TREATMENT OF THE TIME-DEPENDENT MULTI-LEVEL SYSTEM IN QUANTUM MECHANICS ON THE BASIS OF A NEW METHOD OF CALCULATION

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As a consequence of a new foundation of quantum theory, developed by us recently, a new method of calculation for treating time-dependent quantum mechanical problems evolved. Here this method is applied to a multi-level system under time-dependent influences. After presenting the general features of the method the formalism is applied to a 2-level system.

1. *New time-dependent method of calculation*

Recently [1, 2] we presented a new foundation of quantum theory. As a consequence we proposed a new time-dependent method of calculation, the main features of which will be repeated here.

A time-dependent quantum mechanical system may be described by the Schrödinger equation

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

The wave function Ψ is according to

$$\Psi = \sum_{\sigma} S_{\sigma}(t)\phi_{\sigma} \tag{2}$$

expanded with respect to the time-dependent eigenfunctions ϕ_σ obeying the time-dependent eigenvalue equation

$$H\phi_\sigma = h_\sigma \phi_\sigma, \tag{3}$$

where h_σ are the time-dependent eigenvalues (in the above quoted papers we denoted $\phi_\sigma = \hat{\varphi}_\sigma$).

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Orthonormality and completeness read

$$\text{a)} \int \phi_\sigma^* \phi_\mu dq = \delta_{\sigma\mu}, \quad \text{b)} \sum_\sigma \phi_\sigma^*(q', t)\phi_\sigma(q, t) = \delta(q'-q). \tag{4}$$

Hence from the normalization of the wave function we obtain

$$\sum_\sigma S_\sigma^* S_\sigma = 1. \tag{5}$$

Inserting the Fourier expansion (2) into (1) and using (4a) we find the following infinite system of differential equations for the coefficients S_μ:

$$\dot{S}_\mu - \frac{1}{i\hbar} h_\mu S_\mu + \sum_\sigma S_\sigma \varphi_{\mu\sigma} = 0, \tag{6}$$

where

$$\varphi_{\mu\sigma} = \int \phi_\mu^* \frac{\partial \phi_\sigma}{\partial t} dq = -\varphi_{\sigma\mu}^*. \tag{7}$$

For solving (6) we need the time-dependent eigenvalues h_μ and the corresponding time-dependent eigenfunctions ϕ_μ, i.e. we have to solve the eigenvalue problem (3).

For this purpose we decompose the Hamiltonian into a time-independent term and a time-dependent term:

$$H = H^0 + H^t(t) \tag{8}$$

without any restriction concerning the order of magnitude of the contribution. Similarly we decompose

$$h_\mu = E_\mu + h_\mu^t, \tag{9}$$

where the constant eigenvalues E_μ are determined from

$$H^0 \chi_\mu = E_\mu \chi_\mu. \tag{10}$$

We assume that this stationary problem has already been solved and that the time-independent eigenfunctions χ_μ are orthonormal and complete:

$$\text{a)} \int \chi_\sigma^* \chi_\mu dq = \delta_{\sigma\mu}, \quad \text{b)} \sum_\sigma \chi_\sigma^*(q')\chi_\sigma(q) = \delta(q'-q). \tag{11}$$

Let us now use the following expansion

$$\phi_\nu = \sum_\lambda c_{\nu\lambda}(t)\chi_\lambda. \tag{12}$$

Orthonormality and completeness of both sets of eigenfunctions lead to the relations

$$\text{a)} \sum_\lambda c_{\sigma\lambda}^* c_{\mu\lambda} = \delta_{\mu\sigma}, \quad \text{b)} \sum_\lambda c_{\lambda\sigma}^* c_{\lambda\mu} = \delta_{\mu\sigma}. \tag{13}$$

Furthermore, from (7) we find

$$\text{a)}\quad \varphi_{\mu\nu} = \sum_{\lambda} c^*_{\mu\lambda}\dot{c}_{\nu\lambda}, \qquad \text{b)}\quad \dot{c}_{\nu\tau} = \sum_{\mu} c_{\mu\tau}\varphi_{\mu\nu}. \tag{14}$$

Inserting (12) into (3) and using the orthonormality (11a) we obtain the following infinite linear and homogeneous system of equations for the expansion coefficients $c_{\nu\lambda}$:

$$\sum_{\lambda} c_{\nu\lambda}[\delta_{\sigma\lambda}(E_\lambda - E_\nu) + H_{\sigma\lambda} - h^t_\nu \delta_{\sigma\lambda}] = 0, \tag{15}$$

where

$$H_{\sigma\lambda} = \int \chi^*_\sigma H^t \chi_\lambda dq = \langle E_\sigma | H^t | E_\lambda \rangle = H^*_{\lambda\sigma}. \tag{16}$$

Assuming that the convergence properties are fulfilled, the secular equation

$$\det |H_{\sigma\lambda} + \delta_{\sigma\lambda}(E_\lambda - E_\nu - h^t_\nu)| = 0 \tag{17}$$

for the eigenvalue contributions h^t_ν follows from (15).

