i\hbar da/dt = a[(\hbar\omega_0/2)+V_{aa}]+bV_{ab} \tag{3}$$

and similar equations for db/dt, da^*/dt, db^*/dt. The subscripts on V indicate the usual matrix elements. $V_{aa}=V_{bb}=0$ for most all cases of interest, and whenever these can be neglected compared to $\hbar\omega_0/2$, V need be neither small nor of short duration for the results to be exact. Using Eqs. (3) to find the differential equation for $\mathbf{r}$ gives

$$d\mathbf{r}/dt = \boldsymbol{\omega}\times\mathbf{r} \tag{4}$$

where $\boldsymbol{\omega}$ is also a three vector in "$\mathbf{r}$" space defined by the three real components:

$$\begin{aligned}\omega_1 &\equiv (V_{ab}+V_{ba})/\hbar\\ \omega_2 &\equiv i(V_{ab}-V_{ba})/\hbar\\ \omega_3 &\equiv \omega_0.\end{aligned} \tag{5}$$

The $\times$ symbol has the usual vector product meaning. It is easily shown that the remaining real combination aa^*+bb^* is just equal to the length of the $\mathbf{r}$ vector, $(r_1^2+r_2^2+r_3^2)^{\frac{1}{2}}$, and is constant in time. It equals one when ψ is normalized to unity. The motion described by Eq. (4) is of the form for the precession of a classical gyromagnet in a magnetic field. Therefore, it is not surprising that in the case of transitions between the two magnetic levels of a spin $\frac{1}{2}$ particle, this mathematical $\mathbf{r}$ space will be equivalent to physical space with r_1, r_2, r_3 proportional to the expectation values of μ_x, μ_y, μ_z, and ω_1, ω_2, ω_3 proportional to the components of the magnetic field H_x, H_y, H_z respectively. Although in general the formalism does not represent physical space, by analogy any transitions under the stated conditions may be thought of rigorously in terms of the well-known classical vector model for spin precession. The extensive and explicit use of rotating coordinate procedures, as was introduced by Bloch, Ramsey, Rabi, and Schwinger[1,2] for special kinds of magnetic transitions, is generally applicable in dealing with the r space.

INTERPRETATION

The effect of the presence of the quantum systems on the surrounding electromagnetic field is observed in many resonance experiments or devices, so it is of interest to deduce such quantities as the energy given up by the systems and effective polarization densities which, in general, are not linear in the impressed fields. The internal energy, or expectation value of the unperturbed Hamiltonian H at any time t is

$$\langle H\rangle = \int \psi^* H\psi d(\mathrm{Vol}) = (aa^*-bb^*)\hbar\omega_0/2 = r_3\hbar\omega_0/2 \tag{6}$$

or just r_3 in units of $\hbar\omega_0/2$. The total internal energy in any ensemble of these systems is of course the sum of the r_3 values (in units of $\hbar\omega_0/2$) in the region, or the projection on the 3 axis of the vector sum $\mathbf{R}=\sum_i \mathbf{r}^i$ over the region. In fact, any operator x such as the dipole moment operator, which is separable in the systems, has an expectation value of the form

$$x_{ab}\textstyle\sum_i (a^i)^* b^i + x_{ba}\sum_i (b^i)^* a^i + x_{aa}\sum_i (a^i)^* a^i + x_{bb}\sum_i (b^i)^* b^i$$

and is therefore a linear combination of the r_1's, r_2's, and r_3's, or R_1, R_2, and R_3; it is proportional to a projection of $\mathbf{R}$ on some axis, plus perhaps a constant.

It remains to determine the proper projections for particular cases and also state explicitly the values of $\boldsymbol{\omega}$. Since all common microwave transitions such as hyperfine structure, spin flip, molecular rotational and inversion transitions are dipole transitions, we will examine only these cases.

For electric dipole $\Delta m=0$ transitions,

$$V_{ab} = -\mu_{ab}E \tag{7}$$

where μ_{ab} is the matrix element between the two states for the component of the dipole moment along the electric field E. If μ_{ab} is made real by proper choice of the phases of ψ_a and ψ_b, then

$$\begin{aligned}\omega_1 &= (V_{ab}+V_{ba})/\hbar = -(2\mu_{ab}/\hbar)E\\ \omega_2 &= i(V_{ab}-V_{ba})/\hbar = 0\\ \omega_3 &= \omega_0\end{aligned} \tag{8}$$

ω_1 is the electric field strength in units of $-2\mu_{ab}/\hbar$. In this case

$$\langle\mu\rangle = a^*b\mu_{ab}+b^*a\mu_{ba} = r_1\mu_{ab}. \tag{9}$$

This means that the component of the polarization density P along the electric field will equal the average projection of $\mathbf{r}$ on the 1 axis in some small region of space and given in units of $\rho\mu_{ab}$ where ρ is the particle density.

