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Calculation of Transitions in Intense Laserfields with the Magnus Expansion

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Abstract. For bound quantum systems in presence of strong long wavelength electromagnetic fields the time evolution operator is calculated by application of the Magnus expansion in the interaction picture. We find that the first two orders of the Magnus expansion of the interaction picture time evolution operator contain both the momentum-translation transform of H.R. Reiss and terms which give rise to a non-static Stark-effect.

1. Introduction

Since the appearance of Reiss's papers on semiclassical electrodynamics of bound systems in intense fields [1, 2] several attempts have been made to establish the range of validity of this theory and to elucidate its underlying structure. In particular we mention the paper of Tewari [3] in which he has shown that the momentum-translation factor of Reiss can be obtained as an infinite order partial sum of ordinary time-dependent perturbation series. However his method of extracting the Reiss factor as the sum over all one-time integral contributions from the perturbation series requires a lot of laborious calculations. So we feel justified to point on a much simpler and a more natural method for deriving both the Reiss factor and all higher order corrections to it. The method consists in solving the wellknown timedependent Schrödinger equation in the interaction picture not as usual by perturbation theory but to solve it with the help of the far less familiar Magnus expansion [4]. This procedure is carried through in detail for the first two orders of the Magnus expansion in Section 2. In Section 3 we derive the transition matrix from the evolution operator obtained in Section 2 and compare it with the results of Reiss.

2. Theory

The Schrödinger equation for an electron interacting with the static field $V(\mathbf{x})$ and an external electromagnetic field $\mathbf{A}$ in Coulomb gauge is

$$i\hbar \frac{d}{dt} \Psi(t) = H(t)\, \Psi(t), \tag{1}$$

$$H(t) = H_0 + W(t), \tag{2}$$

$$H_0 = \mathbf{p}^2/(2m) + V(\mathbf{x}),$$
$$W(t) = -e\, \mathbf{A}\, \mathbf{p}/(m\, c) + e^2\, \mathbf{A}^2/(2m\, c^2). \tag{3}$$

We take the vectorpotential $\mathbf{A}$ in the position vector independent dipole form

$$\mathbf{A} = \mathbf{A}(t) \tag{4}$$

with

$$\mathbf{A}(t + 2\pi/\omega) = \mathbf{A}(t), \tag{5}$$

and assume that the circular frequency ω of the field $\mathbf{A}$ satisfies the long wavelength condition

$$r_0\, \omega/c \ll 1, \tag{6}$$

where r_0 is a characteristic length for the size of the bound one-electron system without interaction with the field $\mathbf{A}$.
If we define the interaction picture state vector $\Phi(t)$ by

$$\Psi(t) = \exp(-i\, H_0\, t/\hbar)\, \Phi(t), \tag{7}$$

the unitary time evolution operator for $\Phi(t)$

$$\Phi(t_2) = U_I(t_2, t_1)\, \Phi(t_1) \tag{8}$$

satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt_2} U_I(t_2, t_1) = W_I(t_2)\, U_I(t_2, t_1), \tag{9}$$

$$W_I(t) = \exp(i H_0 t/\hbar)\, W(t) \exp(-i H_0 t/\hbar) \tag{10}$$

together with the initial condition

$$U_I(t, t) = 1. \tag{11}$$

In the usual manner [5] we define the position operator in the interaction picture (index I)

$$\mathbf{x}_I(t) = \exp(i H_0 t/\hbar)\, \mathbf{x} \exp(-i H_0 t/\hbar) \tag{12}$$

and the conjugate momentum operator

$$\mathbf{p}_I(t) = \exp(i H_0 t/\hbar)\, \mathbf{p} \exp(-i H_0 t/\hbar), \tag{13}$$

and note the relation

$$\frac{d}{dt} \mathbf{x}_I(t) = \mathbf{p}_I(t)/m. \tag{14}$$

With the help of (3), (4), (13) and (14) the interaction picture potential $W_I(t)$ in (10) can be written in the form

$$\begin{aligned} W_I(t) &= -e\, \mathbf{A}\, \mathbf{p}_I(t)/(m c) + e^2 \mathbf{A}^2(t)/(2m c^2) \\ &= -e\, \mathbf{A} \frac{d}{dt} \mathbf{x}_I(t)/c + e^2 \mathbf{A}^2(t)/(2m c^2). \end{aligned} \tag{15}$$

The Magnus solution [4] of (9) and (11) is

$$U_I(t_2, t_1) = \exp(i\, \Delta(t_2, t_1)), \tag{16}$$

where $\Delta(t_2, t_1)$ is given by the expansion

$$\Delta(t_2, t_1) = \sum_{n=1}^{\infty} \Delta_n(t_2, t_1). \tag{17}$$

Explicitely the first two terms are

$$\Delta_1(t_2, t_1) = -\int_{t_1}^{t_2} d\tau\, W_I(\tau)/\hbar, \tag{18}$$

$$\Delta_2(t_2, t_1) = i \int_{t_1}^{t_2} d\tau \int_{t_1}^{\tau} d\tau_1 [W_I(\tau), W_I(\tau_1)]/(2\hbar^2). \tag{19}$$