For the purpose of comparison it is useful to present the situation in Dirac's perturbation theory: In this method, using the above introduced symbols, the Fourier expansion

$$\Psi = \sum_{\mu} d_\mu(t)\chi_\mu = \sum_{\mu} D_\mu(t) e^{-\frac{iE_\mu t}{\hbar}} \chi_\mu, \tag{18}$$

where the conditions

$$\sum_{\mu} D^*_\mu D_\mu = \sum_{\mu} d^*_\mu d_\mu = 1 \tag{19}$$

hold, leads to the system of differential equations

$$\dot{d}_\mu - \frac{1}{i\hbar} d_\mu E_\mu - \frac{1}{i\hbar} \sum_{\sigma} d_\sigma H_{\mu\sigma} = 0, \tag{20}$$

or because of the relation

$$d_\mu = D_\mu e^{-\frac{iE_\mu t}{\hbar}} \tag{21}$$

to

$$\dot{D}_\mu - \frac{1}{i\hbar} \sum_{\sigma} D_\sigma e^{\frac{i}{\hbar}(E_\mu - E_\sigma)t} H_{\mu\sigma} = 0. \tag{22}$$

The equations (20) or (22) are the counterparts of our system of differential equations (6).

2. Matrix elements, transition probability, probability of presence and initial conditions

The physical background of Dirac's perturbation theory is the stationary system which is affected by a (relatively weak) time-dependent perturbation during a time interval (this basis also corresponds to the ideas of the S-matrix theory). Therefore the matrix elements are defined with respect to the Fourier expansion (18).

For instance, the matrix elements of the dipole moment follow from the expectation value

$$\int \Psi^* \vec{r} \Psi dq = \sum_{\mu,\nu} d_\mu^* d_\nu \int \chi_\mu^* \vec{r} \chi_\nu dq = \frac{1}{e} \sum_{\mu,\nu} d_\mu^* d_\nu \vec{m}_{\mu\nu} \tag{23}$$

in the form of

$$\vec{m}_{\mu\nu} = e \int \chi_\mu^* \vec{r} \chi_\nu dq. \tag{24}$$

Let us take as another example the transition probabilities for the transition from the initial state $\Psi_{(i)}|_{t=0} = \chi_i$ before the perturbation to the final state χ_λ after the perturbation:

$$w_{\lambda(i)} = |(\chi_\lambda, \Psi_{(i)})|^2 = |D_{\lambda(i)}|^2 = \sum_{\sigma,\kappa} S_{\sigma(i)}^* S_{\kappa(i)} c_{\sigma\lambda}^* c_{\kappa\lambda}. \tag{25}$$

According to the interpretation of our foundation of quantum theory in the general case of a time-dependent system, on principle an adiabatic process takes place because of the temporal development of the time-dependent eigenfunctions. Beyond that such a system, e.g. the time-dependent levels, can of course be tested by time-dependent test methods, for instance by means of radiation, similarly to the methods of traditional quantum physics but here on a new level.

As a logical consequence this point of view implies referring to the Fourier expansion (2),

Taking again the example of the matrix elements of the dipole moment we are led to the formula

$$\vec{M}_{\mu\nu} = e \int \phi_\mu^* \vec{r} \phi_\nu dq \tag{26}$$

obtained by considering the expectation value (23) in another decomposition, namely

$$\int \Psi^* \vec{r} \Psi dq = \sum_{\mu,\nu} S_\mu^* S_\nu \int \phi_\mu^* \vec{r} \phi_\nu dq = \frac{1}{e} \sum_{\mu,\nu} S_\mu^* S_\nu \vec{M}_{\mu\nu}. \tag{27}$$

The two kinds of matrix elements are connected by

$$\vec{M}_{\mu\nu} = \sum_{\sigma,\lambda} c_{\mu\sigma}^* c_{\nu\lambda} \vec{m}_{\sigma\lambda}. \tag{28}$$

Consequently, the probability of presence (Aufenthaltswahrscheinlichkeit) of a system, which started from the (time-dependent) initial state $\Psi_{(i)}|_{t=0} = \phi_i(t = 0)$, in the (time-dependent) final state ϕ_λ, where according to our conception the temporal influence is permanently present as a rule, has to be defined by

$$W_{\lambda(i)} = |(\phi_\lambda, \Psi_{(i)})|^2 = |S_{\lambda(i)}|^2. \tag{29}$$

The above fixation of the initial state, namely

$$\Psi_{(i)}|_{t=0} = \phi_i(t = 0)$$

leads us, if we furthermore assume, that $H^t(t = 0) = 0$ may be valid, to the coincidence

$$\phi_\mu(t = 0) = \chi_\sigma, \text{ i.e. } c_{\sigma\lambda}(t = 0) = \delta_{\sigma\lambda} \quad \text{and} \quad S_{\sigma(i)}(t = 0) = \delta_{\sigma i}. \tag{30}$$

Using these results from (15) follows

$$H_{\sigma\nu}(t = 0) = h_\nu^t(t = 0)\delta_{\sigma\nu} = 0. \tag{31}$$

The choice of the transition probability (25) or of the probability of presence (29) depends on the concrete experiment being performed.

