On Nonadiabatic Processes in Inhomogeneous Fields

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The problem of calculating nonadiabatic transition probabilities is considered. It is shown that the general Güttinger equations are incorrect and lead to erroneous results in any case other than that of the rotating magnetic field, which he considered. The corrected equations are applied in the calculation of transition probabilities between the various magnetic states of a field precessing with constant angular velocity.

An atom, or a neutron, moving in an inhomogeneous field is acted on by a time-varying field in the reference system of the particle. If the variation in the field is sufficiently slow, the atom, according to the adiabatic theorem, will remain in the same state with respect to the instantaneous value of the field. The problem of calculating nonadiabatic transition probabilities has been considered by Güttinger,[1] who applied his general equations to the case of a magnetic field rotating with constant angular velocity.

It is the purpose of this paper to point out that Güttinger's equations are incorrect and lead to erroneous results in any case other than that of the rotating field, which he considered. The corrected equations are applied in the calculation of the transition probabilities between the various magnetic states of a field precessing with constant angular velocity.

The Güttinger Equations

Consider an atom whose Hamiltonian contains certain time dependent parameters, such as electric or magnetic field strengths. The eigenstate of the system satisfies the equation

$$i\hbar\frac{\partial}{\partial t}\Psi=\mathcal{H}(t)\Psi. \tag{1}$$

If the system is nondegenerate, Ψ may be expanded in terms of a complete, orthogonal set of eigenstates of $\mathcal{H}(t)$, *viz.:*

$$\Psi=\sum_m C_m(t)\Psi_m(t), \tag{2}$$

where $\qquad \mathcal{H}(t)\Psi_m(t)=E_m(t)\Psi_m(t). \qquad (3)$

[1] P. Güttinger, Zeits. f. Physik **73**, 169 (1931); see also E. Majorana, Nuovo Cimento **9**, 43 (1932); I. I. Rabi, Phys. Rev. **49**, 324 (1936).

It should be emphasized that $E_m(t)$ and $\Psi_m(t)$ are functions of t only in virtue of the time dependence of the parameters contained in $\mathcal{H}(t)$. The equations which the probability amplitudes $C_m(t)$ satisfy are

$$i\hbar\frac{\partial}{\partial t}C_m(t)-E_m(t)C_m(t)=-i\hbar\sum_m\left(\Psi_m,\frac{\partial\Psi_{m'}}{\partial t}\right)C_{m'}. \tag{4}$$

To put this in a more convenient form, consider $(\partial/\partial t)(\Psi_m, \mathcal{H}\Psi_{m'})$. Evidently,

$$\frac{\partial}{\partial t}(\Psi_m,\mathcal{H}\Psi_{m'})=\left(\Psi_m,\frac{\partial\mathcal{H}}{\partial t}\Psi_{m'}\right)+\left(\frac{\partial\Psi_m}{\partial t},\mathcal{H}\Psi_{m'}\right)+\left(\Psi_m,\mathcal{H}\frac{\partial\Psi_{m'}}{\partial t}\right)$$
$$=\left(\Psi_m,\frac{\partial\mathcal{H}}{\partial t}\Psi_{m'}\right)+(E_m-E_{m'})\left(\Psi_m,\frac{\partial\Psi_{m'}}{\partial t}\right). \tag{5}$$

This expression may also be evaluated as $\delta_{m,m'}(\partial E_m/\partial t)$. Therefore,

$$\left(\Psi_m,\frac{\partial\mathcal{H}}{\partial t}\Psi_{m'}\right)+(E_m-E_{m'})\left(\Psi_m,\frac{\partial\Psi_{m'}}{\partial t}\right)=\delta_{m,m'}\frac{\partial E_m}{\partial t}, \tag{6}$$

whence

$$\left(\Psi_m,\frac{\partial\mathcal{H}}{\partial t}\Psi_m\right)\equiv\left(m\left|\frac{\partial\mathcal{H}}{\partial t}\right|m\right)=\frac{\partial E_m}{\partial t}, \tag{7}$$

and

$$\left(\Psi_m,\frac{\partial\Psi_{m'}}{\partial t}\right)=-\frac{(m|\partial\mathcal{H}/\partial t|m')}{E_m-E_{m'}},\quad m\neq m'. \tag{8}$$