Let us discuss the term $\Delta_1(t_2, t_1)$. It is important to note that since we deal with boundstates in external fields, we have the initial switching condition

$$\lim_{t \to -\infty} \mathbf{A}(t) = \mathbf{0}. \tag{20}$$

So we find after insertion of (15) into (18) and integration by parts

$$\Delta_1(t, -\infty) = e\, \mathbf{A}(t)\, \mathbf{x}_I(t)/(\hbar c) + e \int_{-\infty}^{t} d\tau\, \mathbf{E}(\tau)\, \mathbf{x}_I(\tau)/\hbar + \delta, \tag{21}$$

where

$$\delta = -e^2 \int_{-\infty}^{t} d\tau\, \mathbf{A}^2(\tau)/(2\hbar m c^2) \tag{22}$$

and $\mathbf{E}(t)$ is the timedependent electric field vector

$$\mathbf{E}(t) = -\frac{d}{dt} \mathbf{A}(t)/c. \tag{23}$$

As we shall show in Section 3 the term $e\mathbf{A}(t)\, \mathbf{x}_I(t)/(\hbar c)$ in (21) just yields the translation factor of Reiss [1], the term $e \int_{-\infty}^{t} d\tau\, \mathbf{E}(\tau)\, \mathbf{x}_I(\tau)/\hbar$ gives rise to a dynamical Stark-effect and δ is cancelled from a corresponding term which occurs in (19).

Let us first demonstrate how δ is cancelled by adding Δ_2 to Δ_1. Insertion of (15) into (19) yields

$$\begin{aligned} &\Delta_2(t, -\infty) \\ &= i e^2 \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_1 [\mathbf{A}(\tau)\, \mathbf{p}_I(\tau), \mathbf{A}(\tau_1)\, \mathbf{p}_I(\tau_1)]/(2\hbar^2 m^2 c^2). \end{aligned} \tag{24}$$

Making use of (14) we are able to replace $\mathbf{p}_I(\tau_1)$ in (24) by

$$\mathbf{p}_I(\tau_1) = m \frac{d}{d\tau_1} \mathbf{x}_I(\tau_1). \tag{25}$$

Integrating by parts over τ_1 and applying (20) and (23) we find

$$\begin{aligned} \Delta_2(t, -\infty) &= i e^2 \int_{-\infty}^{t} d\tau [\mathbf{A}(\tau)\mathbf{p}_I(\tau), \mathbf{A}(\tau)\mathbf{x}_I(\tau)]/(2\hbar^2 m c^2) \\ &+ i e^2 \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_1 [\mathbf{A}(\tau)\, \mathbf{p}_I(\tau), \mathbf{E}(\tau_1)\, \mathbf{x}_I(\tau_1)]/(2\hbar^2 m c). \end{aligned} \tag{26}$$

With the help of (12) and (13) we infer

$$[\mathbf{A}(\tau)\, \mathbf{p}_I(\tau), \mathbf{A}(\tau)\, \mathbf{x}_I(\tau)] = \hbar\, \mathbf{A}^2(\tau)/i, \tag{27}$$

so that according to (22)

$$\begin{aligned} \Delta_2(t, -\infty) &= -\delta + i e^2 \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_1 \\ &\cdot [\mathbf{A}(\tau)\, \mathbf{p}_I(\tau), \mathbf{E}(\tau_1)\, \mathbf{x}_I(\tau_1)]/(2\hbar^2 m c), \end{aligned} \tag{28}$$

which proves the cancellation of δ if (28) is added to (21). If a further integration by parts over τ is carried through (28) can be brought to final form

$$\begin{aligned} \Delta_2(t, -\infty) &= -\delta + i e^2 \int_{-\infty}^{t} d\tau [\mathbf{A}(t)\mathbf{x}_I(t), \mathbf{E}(\tau)\mathbf{x}_I(\tau)]/(2\hbar^2 c) \\ &+ i e^2 \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau_1 [\mathbf{E}(\tau)\mathbf{x}_I(\tau), \mathbf{E}(\tau_1)\, \mathbf{x}_I(\tau_1)]/(2\hbar^2). \end{aligned} \tag{29}$$

3. The Transition Matrix

In order to calculate the matrixelements of the transition operator for transitions caused by the interaction