3. Application to an N-level system

In Section 1 we presented the theory for the general case of an infinite-dimensional Hilbert space. In practical cases often essential information can already be gained, if a finite-dimensional space (N-level system with $N = 2, 3...$) is considered. According to our theory in the case of a time-dependent Hamiltonian describing the system, the eigenvalues must be calculated from the secular equation (17) being an algebraic equation of degree N for the quantities h_ν^t. Thus we obtain the N roots $h_{\nu(\alpha)}^t$ with $\alpha = 1, 2, ..., N$ for each value of $\nu = 1, 2, ... ,N$. This set of N^2 values reduces to N values, if we take into account that in the special case of time-independency the correspondence

$$h_\nu \to E_\nu, \text{ i.e. } h_\nu^t \to 0 \tag{32}$$

has to be valid, presupposed that degeneracies don't occur (Fig. 1).

According to (15) for a fixed eigenvalue we find a fixed set of coefficients $c_{\gamma\lambda}$ and therefore, according to (12), the corresponding eigenfunction. The fact why N^2 roots appear

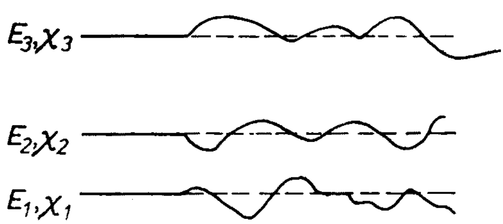

Fig. 1

can be explained as a result of an admissible degeneracy, the maximal degree of which is determined according to the situation mentioned above.

The shift of the levels according to Fig. 1 is a direct consequence of our basic ideas concerning the time-dependent behaviour of quantum systems. If there is any degeneracy, we have to expect a splitting of the spectral lines. This effect, the nature of which is quite different, is usually called "dynamical Stark effect" (compare [3]).

To present our method in detail, we refer to the special case of a 2-level system in the following sections.

4. Eigenvalue problem of the 2-level system.

With a periodic time influence the 2-level problem occurs in different fields of physics (magnetic nuclear resonance, non-linear optics, etc.). Therefore a voluminous literature exists, particularly because the problem has not been exactly solved up to now. Rabi [4] treated the problem approximately, using the so-called "rotating wave approximation". Bloch and Siegert [5] succeeded in an integral equation approach, with the help of which they could find a better approximation than the "rotating wave approximation". They predicted the so-called Bloch–Siegert shift. Some new results are contained in a paper by Shirley [6].

In the following we treat the problem on the basis of our theory.

According to our previous conventions let us begin with the nondegenerate 2-level system:

$$\chi_1 \to E_1,\ \chi_2 \to E_2 \qquad (\Delta E = E_2 - E_1 > 0).$$

The equation (12) reads

$$\text{a)}\quad \phi_1 = c_{11}\chi_1 + c_{12}\chi_2, \qquad \text{b)}\quad \phi_2 = c_{21}\chi_1 + c_{22}\chi_2, \tag{33}$$

while (15) takes the form

$$\left.\begin{aligned} c_{11}(H_{11}-h_1^t)+c_{12}H_{12} &= 0 \\ c_{11}H_{12}^*+c_{12}(H_{22}+\Delta E-h_1^t) &= 0 \end{aligned}\right\}\ \text{system I,} \tag{34}$$

and

$$\left.\begin{aligned} c_{21}(H_{11}-\Delta E-h_2^t)+c_{22}H_{12} &= 0 \\ c_{21}H_{12}^*+c_{22}(H_{22}-h_2^t) &= 0 \end{aligned}\right\}\ \text{system II.} \tag{35}$$

The secular equations of both systems lead to the time-dependent eigenvalue contributions

$$h_1^t = \tfrac{1}{2}\left[H_{11}+H_{22}+\Delta E-\sqrt{(H_{11}-H_{22}-\Delta E)^2+4|H_{12}|^2}\right], \tag{36}$$

$$h_2^t = \tfrac{1}{2}\left[H_{11}+H_{22}-\Delta E+\sqrt{(H_{11}-H_{22}-\Delta E)^2+4|H_{12}|^2}\right] \tag{37}$$

which fulfill the condition (32).

