

Relation between energy shifts and relaxation rates for a small system coupled to a reservoir

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Abstract

For a small system the coupling to a reservoir causes energy shifts as well as transitions between the system's energy levels. We show for a general stationary situation that the energy shifts can essentially be reduced to the relaxation rates. The effects of reservoir fluctuations and self reaction are treated separately. We apply the results to a two-level atom coupled to a reservoir which may be the vacuum of a radiation field.

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1 Introduction

For a small quantum system which is coupled to a reservoir, energy shifts due to the coupling will occur as well as transitions between the system's energy levels. Our aim in the present letter is to derive relations between these relaxation rates and energy shifts which are valid under very general conditions. We consider a system which moves in a stationary way on a possibly accelerated trajectory in a general spacetime (which may be curved or possess nontrivial boundaries). The stationarity of the situation demands that the system moves along the orbits of a timelike Killing vector field. Stationarity is also assumed for the reservoir. The case of an extended system at rest is included. Typical realizations of such a situation are an atom or an elementary particle (system) coupled to a quantized radiation field in the vacuum or a many-photon state (reservoir), whereby the atom may be accelerated. In this case the energy shift is the Lamb shift.

For the description of the system-reservoir interaction we will generalize the formalism which has been established by Dalibard, Dupont-Roc and Cohen-Tannoudji (DDC) [1] and extended in [2, 3] to the situation just described. It leads to a clear and physically appealing interpretation of the processes in terms of the underlying physical mechanisms since it allows the separate discussion of the effects of reservoir fluctuations and self reaction (or radiation reaction).

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2 Reservoir fluctuations and self reaction

First we provide the necessary general relations. We consider a spacetime which is covered by a coordinate system $x = (t, \vec{x})$. The time coordinate t is assumed to be the “natural” time for the description of the reservoir. The system is described by a stationary (accelerated) trajectory $x(\tau) = (t(\tau), \vec{x}(\tau))$. This may be realized for example by a pointlike object moving on this trajectory. The respective proper time variable τ is used for the parametrization of the trajectory.

The time evolution of system and reservoir has to be specified in terms of a single time variable for which we choose the system time τ . The Hamiltonian which governs the dynamics with respect to τ is given by

$$H = H_S(\tau) + H_R(t) \frac{dt}{d\tau} + V(x(\tau)) \quad (1)$$

where H_S is the free Hamiltonian of the system. $H_R(t)$ is the free reservoir Hamiltonian with respect to the time variable t . The factor $dt/d\tau$ in (1) is due to the corresponding change of variables. $V(x(\tau))$ represents the coupling between system and reservoir. It is effective only on the trajectory $x(\tau)$ of the system. It is assumed to have the general linear form

$$V(x(\tau)) = -g \sum_i R_i(\tau) S_i(x(\tau)) \quad (2)$$

with g being a coupling constant. R_i and S_i are hermitean reservoir and system operators. For an extended system at rest, we can set $\tau = t$ and replace $x(\tau)$ by t here and in the equations below.

We can now write down the Heisenberg equations of motion for observables of the system and the reservoir. For our purposes, the following will be important: It is possible in the solution of the Heisenberg equation for the reservoir variable R_i to distinguish on one hand the part which is present even in the absence of the coupling. It is independent of the system and is called the *free part* R_i^f of R_i . The remaining contribution is caused by the presence of the system and contains the coupling constant g . It is called the *source part* R_i^s of R_i :

$$R_i(\tau) = R_i^f(\tau) + R_i^s(\tau). \quad (3)$$

We consider the rate of change of an arbitrary system variable G . Because of the coupling (2), reservoir operators appear in the Heisenberg equations of G . According to (3), they can be divided into their free and source parts. The rate of change of G due to the coupling can therefore be split into two contributions which correspond to two different physical mechanisms: (i) the change in G produced by the fluctuations of the reservoir which are present even in the absence of the system – this portion is related to the free part of the reservoir and is called the contribution of *reservoir fluctuations* to $dG/d\tau$ – and (ii) the change in G due to the interaction with the excitations of the reservoir which are caused by the system itself. This is the contribution of *self reaction* or radiation reaction and is connected with the source part of the field. Following DDC [4], we adopt a symmetric ordering between system and reservoir operators.

In a perturbative approach, we take into account only terms up to second order in g . Since we are interested only in the dynamics of the system, we average over the reservoir degrees of freedom. We assume that the density matrix is factorized into a system and a reservoir part at the initial time $\tau = 0$: $\rho(0) = \rho_S(0) \rho_R(0)$. We select one specific system state $|a\rangle$ and take the expectation value with respect to that state.