$W(t)$ between the eigenvectors $|i\rangle$ and $|f\rangle$ of H_0,

$$H_0|i\rangle = E_i|i\rangle, \tag{30}$$

$$H_0|f\rangle = E_f|f\rangle, \tag{31}$$

$$\langle f|i\rangle = \delta_{fi}, \tag{32}$$

we recall that the S-matrix is [1]

$$S_{fi} = \langle f|\, U_I(+\infty, -\infty)\,|i\rangle. \tag{33}$$

Replacing (9), (11) and (20) by the integralequation

$$U_I(t, -\infty) = 1 - i \int_{-\infty}^{t} d\tau\, W_I(\tau)\, U_I(\tau, -\infty)/\hbar, \tag{34}$$

we obtain from (33) in the limit $t \to +\infty$ the transition-matrix T_{fi} in the form

$$T_{fi} \equiv \langle f|\,[U_I(+\infty, -\infty) - 1]\,|i\rangle = S_{fi} - \delta_{fi}$$

$$= -i \int_{-\infty}^{+\infty} dt \langle f|\, W_I(t)\, U_I(t, -\infty)\,|i\rangle/\hbar. \tag{35}$$

To get complete analogy with Eq. (26) of [1] we insert (10) into (35) and find

$$T_{fi} = -(i/\hbar) \int_{-\infty}^{+\infty} dt \exp(i\, t(E_f - E_i)/\hbar) \langle f|\, W(t)$$

$$\cdot \exp(-i\, H_0\, t/\hbar)\, U_I(t, -\infty) \exp(i\, H_0\, t/\hbar)\,|i\rangle. \tag{36}$$

Now it is straightforward to derive from (36) both the Reiss momentum-translation form of T_{fi} and the corrections to it. We only need to insert (16) into (36). We make use of

$$\exp(-i\, H_0\, t/\hbar) \exp(i\, \Delta(t, -\infty)) \exp(i\, H_0\, t/\hbar)$$

$$= \exp(i\, \tilde{\Delta}(t)), \tag{37}$$

where

$$\tilde{\Delta}(t) = \exp(-i\, H_0\, t/\hbar)\, \Delta(t, -\infty) \exp(i\, H_0\, t/\hbar), \tag{38}$$

so that (36) can be brought into the form

$$T_{fi} = -(i/\hbar) \int_{-\infty}^{+\infty} dt \exp(i\, t(E_f - E_i)/\hbar) \langle f|\, W(t)$$

$$\cdot \exp(i\, \tilde{\Delta}(t))\,|i\rangle. \tag{39}$$

From (17), (21), (29) and (12) written as

$$\exp(-i\, H_0\, t/\hbar)\, \mathbf{x}_I(\tau) \exp(i\, H_0\, t/\hbar) = \mathbf{x}_I(\tau - t), \tag{40}$$

we obtain the first few terms of $\tilde{\Delta}(t)$ in (39), viz.

$$\tilde{\Delta}(t) = \sum_{n=1}^{\infty} \tilde{\Delta}_n(t), \tag{41}$$

where

$$\tilde{\Delta}_1(t) = e\, \mathbf{A}(t)\, \mathbf{x}/(\hbar\, c), \tag{42}$$

$$\tilde{\Delta}_2(t) = e \int_{-\infty}^{t} d\tau\, \mathbf{E}(\tau)\, \mathbf{x}_I(\tau - t)/\hbar, \tag{43}$$

$$\tilde{\Delta}_3(t) = i[\tilde{\Delta}_1(t), \tilde{\Delta}_2(t)]/2, \tag{44}$$

$$\tilde{\Delta}_4(t) = i\, e \int_{-\infty}^{t} d\tau [\mathbf{E}(\tau)\, \mathbf{x}_I(\tau - t), \tilde{\Delta}_2(\tau)]/(2\hbar), \tag{45}$$

and according to (23)

$$\mathbf{E}(t) = -\frac{d}{dt} \mathbf{A}(t)/c. \tag{46}$$

If only the term $\tilde{\Delta}_1(t)$ defined in (42) is retained, the transition matrix (39) becomes

$$T_{fi} \approx T_{fi}^R = -(i/\hbar) \int_{-\infty}^{+\infty} dt \exp(i\, t(E_f - E_i)/\hbar) \langle f|\, W(t)$$

$$\cdot \exp(i\, e\, \mathbf{A}(t)\, \mathbf{x}/(\hbar\, c))\,|i\rangle, \tag{47}$$

which is precisely the transition matrix τ_{fi} Eq. (26) in [1]. The correction terms (43), (44) and (45) produce non-static Stark-effects which are neglected in Reiss's first order theory. A detailed investigation of these corrections will be presented in a forthcoming paper.

4. Conclusion

We have shown how the momentum-translation approximation of Reiss is obtained in a very natural way from the first two orders of the Magnus expansion of the time evolution operator in the interaction picture. In addition our derivation also leads to correction terms which cause a dynamical Stark-effect.

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