Substituting this latter relation into Eq. (4), we obtain:

$$i\hbar\frac{\partial C_m}{\partial t}-E_mC_m=i\hbar\sum_{m'\neq m}\frac{(m|\partial\mathcal{H}/\partial t|m')}{E_m-E_{m'}}C_{m'}-i\hbar\left(\Psi_m,\frac{\partial\Psi_m}{\partial t}\right)C_m. \quad (9)$$

Save for the last term, these equations agree with Güttinger's. Unfortunately, it does not seem possible to find a general expression for this additional term without actually solving Eq. (3). In the next section, we shall solve this equation for a rather general Hamiltonian which includes most of the cases of interest.

Solution of the Eigenstate Equation

In this section, we shall solve Eq. (3) for a Hamiltonian of the form (discarding irrelevant additive terms):

$$\mathcal{H}(t)=-g\mu_0\mathbf{J}\cdot\mathbf{H}(t), \quad (10)$$

where $\mathbf{J}$ is an arbitrary angular momentum vector in units of $\hbar$, and μ_0 is the Bohr magneton. This is the appropriate description of a magnetic field $\mathbf{H}(t)$ interacting with (a) the magnetic moment of a neutron; (b) the electronic magnetic moment of an atom with zero nuclear moment; (c) the nuclear moment of an atom with vanishing electronic moment. Referred to a vector coordinate system fixed in space, $\mathbf{H}$ may be written

$$\mathbf{H}(t)=H(\mathbf{i}\sin\vartheta\cos\varphi+\mathbf{j}\sin\vartheta\sin\varphi+\mathbf{k}\cos\vartheta), \quad (11)$$

with H, ϑ, and φ functions of the time. Hence,

$$\mathcal{H}=-g\mu_0HJ_\zeta, \quad (12)$$

where

$$J_\zeta=\mathbf{J}\cdot\mathbf{H}/H=J_x\sin\vartheta\cos\varphi+J_y\sin\vartheta\sin\varphi+J_z\cos\vartheta. \quad (13)$$

An eigenstate Ψ_m of J_ζ, satisfying the equation

$$J_\zeta\Psi_m=m\Psi_m,\quad -j\leq m\leq j, \quad (14)$$

will be an eigenstate of $\mathcal{H}$ corresponding to the energy,

$$E_m(t)=-mg\mu_0H(t). \quad (15)$$

The solution of Eq. (4) will, therefore, be a solution of Eq. (3) with the eigenvalue (15).

The substitution, $\Psi_m=e^{-iJ_z\varphi}\Psi_m'$, transforms Eq. (14) into:

$$(\sin\vartheta\cos\varphi e^{iJ_z\varphi}J_xe^{-iJ_z\varphi}+\sin\vartheta\sin\varphi e^{iJ_z\varphi}J_ye^{-iJ_z\varphi}+\cos\vartheta J_z)\Psi_m'=m\Psi_m'. \quad (16)$$

Denoting $e^{iJ_z\varphi}J_xe^{-iJ_z\varphi}$, $e^{iJ_z\varphi}J_ye^{-iJ_z\varphi}$, by $A_x(\varphi)$, $A_y(\varphi)$, respectively, we have

$$\begin{aligned}\frac{dA_x(\varphi)}{d\varphi}&=ie^{iJ_z\varphi}(J_zJ_x-J_xJ_z)e^{-iJ_z\varphi}=-A_y(\varphi),\\ \frac{dA_y(\varphi)}{d\varphi}&=ie^{iJ_z\varphi}(J_zJ_y-J_yJ_z)e^{-iJ_z\varphi}=A_x(\varphi).\end{aligned} \quad (17)$$

Therefore,

$$\begin{aligned}A_x(\varphi)&=A_x(0)\cos\varphi-A_y(0)\sin\varphi,\\ A_y(\varphi)&=A_x(0)\sin\varphi+A_y(0)\cos\varphi,\end{aligned} \quad (18)$$

or

$$\begin{aligned}e^{iJ_z\varphi}J_xe^{-iJ_z\varphi}&=J_x\cos\varphi-J_y\sin\varphi,\\ e^{iJ_z\varphi}J_ye^{-iJ_z\varphi}&=J_x\sin\varphi+J_y\cos\varphi.\end{aligned} \quad (19)$$

