Foundations of Physics, Vol. 20, No. 1, 1990

Landau's Density Matrix in Quantum Electrodynamics[1]

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Received August 8, 1988; revised February 27, 1989

This paper is devoted to Landau's concept of the problem of damping in quantum mechanics. It shows that Landau's density matrix formalism should survive in the context of modern quantum electrodynamics. The correct generalized master equation has been derived for the reduced dynamics of the charges. The recent relativistic theory of spontaneous emission becomes reproducible.

1. INTRODUCTION

In 1927 Landau published a paper[1] on the "Problem of damping in wave mechanics." He had in mind the irreversibility of certain quantum mechanical processes, typically the spontaneous decays of excited atomic states. This irreversibility is not inherent in quantum mechanics, though; it must be deduced from the reversible quantum dynamics of the larger system, including the photonic variables also (cf. Ref. 2).

Landau then created the proper formalism to describe the reduced dynamics of the electrons in contact with the electromagnetic fields, which he integrated out. The state vector of the electron system had to be replaced by a matrix, later called the density matrix. This matrix satisfies a linear equation of motion (master equation), which, in contrast to Schrödinger's, contains irreversibility; cf. also in Pauli's famous work.[3] Since in 1927 the full theory of quantum electrodynamics was not within reach, Landau did not elaborate on the exact equation of motion of the electron density matrix. Nevertheless, he did find the proper approxima-

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0015-9018/90/0100-0063$06.00/0

tion, and he calculated the spontaneous decay rates in the electric dipole approximation.

Sixty years later we see much progress in theory and technique. Many years ago a systematic theory of quantum electrodynamics was constructed, and Feynman was able to integrate it over virtual photon states.[4] On the other hand, the density matrix formalism and the theory of master equations have become the most common technique when dealing with quantum damping (see, e.g., Refs. 5 and 6). However, in relativistic field theory the density matrix formalism is still unconventional, and people prefer hand-made calculi for irreversible processes. In spite of this, there exists a very stimulating review[7] on unified treatment of irreversibility in quantum field theory. We also mention some recent papers[8-10] advocating the above technique, e.g., for tasks in cosmological particle physics, where serious irreversibilities are expected.

In this paper we reproduce the original proposal of Landau. Having the equation of quantum electrodynamics, we integrate over the photonic variables and present the exact generalized master equation of the electron system. Deriving an effective Markovian master equation, but not turning to the dipole approximation, we will deduce the relativistic approximation of the spontaneous decay rates, also obtained quite recently in Ref. 11.

2. GENERALIZED MASTER EQUATION

In interaction representation, let $\Phi(t)$ stand for the state vector of the electron–photon system representing the subject of quantum electrodynamics. If one neglects the interactions with any other quantum fields, the state Φ evolves unitarily:

$$\Phi(t) = U(t)\,\Phi(-\infty) \tag{1}$$

$$U(t) = T\exp\left\{-i\int_{x_0<t} J(x)\,A(x)\,dx\right\} \tag{2}$$

where J represents the 4-current, A stands for the 4-potential, and T denotes time ordering. According to the standard quantum electrodynamics, the operator $J(x)$ equals the normal-ordered bilinear form $\bar{\psi}(x)\,\gamma\psi(x)$ times the elementary charge e, where $\psi(x)$ is the field operator of the electrons and γ stands for the four Dirac matrices.

Following Landau,[1] we introduce the density matrix ρ of the electron subsystem by tracing the pure state projector $\Phi\Phi^+$ over the photonic state space:

$$\rho(t) \equiv \mathrm{tr}_A[\Phi(t)\,\Phi^+(t)] \tag{3}$$

We are going to show that Eqs. (1)–(3) lead us to a closed form of generalized master equation governing the time evolution of the electron density matrix (3).