For the following it is convenient to introduce the quantity

$$C = C^* = \tfrac{1}{2}\left[H_{22}-H_{11}+\Delta E-\sqrt{(H_{11}-H_{22}-\Delta E)^2+4|H_{12}|^2}\right]. \tag{38}$$

Solving the systems of equations I and II we find

$$\text{a)}\quad c_{12} = c_{11}\frac{C}{H_{12}}, \qquad \text{b)}\quad c_{21} = -c_{22}\frac{C}{H_{12}^*}, \tag{39}$$

with the help of which the time-dependent eigenfunctions (33) take the form

$$\text{a)}\quad \phi_1 = c_{11}\left(\chi_1 + \frac{C}{H_{12}}\chi_2\right), \qquad \text{b)}\quad \phi_2 = c_{22}\left(\chi_2 - \frac{C}{H_{12}^*}\chi_1\right). \tag{40}$$

Furthermore, from the relations (13) we obtain

$$\text{a)}\quad |c_{11}|^2 = |c_{22}|^2 = \frac{1}{1+\dfrac{C^2}{|H_{12}|^2}}, \quad \text{i.e.} \quad \text{b)}\quad |c_{12}| = |c_{21}|. \tag{41}$$

After some short calculations one straightforwardly finds that the eigenfunctions (40) fulfill the eigenvalue equation (3) and the orthonormality (4a).

From (2) we notice that the phase factor of the eigenfunction can be chosen arbitrarily without any restriction, because it can be absorbed in the coefficients S_σ. Therefore for simplicity we put

$$\text{a)}\quad c_{11} = c_{22} = c_0 = \frac{1}{\sqrt{1+\dfrac{C^2}{|H_{12}|^2}}}, \quad \text{i.e.} \quad \text{b)}\quad c_{12} = c_0 \frac{C}{H_{12}},$$

$$\text{c)}\quad c_{21} = -c_0 \frac{C}{H_{12}^*} = -c_{12}^*. \tag{42}$$

5. System of differential equations for the Fourier coefficients of the 2-level system

Let us first calculate the quantities (7) from (40):

$$\text{a)}\quad \varphi_{11} = c_0\dot{c}_0 + c_{12}^*\dot{c}_{12}, \quad \text{b)}\quad \varphi_{12} = -c_0\dot{c}_{12}^* + c_{12}^*\dot{c}_0,$$

$$\text{c)}\quad \varphi_{21} = -c_{12}\dot{c}_0 + c_0\dot{c}_{12}. \quad \text{d)}\quad \varphi_{22} = c_0\dot{c}_0 + c_{12}\dot{c}_{12}^*. \tag{43}$$

From these results we get

$$\varphi_{11} = \varphi_{22}^*. \tag{44}$$

Furthermore, we realize that the condition (7) is fulfilled:

$$\text{a)}\quad \varphi_{11} = -\varphi_{11}^*, \quad \text{b)}\quad \varphi_{12} = -\varphi_{21}^*, \quad \text{c)}\quad \varphi_{22} = -\varphi_{22}^*. \tag{45}$$

Expressing the coefficients $c_{\mu\nu}$ by means of (42) we find

$$\varphi_{11} = -\tfrac{1}{2}\, c_0^2 C^2 \left[\frac{d}{dt}\frac{1}{|H_{12}|^2} - \frac{H_{12}}{H_{12}^*}\frac{d}{dt}\frac{1}{(H_{12})^2}\right], \tag{46}$$

$$\varphi_{12} = -c_0^2 \frac{d}{dt}\left(\frac{C}{H_{12}^*}\right). \tag{47}$$

For the 2-level system from (6) we obtain the system of differential equations

$$\text{a)}\quad \dot{S}_1 - \frac{h_1}{i\hbar} S_1 + \varphi_{11}S_1 + \varphi_{12}S_2 = 0, \quad \text{b)}\quad \dot{S}_2 - \frac{h_2}{i\hbar} S_2 + \varphi_{11}^* S_2 - \varphi_{12}^* S_1 = 0 \tag{48}$$

for the coefficients $S\sigma$. The quantities (36), (37) as well as (46), (47) should be inserted. From (48) we conclude that the condition (5)

$$S_1^*S_1+S_2^*S_2 = 1 \tag{49}$$

is fulfilled.

To solve the system (48) we rearrange (48a)

$$S_2 = -\frac{1}{\varphi_{12}}\left[\dot{S}_1-\frac{h_1}{i\hbar}S_1+\varphi_{11}S_1\right] \tag{50}$$

and substitute in (48b), the result being

$$\ddot{S}_1-\dot{S}_1\left[\frac{h_1+h_2}{i\hbar}+\frac{\dot{\varphi}_{12}}{\varphi_{12}}\right]+S_1\left[\dot{\varphi}_{11}-\varphi_{11}\frac{\dot{\varphi}_{12}}{\varphi_{12}}-\frac{\dot{h}_1}{i\hbar}+\frac{h_1}{i\hbar}\left(\frac{\dot{\varphi}_{12}}{\varphi_{12}}+\varphi_{11}\right)\right.$$
$$\left.-\frac{h_2}{i\hbar}\varphi_{11}-\frac{h_1h_2}{\hbar^2}+|\varphi_{11}|^2+|\varphi_{12}|^2\right] = 0. \tag{51}$$