Proceeding essentially as in [1], we find for the contribution of reservoir fluctuations

$$\left\langle \frac{dG}{d\tau}(\tau) \right\rangle_{rf} = i \left\langle [H_{rf}^{eff}(\tau), G(\tau)] \right\rangle - \frac{g^2}{2} \sum_i \left\langle [Y_i(\tau), [S_i^f(\tau), G(\tau)]] + [S_i^f(\tau), [Y_i(\tau), G(\tau)]] \right\rangle \quad (4)$$

whereas the contribution of self reaction is (curly brackets denote the anticommutator):

$$\left\langle \frac{dG}{d\tau}(\tau) \right\rangle = i \left\langle [H_{sr}^{eff}(\tau), G(\tau)] \right\rangle - \frac{g^2}{2} \sum_i \left\langle \left\{ Z_i(\tau), [S_i^f(\tau), G(\tau)] \right\} - \left\{ S_i^f(\tau), [Z_i(\tau), G(\tau)] \right\} \right\rangle. \quad (5)$$

In (4) and (5), brackets $\langle \dots \rangle$ denote averaging over the reservoir and taking the expectation value in the system state $|a\rangle$. Furthermore we have introduced the effective Hamiltonians

$$H_{rf}^{eff}(\tau) := \frac{ig^2}{2} \sum_i [Y_i(\tau), S_i^f(\tau)], \quad H_{sr}^{eff}(\tau) := -\frac{ig^2}{2} \sum_i \left\{ Z_i(\tau), S_i^f(\tau) \right\} \quad (6)$$

with

$$Y_i(\tau) := \sum_j \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) S_j^f(\tau'), \quad Z_i(\tau) := \sum_j \int_0^\infty d\tau' \chi_{ij}^R(x(\tau), x(\tau')) S_j^f(\tau') \quad (7)$$

Since we are interested in time scales which are large compared with the correlation time of the reservoir, we have extended the range of integration in (7) to infinity. We have also introduced the symmetric correlation function C_{ij}^R and the linear susceptibility χ_{ij}^R of the reservoir:

$$C_{ij}^R(x(\tau), x(\tau')) := \frac{1}{2} \text{Tr}_R \left(\rho_R(0) \left\{ R_i^f(x(\tau)), R_j^f(x(\tau')) \right\} \right) \quad (8)$$

$$\chi_{ij}^R(x(\tau), x(\tau')) := \frac{1}{2} \text{Tr}_R \left(\rho_R(0) \left[R_i^f(x(\tau)), R_j^f(x(\tau')) \right] \right) \quad (9)$$

Because of the stationarity, C_{ij}^R and χ_{ij}^R are only functions of the time difference $\tau - \tau'$.

3 Energy shifts and relaxation rates

The relaxation rates of the system's energy in the state $|a\rangle$ can be obtained from (4) and (5) with the choice $G = H_S$. We replace $[S_i^f, H_S^f]$ in second order by $i \frac{d}{d\tau} S_i^f$ and find for the contributions of vacuum fluctuations and self reaction to the system's relaxation rate

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{rf} = 2ig^2 \sum_{i,j} \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) \frac{d}{d\tau} \chi_{ij}^S(\tau, \tau') \quad (10)$$

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{sr} = 2ig^2 \sum_{i,j} \int_0^\infty d\tau' \chi_{ij}^R(x(\tau), x(\tau')) \frac{d}{d\tau} C_{ij}^S(\tau, \tau'), \quad (11)$$

with the symmetric correlation function and the linear susceptibility of the system

$$C_{ij}^S(\tau, \tau') := \frac{1}{2} \langle a | \left\{ S_i^f(\tau), S_j^f(\tau') \right\} | a \rangle = \sum_b \text{Re} \left(\langle a | S_i^f(0) | b \rangle \langle b | S_j^f(0) | a \rangle e^{i\omega_{ab}(\tau - \tau')} \right), \quad (12)$$

$$\chi_{ij}^S(\tau, \tau') = \frac{1}{2} \langle a | \left[S_i^f(\tau), S_j^f(\tau') \right] | a \rangle = i \sum_b \text{Im} \left(\langle a | S_i^f(0) | b \rangle \langle b | S_j^f(0) | a \rangle e^{i\omega_{ab}(\tau - \tau')} \right). \quad (13)$$

To evaluate (12) and (13) we have used the stationarity of the situation which allowed us to introduce a complete set of stationary system states $|b\rangle$ (eigenstates of H_S) with energies ω_b and $\omega_{ab} = \omega_a - \omega_b$. The formulas (10) and (11) are the generalizations of the corresponding equations of DDC [1] to the situation considered here. (Note the slight differences in the definition of the correlation functions).