Utilizing these relations in Eq. (16), we find that Ψ_m' satisfies an equation independent of φ, *viz.*:

$$(\sin\vartheta J_x+\cos\vartheta J_z)\Psi_m'=m\Psi_m'. \quad (20)$$

The further substitution,

$$\Psi_m'=\exp(-iJ_y\vartheta)\Psi_m^{(0)},$$

yields:

$$J_z\Psi_m^{(0)}=m\Psi_m^{(0)}, \quad (21)$$

with the aid of the relations

$$\begin{aligned}e^{iJ_y\vartheta}J_xe^{-iJ_y\vartheta}&=\cos\vartheta J_x+\sin\vartheta J_z,\\ e^{iJ_y\vartheta}J_ze^{-iJ_y\vartheta}&=-\sin\vartheta J_x+\cos\vartheta J_z.\end{aligned} \quad (22)$$

Consequently, $\Psi_m^{(0)}$ is an eigenstate of the z component of angular momentum corresponding to the eigenvalue m. Combining the two substitutions, we obtain, finally:

$$\Psi_m=e^{-iJ_z\varphi}e^{-iJ_y\vartheta}\Psi_m^{(0)}. \quad (23)$$

Having found the eigenstates, we can substitute directly into Eq. (4), without using the corrected Güttinger equations. One need merely evaluate

$$\left(\Psi_m, \frac{\partial\Psi_{m'}}{\partial t}\right). \text{ Now,}$$

$$\frac{\partial\Psi_{m'}}{\partial t} = -i\dot{\varphi}J_z e^{-iJ_z\varphi}e^{-iJ_y\vartheta}\Psi_{m'}{}^{(0)} - i\dot{\vartheta}e^{-iJ_z\varphi}J_y e^{-iJ_y\vartheta}\Psi_{m'}{}^{(0)}, \quad (24)$$

whence we obtain:

$$\begin{aligned}\left(\Psi_m, \frac{\partial\Psi_{m'}}{\partial t}\right) &= -i\dot{\varphi}(\Psi_m{}^{(0)}, e^{iJ_y\vartheta}J_z e^{-iJ_y\vartheta}\Psi_{m'}{}^{(0)}) - i\dot{\vartheta}(\Psi_m{}^{(0)}, J_y\Psi_{m'}{}^{(0)}) \\ &= -i\dot{\varphi}\cos\vartheta(m|J_z|m') + i\dot{\varphi}\sin\vartheta(m|J_x|m') - i\dot{\vartheta}(m|J_y|m'), \quad (25)\end{aligned}$$

using the second relation of Eq. (22). The only nonvanishing expressions of this type are:

$$\begin{aligned}\left(\Psi_m, \frac{\partial\Psi_m}{\partial t}\right) &= -i\dot{\varphi}\cos\vartheta m, \\ \left(\Psi_m, \frac{\partial\Psi_{m-1}}{\partial t}\right) &= (i\dot{\varphi}\sin\vartheta - \dot{\vartheta})\tfrac{1}{2}((j+m)(j-m+1))^{\frac{1}{2}}, \\ \left(\Psi_m, \frac{\partial\Psi_{m+1}}{\partial t}\right) &= (i\dot{\varphi}\sin\vartheta + \dot{\vartheta})\tfrac{1}{2}((j-m)(j+m+1))^{\frac{1}{2}}. \quad (26)\end{aligned}$$

Hence, the differential equations for the probability amplitudes become:

$$\begin{aligned}i\hbar\frac{\partial C_m}{\partial t} + mg\mu_0 H C_m = &-\hbar\dot{\varphi}\cos\vartheta m C_m \\ &+\tfrac{1}{2}\hbar(\dot{\varphi}\sin\vartheta + i\dot{\vartheta})((j+m)(j-m+1))^{\frac{1}{2}}C_{m-1} \\ &+\tfrac{1}{2}\hbar(\dot{\varphi}\sin\vartheta - i\dot{\vartheta})((j-m)(j+m+1))^{\frac{1}{2}}C_{m+1}. \quad (27)\end{aligned}$$