For mathematical reasons it is convenient to pass over to the new coefficients s_σ defined by

$$S_\sigma = s_\sigma e^{i\chi\sigma}, \tag{52}$$

where

$$\text{a)}\quad \hat{\chi}_1 = \int\limits_{t=0}^{t}\left(i\varphi_{11}-\frac{h_1}{\hbar}\right)dt+\chi_{10},\qquad \text{b)}\quad \hat{\chi}_2 = \int\limits_{t=0}^{t}\left(i\varphi_{11}^*-\frac{h_2}{\hbar}\right)dt+\chi_{20}$$

$$(\chi_\bullet = \chi_{2\bullet}-\chi_{1\bullet}) \tag{53}$$

and because of (49)

$$s_1^*s_1+s_2^*s_2 = 1 \tag{53c}$$

is valid. Under these conditions the system (48) takes the much simpler form

$$\text{a)}\quad \dot{s}_1 = -s_2\varphi_{12}e^{i(\hat{\chi}_2-\hat{\chi}_1)},\qquad b)\quad \dot{s}_2 = s_1\varphi_{12}^*e^{-i(\hat{\chi}_2-\hat{\chi}_1)}, \tag{54}$$

while instead of (51) we obtain

$$\ddot{s}_1+\dot{s}_1\left[\frac{h_1-h_2}{i\hbar}-2\varphi_{11}-\frac{\dot{\varphi}_{12}}{\varphi_{12}}\right]+s_1|\varphi_{12}|^2 = 0. \tag{55}$$

For comparison with Dirac's method it is useful to apply (22) to the 2-level system. We find $\left(\Delta\omega = \frac{\Delta E}{\hbar}\right)$

$$\text{a)}\quad \dot{D}_1 = \frac{1}{i\hbar}H_{11}D_1+\frac{1}{i\hbar}H_{12}D_2e^{-i\Delta\omega t},\qquad \text{b)}\quad \dot{D}_2 = \frac{1}{i\hbar}H_{12}^*D_1e^{i\Delta\omega t}+\frac{1}{i\hbar}H_{22}D_2, \tag{56}$$

where

$$D_1^* D_1 + D_2^* D_2 = 1, \tag{56c}$$

and by elimination of D_2 the differential equation

$$\ddot{D}_1 + \frac{i}{\hbar}\dot{D}_1\left[H_{11}+H_{22}+\Delta\omega\hbar+i\hbar\frac{\dot{H}_{12}}{H_{12}}\right] - \frac{D_1}{\hbar^2}\left[H_{11}H_{22}-|H_{12}|^2 - \frac{i\hbar}{H_{12}}(\dot{H}_{11}H_{12}-H_{11}\dot{H}_{12})+\Delta\omega\hbar H_{11}\right] = 0 \tag{57}$$

for D_1 as a counterpart to our result (55). In concrete cases of application it has to be decided whether our method using (55) or Dirac's method using (57) is of greater advantage.

Proceeding this section we notice the relationships between Dirac's coefficients D_μ and our coefficients S_μ:

$$\text{a)}\quad D_1 = c_0 e^{\frac{iE_1 t}{\hbar}}\left(S_1 - \frac{C}{H_{12}^*}S_2\right), \qquad \text{b)}\quad D_2 = c_0 e^{\frac{iE_2 t}{\hbar}}\left(S_2 + \frac{C}{H_{12}}S_1\right) \tag{58}$$

resp.

$$\text{a)}\quad S_1 = c_0 e^{-\frac{iE_1 t}{\hbar}}\left(D_1 + \frac{C}{H_{12}^*}e^{-i\Delta\omega t}\right), \qquad \text{b)}\quad S_2 = c_0 e^{-\frac{iE_2 t}{\hbar}}\left(D_2 - \frac{C}{H_{12}}e^{i\Delta\omega t}D_1\right). \tag{59}$$

The initial conditions (30) take the form

$$\text{a)}\quad D_1(t=0) = 1, \qquad \text{b)}\quad D_2(t=0) = 0 \tag{60}$$

resp.

$$\text{a)}\quad S_1(t=0) = c_0(t=0) = 1, \qquad \text{b)}\quad S_2(t=0) = -c_0(t=0)\left(\frac{C}{H_{12}}\right)_{t=0} = 0. \tag{61}$$

For the transition probabilities (25) resp. (29) we find

$$w_{2(1)} = |D_{2(1)}|^2 = c_0^2\left[|S_2|^2 + \frac{C^2}{|H_{12}|^2}|S_1|^2 + C\left(\frac{S_1^* S_2}{H_{12}^*} + \frac{S_2^* S_1}{H_{12}}\right)\right] \tag{62}$$

resp.