In the case of magnetic dipole $\Delta m=0$ transitions, the same formulas apply substituting H for E and the appropriate magnetic dipole for μ.

In the case of electric or magnetic $\Delta m=\pm 1$ dipole transitions, considering E_x and E_y to be the relevant spacial components of either the electric or magnetic fields,

$$V = (-1/2)(\mu^+E^- + \mu^-E^+) \tag{10}$$

where $E^\pm \equiv E_x \pm iE_y$ and $\mu^\pm \equiv \mu_x \pm i\mu_y$. By the well-known properties of the $\mu^\pm$ operators:

$$\begin{aligned}V_{ab} &= -(1/2)\mu_{ab}{}^+(E_x-iE_y)\\ V_{ba} &= -(1/2)\mu_{ba}{}^-(E_x+iE_y).\end{aligned} \tag{11}$$

Choosing the phases of ψ_a and ψ_b such that $\mu_{ab}{}^+$ is a real number γ, then $\mu_{ab}{}^+ = \mu_{ba}{}^-$ by their definitions, and:

$$\begin{aligned}\omega_1 &= -(\gamma/\hbar)E_x\\ \omega_2 &= -(\gamma/\hbar)E_y;\end{aligned} \tag{12}$$

thus $\boldsymbol{\omega}$ behaves in the 1–2 plane exactly as does E in

[1] Rabi, Ramsey, and Schwinger, Revs. Modern Phys. 26, 167 (1954).
[2] R. K. Wangsness, Am. J. Phys. 24, 60 (1956).

the $x-y$ plane of space. By noting that $\langle\mu^+\rangle=\gamma a^*b$ and $\langle\mu^-\rangle=\gamma b^*a$, we find:

$$\langle\mu_x\rangle=(\gamma/2)r_1$$
$$\langle\mu_y\rangle=(\gamma/2)r_2. \tag{13}$$

If there exists a component μ_z such that $-\mu_z E_z=H$, then it can be seen that the mathematical "**r**" space reduces to physical space, as in the case of free spin $\frac{1}{2}$ Zeeman transitions. By similar procedures any kind of perturbation affecting only two levels can be thought of in terms of the familiar behavior of vectors rotating in space, according to $d\mathbf{r}/dt=\boldsymbol{\omega}\times\mathbf{r}$.

SAMPLE APPLICATIONS

Beam Type Maser Oscillator[3]

To examine how this viewpoint leads to the solution of a particular problem, we first solve the effect of a given field on the particles involved; secondly, we formulate the classical field equations in a way suitable to the experimental situation, and using the proper projections of the **r** vector we find the conditions which satisfy both Schrödinger's and Maxwell's equations simultaneously. Consider a beam of molecules which enters a microwave cavity which is near resonance with a $\Delta m=0$ transition of the molecule. The molecules have been prepared so that only those in the higher energy state enter the cavity. Assume for simplicity that the cavity mode shape is such that the molecules see an oscillatory field of constant amplitude and phase as they pass through the cavity. The oscillating ω_1 can be separated into two counter-rotating components in the 1–2 plane. For coherent perturbations such as this it is convenient to transform to a coordinate frame in which the appropriate component of ω_1 appears stationary, and neglect the other counter-rotating component. The rotating axes will be designated the *I*, *II*, and *III* axes. We take the *I* axis in the plane of the stationary driving torque which now has the following constant components (see Fig. 1):

$$\omega_I=1/2|\omega_1|$$
$$\omega_{II}=0$$
$$\omega_{III}=\omega_0-\omega.$$

ω is the frequency of the perturbation. The molecules enter the cavity with $\mathbf{r}=\mathbf{III}$ and at a time t later the components r_I and r_{II} can be seen by inspection of Fig. 1 to be

$$r_I=\frac{\omega_I(\omega_0-\omega)}{\Omega^2}[1-\cos(\Omega t)]$$
$$r_{II}=-\frac{\omega_I}{\Omega}\sin(\Omega t). \tag{14}$$

Ω is the magnitude $[\omega_I^2+(\omega_0-\omega)^2]^{\frac{1}{2}}$ of the driving torque as seen in the rotating frame.

[3] Gordon, Zeiger, and Townes, Phys. Rev. **95**, 282 (1954).

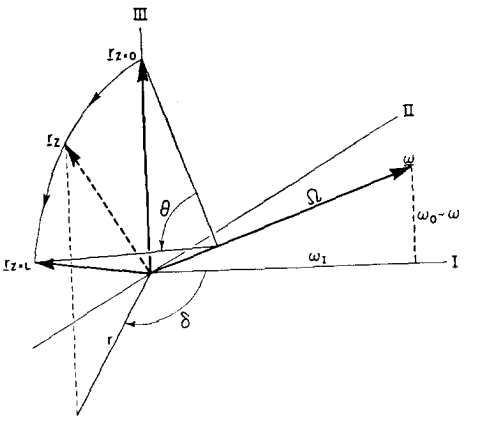

FIG. 1. MASER oscillator diagram in rotating coordinates.