Throughout this paper we assume that at $t = -\infty$ there were no photons but only bare charges. Then we can take $\Phi(-\infty)\,\Phi^+(-\infty)$ in the form

$$\Phi(-\infty)\,\Phi^+(-\infty) = |O_A\rangle\, \rho(-\infty)\, \langle O_A| \tag{4}$$

where $|O_A\rangle$ denotes the photonic vacuum state and $\rho(-\infty)$ stands for the initial (pure) state of the electron system. (Note that all results below remain valid if $\rho(-\infty)$ is a mixed state.) By substituting Eqs. (1) and (4) into Eq. (3), we obtain

$$\begin{aligned}\rho(t) &= \mathrm{tr}_A[U(t)\,|O_A\rangle\, \rho(-\infty) \langle O_A|\, U^+(t)] \\ &= \langle O_A|\, U^+(t) \circ U(t)\, |O_A\rangle\, \rho(-\infty)\end{aligned} \tag{5}$$

Here the super-operator $U^+ \circ U$ is, by definition, the ordinary product of U^+ and U on the photonic state space but a tensor product on the electron state space. Generally, the word "super-operator" means any linear combination of tensorial (direct) products of two ordinary operators. Consequently, the expectation value $\langle O_A|\, U^+(t) \circ U(t)\, |O_A\rangle$ of the super-operator $U^+ \circ U$ is still a super-operator acting on the space of mixed electron states ρ; cf. Eq. (5).

Our next task is to evaluate this expectation value. From (2), we see that $U^+ \circ U$ is the direct product of a time-ordered exponential expression and another anti-time-ordered one. In fact, one can generalize the time-ordering convention and, as a result, obtain a single exponential form for $U^+ \circ U$, which is evaluated easily between states $\langle O_A|$, $|O_A\rangle$. We shall not present the details of these calculations, which the reader can understand from Ref. 7. We only summarize the result: Let us append a + or − index to the operator field J to indicate whether J is to act from the left or from the right. For example,

$$J_+\rho \equiv J\rho, \qquad J_-\rho \equiv \rho J \tag{6}$$

Furthermore, let us introduce the symbol $\hat{T}$ which represents time-ordering (T) for J_+ fields and anti-time-ordering ($\bar{T}$) for J_- fields. Inserting Eq. (2) into the RHS of (5) and applying the notations (6), we obtain the following relation:

$$\rho(t)=\hat{T}\exp\left\{\frac{1}{2}i\iint_{x_0,\,y_0<t}dx\,dy[D^{(F)}(x-y)\,J_+(x)\,J_+(y)\right.$$
$$+D^{(\bar{F})}(x-y)\,J_-(x)\,J_-(y)-D^{(+)}(x-y)\,J_+(x)\,J_-(y)$$
$$\left.-D^{(-)}(x-y)\,J_-(x)\,J_+(y)]\right\}\rho(-\infty) \tag{7}$$

where

$$D^{(F)}(x)=i\langle O_A|\,TA(x)\,A(O)\,|O_A\rangle=(2\pi)^{-4}\int dp\,e^{-ipx}[p^2+i\varepsilon]^{-1} \tag{8a}$$

$$D^{(\bar{F})}(x)=i\langle O_A|\,\bar{T}A(x)\,A(O)\,|O_A\rangle=-(2\pi)^{-4}\int dp\,e^{-ipx}[p^2-i\varepsilon]^{-1} \tag{8b}$$

$$D^{(+)}(x)=i\langle O_A|\,A(O)\,A(x)\,|O_A\rangle$$
$$=(2\pi)^{-4}\int dp\,e^{-ipx}[-2\pi i\theta(-p_0)\,\delta(p^2)] \tag{8c}$$

$$D^{(-)}(x)=i\langle O_A|\,A(x)\,A(O)\,|O_A\rangle$$
$$=(2\pi)^{-4}\int dp\,e^{-ipx}[-2\pi i\theta(p_0)\,\delta(p^2)] \tag{8d}$$

Equation (7) is the central point of our paper. Such generalized (i.e., not Markovian) master equations of the same mathematical structure are well known from nonrelativistic quantum mechanics. In terms of the latter, Eq. (7) is just the effective equation for the reduced dynamics of the electrons and positrons surrounded by a natural reservoir (cf. Ref. 5), which is, in our case, the fluctuating electromagnetic vacuum.

This generalized master equation is equivalent to the whole apparatus of quantum electrodynamics if we suppose that our electrodynamical experience is deduced, *ad extremum*, only from the motion of charges (J) and we use the notion of electromagnetic field (A) merely for the convenience of locality.