$$W_{2(1)} = |S_{2(1)}|^2. \tag{63}$$

6. *Quantum mechanical system under the influence of an electromagnetic wave*

Up to now the above theory was developed without taking into consideration a specified time-dependency. In this section we treat the case of an electromagnetic wave, described by

$$\vec{A} = \vec{A}_0 \sin(\vec{k}\vec{r} - \omega t), \tag{64}$$

where

$$\vec{A}^{+} = \vec{A}, \quad \vec{A}_0\vec{k} = 0 \text{ (Coulomb gauge)}, \tag{65}$$

which acts on a quantum particle. Including the interaction in a rather general case the Hamiltonian is given by

$$H = \frac{1}{2m_0}\left(\vec{P} - \frac{e}{c}\vec{A}\right)^2 + V + \mu\vec{\sigma}\left[\vec{B} + \frac{1}{2m_0c}\vec{E}\times\left(\vec{P} - \frac{e}{c}\vec{A}\right)\right] \tag{66}$$

(m_0 mass, e electric charge, $\vec{\sigma}$ spin vector, μ magnetic moment). If we assume that the potential energy $V = e\varphi$ is time-independent, according to the decomposition (8) we are led to the identification

$$H^0 = \frac{1}{2m_0}\vec{P}^2 + V, \tag{67}$$

$$H^{\mathfrak{t}} = H^{\mathfrak{t}}_P + H^{\mathfrak{t}}_A + H^{\mathfrak{t}}_S, \tag{68}$$

where

$$\text{a)} \quad H^{\mathfrak{t}}_P = -\frac{e}{2m_0c}(\vec{P}\vec{A} + \vec{A}\vec{P}), \qquad \text{b)} \quad H^{\mathfrak{t}}_A = \frac{e^2\vec{A}^2}{2m_0c^2},$$

$$\text{c)} \quad H^{\mathfrak{t}}_S = \mu\vec{\sigma}\left[\vec{B} + \frac{1}{2m_0c}\vec{E}\times\left(\vec{P} - \frac{e}{c}\vec{A}\right)\right]. \tag{69}$$

Inserting the expression (64) we find

$$H^{\mathfrak{t}}_P = ae^{i\omega t} + a^{+}e^{-i\omega t}, \tag{70}$$

where

$$a = \frac{e\vec{A}_0}{2m_0ci}e^{-i\vec{k}\vec{r}}\vec{P}. \tag{71}$$

Further we obtain

$$H^{\mathfrak{t}}_A = \frac{e^2\vec{A}_0^2}{2m_0c^2}\sin^2(\vec{k}\vec{r} - \omega t) \tag{72}$$

and

$$H^{\mathfrak{t}}_S = \mu\vec{\sigma}\left[\vec{k}\times\vec{A}_0\cos(\vec{k}\vec{r} - \omega t) - \frac{e}{2m_0c^2}\vec{A}_0\times \operatorname{grad}\varphi\sin(\vec{k}\vec{r} - \omega t)\right.$$
$$\left. + \frac{1}{2m_0c}\left\{-\operatorname{grad}\varphi + \frac{\omega}{c}\vec{A}_0\cos(\vec{k}\vec{r} - \omega t)\right\}\times\vec{P}\right]. \tag{37}$$

Passing over to the dipole approximation the matrix elements (16) take the form

$$H_{P\mu\sigma} = \langle E_\mu | H_P^t | E_\sigma \rangle = v_{\mu\sigma} \sin \omega t, \tag{74}$$

where

$$v_{\mu\sigma} = \frac{e\vec{A}_0 \hbar}{i m_0 c} \int \chi_\mu^* \operatorname{grad} \chi_\sigma dq = v_{\sigma\mu}^*. \tag{75}$$

Further results are

$$H_{A\mu\sigma} = \frac{e^2 \vec{A}_0^2}{2 m_0 c^2} \delta_{\mu\sigma} \sin^2 \omega t \tag{76}$$

and

$$H_{S\mu\sigma} = \mu\vec{\sigma} \left[\vec{k} \times \vec{A}_0 \delta_{\mu\sigma} \cos \omega t + \frac{e}{2 m_0 c^2} \sin \omega t \vec{A}_0 \times \int \chi_\mu^* \operatorname{grad} \varphi \chi_\sigma dq \right.$$
$$\left. - \frac{\hbar}{2 m_0 c i} \int \chi_\mu^* \operatorname{grad} \varphi \times \operatorname{grad} \chi_\sigma dq + \frac{\omega \hbar}{2 m_0 c^2 i} \cos \omega t \vec{A}_0 \times \int \chi_\mu^* \operatorname{grad} \chi_\sigma dq \right]. \tag{77}$$

7. *A special model*

7.1. General

To study some features of the theory pointed out above we consider the following special case which often is applied in experimental physics as a model:

$$\text{a)} \quad H_{11} = 0, \quad \text{b)} \quad H_{22} = 0 \text{ (no permanent moments),}$$
$$\text{c)} \quad H_{12} = v \sin \omega t = v_0 e^{i\lambda} \sin \omega t \quad (v = \text{const}). \tag{78}$$

Hence from (38, (46) and (47) we find

$$C = \frac{\hbar \Delta\omega}{2} [1 - \sqrt{1 + 4 V_0^2 \sin^2 \omega t}] \quad \left(V_0 = \frac{v_0}{\hbar \Delta\omega} \right), \tag{79}$$

$$\text{a)} \quad \varphi_{11} = 0, \quad \text{b)} \quad \varphi_{12} = \frac{V_0 e^{i\lambda} \omega \cos \omega t}{1 + 4 V_0^2 \sin^2 \omega t}. \tag{80}$$

In the case of an electromagnetic wave the parameter V_0 has the following physical meaning

$$V_0 = \frac{\mu E_0}{\omega \hbar}$$

(μ dipole moment, E_0 wave amplitude, ω wave frequency).