Beneath that, the system-reservoir coupling leads to a shift of the system's energy levels. The second order radiative shift of state $|a\rangle$ is given by the expectation value of the effective Hamiltonians (6) in that level. Again, the total shift can be split into the contributions of vacuum fluctuations and radiation reaction:

$$(\delta E_a)_{rf} = -ig^2 \sum_{i,j} \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) \chi_{ij}^S(\tau, \tau') \quad (14)$$

$$(\delta E_a)_{sr} = -ig^2 \sum_{i,j} \int_0^\infty d\tau' \chi_{ij}^R(x(\tau), x(\tau')) C_{ij}^S(\tau, \tau') \quad (15)$$

These formulas too are generalizations of those in [1]. Because C_{ij}^R (χ_{ij}^R) is symmetric (antisymmetric) in i and j , terms with $\omega_{ab} = 0$ do not contribute to the relaxation rates and energy shifts. The proof, which we omit, is based on the stationarity. Without restriction, we can therefore exclude these terms below from all b summations.

4 Relation between energy shifts and relaxation rates

We now come to the main point of this letter. We will prove to second order in g for a system in the state $|a\rangle$ quite general relations between the corresponding relaxation rates (10) and (11) and the energy shifts (14) and (15). We start with the contribution of reservoir fluctuations. Using the explicit formula (13) for the system's linear susceptibility, the energy shift (14) can be written

$$(\delta E_a)_{rf} = -g^2 \sum_{i,j,b} \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) \frac{d}{d\tau} \text{Re} \left(\langle a|S_i^f(0)|b\rangle \langle b|S_j^f(0)|a\rangle \frac{1}{\omega_{ab}} e^{i\omega_{ab}(\tau-\tau')} \right) \quad (16)$$

Now we can apply the Kramers-Kronig relation [5]

$$\text{Re}(f(\omega_{ab})) = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \text{Im}(f(\omega')) \frac{\mathcal{P}}{\omega' - \omega_{ab}} \quad (17)$$

to the function $f(\omega_{ab}) = \langle a|S_i^f(0)|b\rangle \langle b|S_j^f(0)|a\rangle \omega_{ab}^{-1} e^{i\omega_{ab}(\tau-\tau')}$ which is analytic for $\omega_{ab} \neq 0$ and vanishes for $\omega_{ab} \rightarrow i\infty$. We find

$$\begin{aligned} (\delta E_a)_{rf} &= -\frac{g^2}{\pi} \sum_{i,j,b} \int_{-\infty}^{+\infty} d\omega' \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) \\ &\quad \times \frac{d}{d\tau} \text{Im} \left(\langle a|S_i^f(0)|b\rangle \langle b|S_j^f(0)|a\rangle \frac{1}{\omega'} e^{i\omega'(\tau-\tau')} \right) \frac{\mathcal{P}}{\omega' - \omega_{ab}} \end{aligned} \quad (18)$$

Introducing the quantity $\Gamma_{ab}^{rf}(\omega')$ by the definition

$$\Gamma_{ab}^{rf}(\omega') := -2g^2 \sum_{i,j} \int_0^\infty d\tau' C_{ij}^R(x(\tau), x(\tau')) \frac{d}{d\tau} \text{Im} \left(\langle a|S_i^f(0)|b\rangle \langle b|S_j^f(0)|a\rangle e^{i\omega'(\tau-\tau')} \right) \quad (19)$$

we obtain the desired relation

$$(\delta E_a)_{rf} = \frac{1}{2\pi} \sum_b \int_{-\infty}^{+\infty} d\omega' \frac{\Gamma_{ab}^{rf}(\omega')}{\omega'} \frac{\mathcal{P}}{\omega' - \omega_{ab}}. \quad (20)$$

Eq. (20) connects energy shift and relaxation rate since the latter can be expressed easily in terms of Γ_{ab}^{rf} :

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{rf} = \sum_b \Gamma_{ab}^{rf}(\omega_{ab}), \quad (21)$$

where we have used Eqs. (10) and (13). Following essentially the same procedure, an equation analogous to (20) can be derived for the contribution of self reaction to the energy shift

$$(\delta E_a)_{sr} = \frac{1}{2\pi} \sum_b \int_{-\infty}^{+\infty} d\omega' \frac{\Gamma_{ab}^{sr}(\omega')}{\omega'} \frac{\mathcal{P}}{\omega' - \omega_{ab}}, \quad (22)$$

where

$$\Gamma_{ab}^{sr}(\omega') := 2ig^2 \sum_{i,j} \int_0^\infty d\tau' \chi_{ij}^R(x(\tau), x(\tau')) \frac{d}{d\tau} \text{Re} \left(\langle a|S_i^f(0)|b\rangle \langle b|S_j^f(0)|a\rangle e^{i\omega'(\tau-\tau')} \right) \quad (23)$$

and Eq. (21) holds correspondingly (replace rf by sr). Note that $\Gamma_{ab}^{rf/sr}$ do not depend on τ because of the stationarity of the physical situation.