To reduce these results to the stationary frame we choose the time reference such that $\omega_1=2\omega_I\cos(\omega t)$. Then $r_1=r(t)\cos[\omega t+\delta(t)]$ where $r(t)$ is the magnitude of the projection of **r** on the 1–2 plane and $\delta(t)=\tan^{-1}r_{II}/r_I$. If we use complex quantities to represent time dependence at frequency ω, it is evident if ω_1 is represented by ω_I then r_1 is represented by (r_I+ir_{II}). Assuming all the molecules to have a velocity v then the complex polarization density P at a distance z along the cavity is the simple expression $\rho\mu_{ab}(r_I+ir_{II})$ with $t=z/v$.[4] In a thin beam, P_z, the polarization per unit length of beam is $(n/v)\mu_{ab}\times(r_I+ir_{II})$. n is number per second entering the cavity. Thus in practice one obtains the quantities of interest directly from the rotating frame.

The electric field configuration in the cavity has been assumed to be the normal configuration $\mathbf{E}_c(x,y,z)$ of the nondegenerate mode employed, where the normalization is taken such that $\int|\mathbf{E}_c|^2d\mathcal{V}=1$. $|\mathbf{E}_c|$ at the beam is taken to be the constant $f\mathcal{V}^{-\frac{1}{2}}$. $\mathcal{V}$ is the volume of the cavity. f is a form factor which would be unity were the field uniform throughout. The electric field may be written $\mathbf{E}=\mathbf{E}_c(x,y,z)\mathcal{E}(t)e^{i\omega t}$ where $\mathcal{E}$ is a real amplitude, constant in the steady state of oscillation. Then Maxwell's equations in complex form give

$$-\omega^2[\mathcal{E}\mathbf{E}_c+(4\pi\mathbf{E}_c/|\mathbf{E}_c|)P]+i(\omega\omega_c/Q)\mathbf{E}_c\mathcal{E}+\omega_c^2\mathbf{E}_c\mathcal{E}=0. \tag{15}$$

ω_c is the resonant frequency of the cavity and Q is quality factor of the cavity. Integrating Eq. (15) by $\cdot\mathbf{E}_c$ over the cavity volume gives in the case of a very thin beam

$$-\omega^2\left[\mathcal{E}+(4\pi n/v)\mu_{ab}\int_0^L f\mathcal{V}^{-\frac{1}{2}}(r_I+ir_{II})dz\right]+i(\omega\omega_c/Q)\mathcal{E}+\omega_c^2\mathcal{E}=0. \tag{16}$$

Performing the indicated integration, the imaginary

[4] J. Helmer, M. L. Report No. 311, Signal Corps Contract DA 36-039 SC-71178, Stanford University.

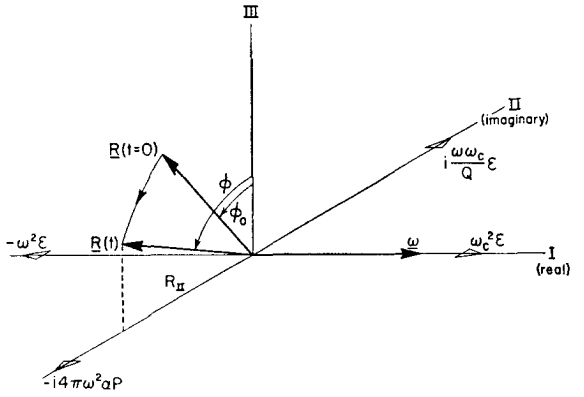

FIG. 2. Representation of "radiation damping" with the complex Maxwell's equations represented on the $I-II$ plane by the hollow arrows. $\mathbf{R}=\Sigma i\mathbf{r}^i$, $\alpha=fV^{-\frac{1}{2}}\mu_{ab}$, P=total polarization (or magnetization).

part of Eq. (16) gives

$$\frac{n}{n_{th}}=\frac{\theta^2}{2(1-\cos\theta)}. \tag{17}$$

$n_{th}\equiv\hbar\mathcal{V}v^2/2\pi f^2\mu_{ab}^2L^2Q$ and is the threshold number per second required to sustain oscillation. θ is the total angle $\Omega L/v$ through which each r precesses about the effective $\boldsymbol{\omega}$.

Equation (17) gives θ if n is known and thus the spread of frequencies at which oscillation is possible. To determine the magnitude of the electric field and the frequency of oscillation for a particular ω_c and cavity Q consider the real part of Eq. (16).