Under these circumstances from (55) and (57) there result the differential equations

$$\ddot{s}_1+\dot{s}_1\left[i\Delta\omega\sqrt{1+4V_0^2\sin^2\omega t}+\omega\tan\omega t+\frac{8V_0^2\omega\sin\omega t\cos\omega t}{1+4V_0^2\sin^2\omega t}\right]$$

$$+s_1\frac{V_0^2\omega^2\cos^2\omega t}{(1+4V_0^2\sin^2\omega t)^2}=0 \tag{81}$$

and

$$\ddot{D}_1+\dot{D}_1[i\Delta\omega-\omega\cot\omega t]+D_1\frac{v_0^2\sin^2\omega t}{\hbar^2}=0. \tag{82}$$

7.2. Weak intensity ($V_0^2 \ll 1$)

This case can be treated in different ways: First, we can immediately apply the perfect formulae from literature presenting Dirac's perturbation theory. In first order one has to perform the integration

$$D_{2(1)}=-\frac{iv^*}{\hbar}\int_0^t\sin\omega t e^{i\Delta\omega t}dt \tag{83}$$

and then finds from (62)

$$w_{2(1)}=\frac{v_0^2}{2\hbar^2[\omega^2-(\Delta\omega)^2]^2}[3\omega^2+(\Delta\omega)^2+\{\omega^2-(\Delta\omega)^2\}\cos 2\omega t$$

$$-2\omega(\omega-\Delta\omega)\cos(\omega+\Delta\omega)t-2\omega(\omega+\Delta\omega)\cos(\omega-\Delta\omega)t] \tag{84}$$

and further near resonance ($\varrho=\omega-\Delta\omega$)

$$w_{2(1)}|_{\text{res}}=\frac{v_0^2}{\hbar^2\varrho^2}\sin^2\left(\frac{\varrho t}{2}\right). \tag{85}$$

Second, we can also approach this problem, starting from equation (81) which leads to the differential equation

$$\ddot{s}_1+\dot{s}_1[i\Delta\omega+\omega\tan\omega t]+s_1V_0^2\omega^2\cos^2\omega t=0 \tag{86}$$

with the solutions

$$s_1=s_{10}+V_0^2s_{11}(t)\qquad(s_{10}=\text{const}), \tag{87}$$

where

$$s_{11}(t)=\frac{\Lambda_0}{2}\left(\frac{e^{i(\omega-\Delta\omega)t}}{\omega-\Delta\omega}-\frac{e^{i(\omega+\Delta\omega)t}}{\omega+\Delta\omega}\right)-\frac{s_{10}\omega^2}{4i}\left(\frac{e^{2i\omega t}}{2i\omega(\omega+\Delta\omega)}+\frac{e^{-2i\omega t}}{2i\omega(\omega-\Delta\omega)}\right.$$

$$\left.+\frac{t}{\omega+\Delta\omega}-\frac{t}{\omega-\Delta\omega}\right), \tag{88}$$

and

$$s_2 = -iV_0 e^{-i(\lambda+\chi_0)} \left[\frac{\Lambda_0}{\omega} + \frac{s_{10}\omega}{2} \left(\frac{e^{i(\omega+\Delta\omega)t}}{\omega+\Delta\omega} - \frac{e^{-i(\omega-\Delta\omega)t}}{\omega-\Delta\omega} \right) \right]. \tag{89}$$

According to (62) we also find (84).

For comparison we also note down the result for our transition probability (63)

$$W_{2(1)} = \frac{V_0^2\omega^2}{2[\omega^2-(\Delta\omega)^2]^2} [\omega^2+3(\Delta\omega)^2 - \{\omega^2-(\Delta\omega)^2\} \cos 2\omega t$$

$$+2\Delta\omega(\omega-\Delta\omega) \cos(\omega+\Delta\omega)t - 2\Delta\omega(\omega+\Delta\omega)\cos(\omega-\Delta\omega)t]. \tag{90}$$

7.3. Strong intensity ($V_0 \gg 1$)

In this case our differential equation (81) shows significant advantages in contrast to (82). Namely, from (81) we get

$$\ddot{s}_1 + \dot{s}_1 [i\Delta\omega \sqrt{1+4V_0^2 \sin^2 \omega t} + \omega \tan \omega t + 2\omega \cot \omega t] = 0. \tag{91}$$