It is instructive to observe that the J_+J_+ and J_-J_- combinations in Eq. (7) correspond to tracing over virtual photon states, while J_+J_- combinations account for inelastically produced real photons. Had we omitted the J_+J_- combinations, the RHS of (7) would factorize as follows:

$$\rho(t)\approx V(t)\,\rho(-\infty)\,V^+(t) \tag{9a}$$

$$V(t)=T\exp\left\{\frac{1}{2}i\iint_{x_0,\,y_0<t}dx\,dy\,D^{(F)}(x-y)\,J(x)\,J(y)\right\} \tag{9b}$$

which is just Feynman's famous result.[4] Of course, Eq. (9a) does not take into account the inelastically produced real photons, and it therefore will not preserve the trace of $\rho(t)$. The generalized master equation (7) does, by construction, preserve the normalization and positivity of the density matrix ρ; this fact would deserve an explicit demonstration also.

3. MARKOVIAN EFFECTIVE MASTER EQUATION

In this section, we approximate the exact master equation (7) of the electron system by an effective Markovian master equation[5] $\dot{\rho}(t) = L\rho(t)$ applicable at large enough time scales. The evolution (super-)operator L is introduced by the definition

$$\lim_{T\to\infty} 1/T\left[\rho\left(\frac{1}{2}T\right) - \rho\left(-\frac{1}{2}T\right)\right] \equiv L\rho(O) \tag{10}$$

We are going to find the evolution operator L perturbatively. Remember that J is proportional to the elementary charge e, which is a small quantity. In the lowest nonvanishing order of e, the generalized master equation (7) yields the approximation of the order of e^2:

$$\rho(\infty) - \rho(-\infty) = \frac{1}{2} i \iint dx\, dy [D^{(F)}(x-y)\, T(J(x)\, J(y))\, \rho(-\infty) - D^{(+)}(x-y)\, J(x)\, \rho(-\infty)\, J(y)] + \text{H.C.} \tag{11}$$

When the Fourier transform (8a)–(8c) of the Green functions and of the currents is applied, the above equation assumes the form

$$\begin{aligned}\rho(\infty) - \rho(-\infty) = (2\pi)^{-4} \int dp\, 1/(2\,|\mathbf{p}|) \\ \times [i(p_0 + |\mathbf{p}|)^{-1} [\tilde{J}^+(p)\, \tilde{J}(p), \rho(-\infty)] \\ + \pi\delta(p_0 + |\mathbf{p}|)\, \{\tilde{J}^+(p)\, \tilde{J}(p), \rho(-\infty)\} \\ - 2\pi\delta(p_0 - |\mathbf{p}|)\, \tilde{J}^+(p)\, \rho(-\infty)\, \tilde{J}(p)]\end{aligned} \tag{12}$$

From now on, we assume that the unperturbed Hamiltonian of the electron system is time independent and the eigenstates are labelled by small Latin indices. Then, in the energy representation, the time dependence of the matrix elements J_{mn} of the current operator will be trivial:

$$J_{mn}(x) = \exp(i\omega_{mn} x_0)\, J_{mn}(\mathbf{x}) \tag{13a}$$

$$\tilde{J}_{mn}(p) = 2\pi\delta(p_0 + \omega_{nm})\, \tilde{J}_{nm}(\mathbf{p}) \tag{13b}$$

where ω_{mn} is the relative energy $E_m - E_n$ between the mth and nth stationary states; $J(\mathbf{x})$, $\tilde{J}(\mathbf{p})$ are the current operator and its Fourier transform, respectively, in the Schrödinger picture. From Eq. (13b), one can derive the following useful relation for the product of two currents, which is needed on the RHS of Eq. (12):

$$\begin{aligned}\tilde{J}^*_{nm}(p)\,\tilde{J}_{rs}(p) &= 4\pi^2[\delta(p_0 + \omega_{nm})]^2\, \delta_{nr}\delta_{ms}\tilde{J}^*_{nm}(\mathbf{p})\,\tilde{J}_{rs}(\mathbf{p}) \\ &\approx 2\pi T\delta(p_0 + \omega_{nm})\,\delta_{nr}\delta_{ms}\tilde{J}^*_{nm}(\mathbf{p})\,\tilde{J}_{rs}(\mathbf{p})\end{aligned} \tag{14}$$

The substitution in the second line (well known from the elements of quantum mechanical perturbation theory) is valid in the limit $T \to \infty$, T representing the time interval for which the electron–photon interactions are switched on.