The Precessing Field

The most general field giving rise to a set of equations for the C_m with constant coefficients satisfies the conditions:

$$\frac{dH}{dt} = 0, \quad \dot{\vartheta} = 0, \quad \dot{\varphi} = \omega = \text{const.}, \quad (28)$$

which is the mathematical description of a field precessing with constant angular velocity ω around the z axis. In this case, Eq. (27) reduces to:

$$\begin{aligned}i\hbar\frac{\partial C_m}{\partial t} = &-m(g\mu_0 H + \hbar\omega\cos\vartheta)C_m \\ &+\tfrac{1}{2}\hbar\omega\sin\vartheta((j+m)(j-m+1))^{\frac{1}{2}}C_{m-1} \\ &+\tfrac{1}{2}\hbar\omega\sin\vartheta((j-m)(j+m+1))^{\frac{1}{2}}C_{m+1}. \quad (29)\end{aligned}$$

To solve this set of equations, let us introduce the eigenstate Φ, defined by

$$\Phi = \sum_m C_m(t)\Psi_m{}^{(0)}. \quad (30)$$

It is easily verified that $\Phi(t)$ satisfies a differential equation of Hamiltonian form, namely:

$$i\hbar\frac{\partial}{\partial t}\Phi = \{-(g\mu_0 H + \hbar\omega\cos\vartheta)J_z + \hbar\omega\sin\vartheta J_x\}\Phi. \quad (31)$$

In terms of the angle Θ, defined by

$$\tan\Theta = \frac{\hbar\omega\sin\vartheta}{\hbar\omega\cos\vartheta + g\mu_0 H}, \quad (32)$$

this may be written

$$i\hbar\frac{\partial}{\partial t}\Phi = -\frac{\hbar\omega\sin\vartheta}{\sin\Theta}(\cos\Theta J_z - \sin\Theta J_x)\Phi. \quad (33)$$

The transformation, $\Phi = e^{iJ_y\Theta}\Phi'$, simplifies this equation to

$$i\hbar\frac{\partial}{\partial t}\Phi' = -\frac{\hbar\omega\sin\vartheta}{\sin\Theta}J_z\Phi', \quad (34)$$

the solution of which is

$$\Phi' = \sum_m C_m'\Psi_m{}^{(0)}e^{-(i/\hbar)E_m' t}. \quad (35)$$

Here, the C_m' are arbitrary integration constants, and

$$\begin{aligned}E_m' &= -m\frac{\hbar\omega\sin\vartheta}{\sin\Theta} \\ &= -m(g^2\mu_0{}^2H^2 + 2g\mu_0 H\hbar\omega\cos\vartheta + \hbar^2\omega^2)^{\frac{1}{2}}. \quad (36)\end{aligned}$$

Therefore,

$$\Phi = e^{iJ_y\Theta}\sum_m C_m'\Psi_m{}^{(0)}e^{-(i/\hbar)E_m' t}, \quad (37)$$

from which we obtain

$$C_m(t)=(\Psi_m^{(0)},\Phi)$$
$$=\sum_{m'}(m|e^{iJ_y\Theta}|m')C_{m'}'e^{-(i/\hbar)E_{m'}'t}. \quad (38)$$

The integration constants C_m' are easily evaluated in terms of the initial conditions. By Eq. (38) we have

$$C_m(0)=\sum_{m'}(m|e^{iJ_y\Theta}|m')C_{m'}', \quad (39)$$

whence we obtain

$$\sum_{m'}(m|e^{-iJ_y\Theta}|m')C_{m'}(0)$$
$$=\sum_{m',m''}(m|e^{-iJ_y\Theta}|m')(m'|e^{iJ_y\Theta}|m'')C_{m''}'$$
$$=C_m', \quad (40)$$

by the matrix law of multiplication. Hence,

$$C_m(t)=\sum_{m',m''}(m|e^{iJ_y\Theta}|m')e^{-(i/\hbar)E_{m'}'t}$$
$$\times(m'|e^{-iJ_y\Theta}|m'')C_{m''}(0). \quad (41)$$