Integration yields

$$\dot{s}_1 = \alpha \frac{\cos \omega t}{\sin^2 \omega t} e^{-i\Delta\omega \int \sqrt{1+4V_0^2 \sin^2 \omega t}\, dt}. \tag{92}$$

Hence from (54a) we find

$$s_2 = \text{const.} \tag{93}$$

From (53c) with the aid of this result we can conclude

$$s_1 = \text{const, i. e.} \quad \alpha = 0. \tag{94}$$

Considering the initial conditions (61) which here take the form

$$\text{a) } s_1(t=0) = 1, \quad \text{b) } s_2(t=0) = 0 \tag{95}$$

we finally find for this limiting case $V_0 \to \infty$

$$\text{a) } s_1 = 1, \quad \text{b) } s_2 = 0. \tag{96}$$

According to (62) and (63) for the transition probabilities we obtain without averaging straightforwardly

$$\text{a) } w_{2(1)} = \tfrac{1}{2}\,(t>0), \quad \text{b) } W_{2(1)} = 0 \quad (t>0). \tag{97}$$

8. Rotating wave approximation

Only for the purpose of illustration let us finally sketch the situation in the "rotating wave approximation".

Because of the complications in an exact treating of the equation (82) in contrast to (78) the following simplified problem is studied:

$$\text{a) } H_{11} = 0, \quad \text{b) } H_{22} = 0, \quad \text{c) } H_{12} = ue^{i\omega t} = u_0 e^{i\omega t + i\tau}. \tag{98}$$

In this case the differential equations (56a, b) lead to

$$\text{a)}\quad \dot{D}_1 = \frac{D_2}{i\hbar}\,[e^{i(\omega-\Delta\omega)t}\langle E_1|a|E_2\rangle + \underline{e^{-i(\omega+\Delta\omega)t}\langle E_1|a^+|E_2\rangle}],$$

$$\text{b)}\quad \dot{D}_2 = \frac{D_1}{i\hbar}\,[\underline{e^{i(\omega+\Delta\omega)t}\langle E_2|a|E_1\rangle} + e^{-i(\omega-\Delta\omega)t}\langle E_2|a^+|E_1\rangle]. \tag{99}$$

The next simplifying step consists in setting

$$\langle E_1|a^+|E_2\rangle = 0, \qquad \text{i. e. } \langle E_2|a|E_1\rangle = 0, \tag{100}$$

justified by the fact that near resonance ($\omega \approx \Delta\omega$) the underlined terms occur with double frequency. Under these circumstances the differential equation (57) exhibits constant coefficients and can be solved in the usual way with the result ("rotating wave approximation" [4]):

$$w_{2(1)} = \frac{4u_0^2}{\hbar^2\left(\varrho^2 + \dfrac{4u_0^2}{\hbar^2}\right)}\sin^2\left(\frac{t}{2}\sqrt{\varrho^2 + \frac{4u_0^2}{\hbar^2}}\right), \tag{101}$$

Comparing (78) with (98), one states a correspondence between u_0 and v_0. Because of the neglected terms the relation

$$v_0^2 = 4u_0^2 \tag{102}$$

is valid, as it can be seen from (85) and (101) for the limiting case $v_0 \to 0$.

The same results follow from our method, taking into account

$$\text{a)}\quad |H_{12}|^2 = u_0^2, \qquad \text{b)}\quad C = \frac{\Delta\omega\hbar}{2}\left[1 - \sqrt{1 + \frac{4u_0^2}{(\Delta\omega)^2\hbar^2}}\right],$$

$$\text{c)}\quad \varphi_{11} = -\frac{ic_0^2C^2\omega}{u_0^2}, \qquad \text{d)}\quad \varphi_{12} = -ic_0^2\omega\,\frac{C}{u_0}\,e^{i\omega t + i\tau} \tag{103}$$

and solving the differential equation (55).

This example shows in detail that our method using time-dependent eigenfunctions works correctly.

Finally we mention that according to the definition (63) of the transition probability we find

$$W_{2(1)} = \frac{4\omega^2C^2}{u_0^2\left(1 + \dfrac{C^2}{u_0^2}\right)^2\left(\varrho^2 + \dfrac{4u_0^2}{\hbar^2}\right)}\sin^2\left(\frac{t}{2}\sqrt{\varrho^2 + \frac{4u_0^2}{\hbar^2}}\right). \tag{104}$$

The difference of both definitions of the transition probabilities can be learned from

$$\frac{W_{2(1)}}{w_{2(1)}} = \frac{\omega^2 C^2 \hbar^2}{u_0^2\left(1+\dfrac{C^2}{u_0^2}\right)^2} \to \begin{cases} 1 \text{ for } V_0^2 \ll 1 \\ 0 \text{ for } V_0^2 \gg 1 \end{cases} \quad \text{(near resonance),} \tag{105}$$

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