This may be written as

$$\frac{\omega_0-\omega}{\omega-\omega_c}=\frac{Q}{\pi Q_B}\frac{1-\cos\theta}{1-(\sin\theta)/\theta}\approx\frac{\omega_0-\omega}{\omega_0-\omega_c} \tag{18}$$

where $Q_B\equiv 2\pi\omega_0L/v\approx\omega_0/\Delta\omega$ is a parameter describing the natural molecular resonance line width $\Delta\omega$. Given the amount of cavity detuning $\omega_0-\omega_c$ and θ from Eq. (17), Eq. (18) enables one to determine the frequency of oscillation ω and then $\mathcal{E}\sim\omega_I$ by using the definition of θ. These are essentially the results of Shimoda, Wang, and Townes,[5] though it appears here that no restrictions need be placed on ω to obtain them. Since the parameters θ, $\omega-\omega_0$, $\omega_I\sim\mathcal{E}$, the internal energy, and the dipole moment all appear as geometrical quantities in Fig. 1, it is easy to visualize the effects of changing any of them. Also, it is often easy to visualize, if not to solve, more complicated situations such as those which involve cavities with nonuniform modes, multiple cavities, or externally-driven cavities.

To picture the coupling of the molecules, governed by the Schrödinger equation, with the field, governed by Maxwell's equation, it is useful to think of the $I-II$ plane in the rotating frame as a complex plane representing relative time phase, with the II axis as the imaginary axis. Then the complex Maxwell's equation (16) can be drawn on the $I-II$ plane and the way in which the various quantities must vary to balance the equation to zero (or to some other driving force, if present) can be visualized. Imagining the $I-II$ plane as complex is especially useful when the $\mathbf{r}$ vectors throughout the cavity have all seen the same perturbation for the same length of time, in which case the integrals are just proportional at any time to the resultant $\mathbf{R}=\sum_i\mathbf{r}^i$ which behaves in the same manner as the individual $\mathbf{r}$'s, i.e., $d\mathbf{R}/dt=\boldsymbol{\omega}\times\mathbf{R}$. This picture is easily applied to the phenomenon of "radiation damping."[6,7]

Radiation Damping

To examine the spontaneous behavior of an ensemble of dipoles in an arbitrary state (represented by an $\mathbf{R}$) and enclosed in some small portion of a microwave cavity, we may write Maxwell's equations for the cavity as before. When the ensemble is in thermal equilibrium $\mathbf{R}$ is $-\mathbf{III}R_0$ where R_0 is given by the number present and Boltzmann statistics. Assume some other $\mathbf{R}$ state is obtained (this can be done by applying a short intense rf pulse at ω_0) and $\mathbf{R}$ is left tipped at an angle ϕ_0 to the III axis in the II, III plane ($R_I=0$). Further, we assume that the cavity is tuned to the molecular resonant frequency so that in this case $\omega=\omega_0=\omega_c$. Figure 2 is drawn for this case. $R_{II}=R_0\sin\phi$ is proportional to $\mathcal{E}$ from balancing imaginary parts of the diagram. We must now assume that $d\mathcal{E}/dt\ll(\omega_0/Q)\mathcal{E}$ and $(\omega_I/\omega_0)^2\ll 1$ as we have replaced time derivatives by $i\omega$ only. Now $d\mathbf{R}/dt=\boldsymbol{\omega}\times\mathbf{R}$ means that $d\phi/dt\sim\sin\phi$. So the radiation damping obeys $d\phi/dt\sim\sin\phi$ at resonance. The solution with constants evaluated is

$$\tan(\phi/2)=\tan(\phi_0/2)e^{t/\tau}. \tag{19}$$

$\tau=\mathcal{V}\hbar/4\pi f^2\mu_{ab}^2QR_0$ for $\Delta m=0$ transitions, and $\tau=\mathcal{V}\hbar/\pi f^2\gamma^2R_0Q$ for the case of $\Delta m=\pm 1$ transitions in a linearly polarized field (that is, a nondegenerate cavity mode). The case of a circularly polarized field involving two cavity modes and $\Delta m=\pm 1$ transitions is more complicated and involves both $\langle\mu_x\rangle$ and $\langle\mu_y\rangle$ each coupling to a separate mode.

In conclusion, we wish to emphasize the usefulness of the geometrical model in visualizing and solving problems involving transitions between two levels. However, the way in which this model would be interpreted and used in a given situation depends upon the particular problem as is indicated by the two examples given. This technique of using the geometrical model does not make solutions of problems possible which were not solvable previously. However, even in many of these insoluble cases one can gain considerable insight into the behavior of the processes being investigated by observing how the parameters in the model vary.

[5] Shimoda, Wang, and Townes, Phys. Rev. **102**, 1308 (1956).

[6] N. Bloembergen and R. V. Pound, Phys. Rev. **95**, 8 (1954).

[7] R. H. Dicke, Phys. Rev. **93**, 99 (1954).