We have studied above a very general stationary situation: arbitrary linear system-reservoir coupling, arbitrary stationary motion in a flat or curved spacetime, nontrivial boundary conditions allowed, arbitrary state of the reservoir. We have shown that the determination of energy shift and relaxation rate can be reduced in a unified way directly to the calculation of the coefficients $\Gamma_{ab}^{rf/sr}$. They turn out to be the fundamental underlying quantities. The calculation of the energy shift has thereby been simplified as compared to (14) and (15). Equations (20), (21) and (22) show that the $\Gamma_{ab}^{rf/sr}$ refer to particular

transitions $|a\rangle \rightarrow |b\rangle$. This becomes even more evident when the system has only a few energy states as will be demonstrated in the next section. In addition we see that the mutual dependence between energy shifts and relaxation rates holds for the reservoir fluctuation terms and for the self reaction terms separately. This supports the view that the distinction of these two mechanisms is physically reasonable. Finally we mention that for concrete physical situations it may be necessary to introduce a frequency cutoff in order to regularize $(\delta E_a)_{rf/sr}$. As compared with (14) and (15), the new expressions (20) and (22) are directly prepared for this.

5 Application: Two-level atom

To demonstrate the usefulness of the proposed scheme we consider a two-level system moving on a stationary trajectory and derive several statements which are valid under very general conditions. This illustrates at the same time the physical concepts. We assume two stationary states $|+\rangle$ and $|-\rangle$ with energies $\pm \frac{1}{2}\omega_0$. The atomic Hamiltonian can be written with the help of the pseudospin operator $S_3 = \frac{1}{2}|+\rangle\langle+| - \frac{1}{2}|-\rangle\langle-|$ as

$$H_S = \omega_0 S_3(\tau) \quad (24)$$

The coupling to the reservoir is linear and connects only different levels of the system:

$$V = -g S_2(\tau) R(x(\tau)) \quad (25)$$

with $S_2 = \frac{i}{2}(S_+ - S_-)$ and $S_{\pm} = |\pm\rangle\langle\mp|$. We rewrite $\Gamma_{ab}^{rf/sr}$ from Eqs. (19) and (23) as

$$\Gamma_{ab}^{rf/sr}(\omega_{ab}) = -2\omega_{ab} |\langle a|S_2^f(0)|b\rangle|^2 \gamma^{rf/sr}(\omega_{ab}) \quad (26)$$

where we have simply $|\langle a|S_2^f(0)|b\rangle|^2 = \frac{1}{4}$ for $a \neq b$. Here,

$$\gamma^{rf}(\omega_{ab}) = g^2 \int_0^\infty d\tau' C^R(x(\tau), x(\tau')) \cos \omega_{ab}(\tau - \tau'), \quad (27)$$

$$\gamma^{sr}(\omega_{ab}) = ig^2 \int_0^\infty d\tau' \chi^R(x(\tau), x(\tau')) \sin \omega_{ab}(\tau - \tau'), \quad (28)$$

and $\omega_{ab} = \pm\omega_0$ for $a > b$ ($a < b$).

Using the general expression (21) for the relaxation rate together with (26), we can write

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{rf} = -2 \sum_b \omega_{ab} |\langle a|S_2^f(0)|b\rangle|^2 \gamma^{rf}(\omega_{ab}) \quad (29)$$

Since γ^{rf} is symmetric in ω_{ab} , it follows that

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{rf} = -2\omega_0 \gamma^{rf}(\omega_0) \left(\sum_{b<a} |\langle a|S_2^f(0)|b\rangle|^2 + \sum_{b>a} |\langle a|S_2^f(0)|b\rangle|^2 \right) \quad (30)$$

Analogously, we find for the contribution of self reaction to the relaxation rate

$$\left\langle \frac{dH_S}{d\tau} \right\rangle_{sr} = -2\omega_0 \gamma^{sr}(\omega_0) \left(\sum_{b<a} |\langle a|S_2^f(0)|b\rangle|^2 - \sum_{b>a} |\langle a|S_2^f(0)|b\rangle|^2 \right). \quad (31)$$