Now, by exploiting the asymptotic formula (14), we evaluate the RHS of Eq. (12) and take the time average (10). Then T cancels, and one obtains the following Markovian master equation for the density matrix elements of the electron system:

$$\dot{\rho}_{nn} = -\Gamma_n \rho_{nn} + \sum_r \Gamma_{r \to n}\rho_{rr} \tag{15a}$$

$$\dot{\rho}_{nm} = \left[-i(\Delta E_n - \Delta E_m) - \frac{1}{2}(\Gamma_n + \Gamma_m)\right]\rho_{nm}, \qquad n \neq m \tag{15b}$$

For the energy shifts ΔE_n and for the transition rates $\Gamma_{r\to n}$ we obtain, respectively, the following expressions:[3]

$$\Delta E_n = -(2\pi)^{-3} \sum_r \int d\mathbf{p}[2\,|\mathbf{p}|(|\mathbf{p}| - \omega_{rn})]^{-1}\, \tilde{J}^*_{rn}(\mathbf{p})\,\tilde{J}_{rn}(\mathbf{p}) \tag{16}$$

$$\Gamma_{r\to n} = -(2\pi)^{-3} \int d\mathbf{p}(\pi/|\mathbf{p}|)\,\delta(|\mathbf{p}| - \omega_{rn})\,\tilde{J}^*_{rn}(\mathbf{p})\,\tilde{J}_{rn}(\mathbf{p}) \tag{17}$$

and the full decay rate of the nth level is defined by

$$\Gamma_n = \sum_r \Gamma_{n\to r} \tag{18}$$

[3] Equations (16) and (17) were given previously by A. O. Barut in *Quantum Theory and the Structure of Space and Time*, L. Castelland C. F. von Weiszäcker, eds. (Hanser, Munich, 1986).

Notice that the transition rates (17) are nonzero only in the case in which the final state possesses a lower energy than the initial one.

The master equation (15) was first derived in Landau's paper,[1] but he calculated the coefficients in the dipole approximation. Recently Barut and Salamin[11] calculated the spontaneous emission rate, without using the dipole approximation, and our result is identical to theirs.

The reader may notice that the Lorentz indices have been supressed everywhere. If one restore them, it is straightforward to see that, due to the current conservation $p_\mu \tilde{J}^\mu(p) \equiv 0$, one can eliminate the 0th component of the current from all of the above formulas. In this special gauge, the positivity of the transition rate (17) can be explicitly seen:

$$\Gamma_{r \to n} = (2\pi)^{-3} \int d\mathbf{p}(\pi/|\mathbf{p}|)\, \delta(|\mathbf{p}| - \omega_{rn})\, \tilde{J}^*_{rn}(\mathbf{p})(\mathbb{1} - \mathbf{n} \circ \mathbf{n})\, \tilde{J}_{rn}(\mathbf{p}) \qquad (19)$$

where $\mathbf{n} = \mathbf{p}/|\mathbf{p}|$. Restricting this formula to the dipole approximation $\tilde{J}_{rn}(\mathbf{p}) \approx \tilde{J}_{rn}(\mathbf{O}) = -i\omega_{rn}\sqrt{4\pi}\,\mathbf{D}_{rn}$, we can evaluate the integral on the RHS of Eq. (19):

$$\Gamma_{r \to n} = (4/3)\, \omega_{rn}\, |\mathbf{D}_{rn}|^2, \qquad \text{if} \quad \omega_{rn} > 0 \qquad (20)$$

This is the classical result[2] for the spontaneous emission rate. Although it was known to Landau, its illuminating derivation from the first principles of the quantum theory is due to him.[1]

4. CONCLUDING REMARKS

In this paper we have reconsidered Landau's concept of the problem of damping in quantum mechanics. We have shown that Landau's density-matrix formalism can be generalized by using the technique of modern quantum electrodynamics. We have derived the generalized master equation for the reduced dynamics of the charges. It would be interesting to discuss whether such a formalism may provide essential help to treat strong irreversibilities in other branches of field theory. One would consider, for example, cosmological particle creation, relativistic heavy ion physics, and especially hadronization processes in quantum chromodynamics.

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