$e^{-(i/\hbar)E_{m}'t}$ is the diagonal matrix element of the operator $e^{(i/\hbar)\gamma tJ_z}$, where γ denotes $(g^2\mu_0^2H^2+2g\mu_0H\hbar\omega\cos\vartheta+\hbar^2\omega^2)^{\frac{1}{2}}$. Therefore,

$$C_m(t)=\sum(m|e^{iJ_y\Theta}|m')(m'|e^{(i/\hbar)\gamma tJ_z}|m'')$$
$$\times(m''|e^{-iJ_y\Theta}|m''')C_{m'''}(0)$$
$$=\sum_{m'}(m|e^{iJ_y\Theta}e^{(i/\hbar)\gamma tJ_z}e^{-iJ_y\Theta}|m')C_{m'}(0). \quad (42)$$

If the system is initially in a state with magnetic quantum number m, i.e., $C_m(0)=1$, the probability that the system is in a state m' after a time t is:

$$W(m,m';t)=|(m'|e^{iJ_y\Theta}e^{(i/\hbar)\gamma tJ_z}e^{-iJ_y\Theta}|m)|^2$$
$$=|(m'|e^{(i/\hbar)\gamma t(J_z\cos\Theta-J_x\sin\Theta)}|m)|^2. \quad (43)$$

It is immediately verified that

$$\sum_{m'}W(m,m';t)=1. \quad (44)$$

In the simple case of $j=\frac{1}{2}$, the matrix element (43) is easily evaluated. An angular momentum with $j=\frac{1}{2}$ can be considered as a spin and represented in terms of the Pauli matrices, i.e., $\mathbf{J}=\frac{1}{2}\boldsymbol{\sigma}$. Since $(\sigma_z\cos\Theta-\sigma_x\sin\Theta)^2=1$, we have

$$W(m,m';t)=\left|\left(m'\left|\cos\frac{\gamma t}{2\hbar}\right.\right.\right.$$
$$\left.\left.\left.+i(\sigma_z\cos\Theta-\sigma_x\sin\Theta)\sin\frac{\gamma t}{2\hbar}\right|m\right)\right|^2. \quad (45)$$

Therefore,

$$W(\tfrac{1}{2},-\tfrac{1}{2};t)=W(-\tfrac{1}{2},\tfrac{1}{2};t)=\sin^2\Theta\sin^2\frac{\gamma t}{2\hbar}$$
$$=\frac{\hbar^2\omega^2\sin^2\vartheta}{g^2\mu_0^2H^2+2g\mu_0H\hbar\omega\cos\vartheta+\hbar^2\omega^2}\sin^2\frac{t}{2\hbar}$$
$$\times(g^2\mu_0^2H^2+2g\mu_0H\hbar\omega\cos\vartheta+\hbar^2\omega^2)^{\frac{1}{2}}. \quad (46)$$

If these transition probabilities are written as $\sin^2\frac{1}{2}\alpha$, it is evident that

$$W(\tfrac{1}{2},\tfrac{1}{2};t)=W(-\tfrac{1}{2},-\tfrac{1}{2};t)=\cos^2\tfrac{1}{2}\alpha. \quad (47)$$

The uncorrected Güttinger equations result in an *umklappwahrsheinlichkeit* which depends only upon ω^2, namely:

$$W(\tfrac{1}{2},-\tfrac{1}{2};t)=\frac{\hbar^2\omega^2\sin^2\vartheta}{g^2\mu_0^2H^2+\hbar^2\omega^2\sin^2\vartheta}\sin^2\frac{t}{2\hbar}$$
$$\times(g^2\mu_0^2H^2+\hbar^2\omega^2\sin^2\vartheta)^{\frac{1}{2}}. \quad (48)$$

A discussion of the measurement of magnetic moments by means of a precessing field, which depends upon the fact that the transition probabilities involve ω explicitly, has been given by Professor Rabi in an accompanying paper.

The evaluation of the matrix element (43) may be carried out, for an arbitrary j, by a method which will not be given here. The results are in complete agreement with those obtained from Majorana's general theorem (see the accompanying paper of Professor Rabi).

In conclusion, the author wishes to express his indebtedness to Dr. Lloyd Motz for pointing out the contradiction between the results obtained by Professor Rabi and those obtained with the Güttinger equations, and to Professor I. I. Rabi for his continued interest throughout the course of this investigation.