From these general relations, it is possible to find expressions for the atom's evolution into equilibrium as well as for the Einstein coefficients $A_\uparrow$ and $A_\downarrow$ corresponding to upwards and downwards transitions. We consider the total transition rate $\langle \frac{dH_S}{d\tau} \rangle_{tot} = \langle \frac{dH_S}{d\tau} \rangle_{rf} + \langle \frac{dH_S}{d\tau} \rangle_{sr}$. Using (30) and (31), it can be simplified by noting

$$\sum_{b>a} |\langle a|S_2^f(0)|b\rangle|^2 \pm \sum_{b<a} |\langle a|S_2^f(0)|b\rangle|^2 = \begin{cases} \frac{1}{4} \\ -\frac{1}{2\omega_0} \langle a|H_S|a \rangle \end{cases} \quad (32)$$

Here we have replaced H_S^f by the total system Hamiltonian, which is justified in order g^2 . We thus obtain a differential equation for the evolution of the mean atomic excitation energy

$$\left\langle \frac{dH_S}{d\tau}(\tau) \right\rangle_{tot} = -\frac{1}{2}\omega_0 \gamma^{sr}(\omega_0) - \gamma^{rf}(\omega_0) \langle H_S(\tau) \rangle \quad (33)$$

which has the solution

$$\langle H_S(\tau) \rangle = -\frac{1}{2}\omega_0 + \frac{1}{2}\omega_0 \frac{\gamma^{rf} - \gamma^{sr}}{\gamma^{rf}} + \left(\langle H_S(0) \rangle + \frac{1}{2}\omega_0 \frac{\gamma^{sr}}{\gamma^{rf}} \right) e^{-\gamma^{rf}\tau} \quad (34)$$

A number of interesting points can be inferred from (34): First the relaxation into equilibrium is always exponential, without oscillations, no matter what the trajectory of the atom or the state of the reservoir is. Its rate is determined by the contribution of reservoir fluctuations γ^{rf} alone. Furthermore, the first two terms of (34) show that the equilibrium excitation above the ground state $-\frac{1}{2}\omega_0$ is governed by the relative magnitude of γ^{rf} and γ^{sr} .

The Einstein coefficients $A_\uparrow$ and $A_\downarrow$ can be identified by comparison of (34) with an appropriate rate equation (Eq. (65) of [2]). One finds

$$A_\uparrow = \frac{1}{2}\gamma^{rf} - \frac{1}{2}\gamma^{sr}, \quad A_\downarrow = \frac{1}{2}\gamma^{rf} + \frac{1}{2}\gamma^{sr}. \quad (35)$$

The important consequence is that γ^{rf} and γ^{sr} (and therefore Γ_{ab}^{rf} and Γ_{ab}^{sr}) can separately be determined as functions of the Einstein coefficients. In principle they are therefore measurable quantities. Beyond that one can read off from (35) the physical origin of the Unruh effect [6]. Taking as reservoir the vacuum, the spontaneous excitation of an accelerated two-level atom results from an imbalance between the contributions of vacuum fluctuations and radiation reaction as has been discussed in detail in [2].

The radiative energy shift, which in this case is called the Lamb shift of the two-level atom can now be obtained by application of the formulas (20) and (22). First we notice that generally the contribution of self reaction does not contribute to the relative shift of the two levels. From (22) it follows after a short calculation that

$$\Delta_{sr} = \delta E_+^{sr} - \delta E_-^{sr} = 0. \quad (36)$$

On the other hand, the contribution of reservoir fluctuations is

$$\begin{aligned} \Delta_{tot} &= \Delta_{rf} = \delta E_+^{rf} - \delta E_-^{rf} \\ &= \frac{1}{2\pi} \int_0^\infty d\omega' \gamma^{rf}(\omega') \left(\frac{\mathcal{P}}{\omega' + \omega_0} - \frac{\mathcal{P}}{\omega' - \omega_0} \right), \end{aligned} \quad (37)$$

where the symmetry properties of $\gamma^{rf}(\omega')$ have been used. It is determined by the fluctuations of the reservoir in accordance with the heuristic picture of Welton [7]. In the derivation of Eq. (37), no other properties of the reservoir and no further assumptions about boundaries or the atomic trajectory were used. Their influences are contained in the form of γ^{rf} . Note that the energy shift can be determined once the functional form of the Einstein coefficients (35) is known. This is so much the more remarkable since, in contrast to the usual expression for the Lamb shift, they can be calculated easily for a given system, for example from Fermi's golden rule.

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