# Master Equation for Electromagnetic Dissipation and Decoherence of Density Matrix

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We set up a forward–backward path integral for a point particle in a bath of photons to derive a master equation for the density matrix which describes electromagnetic dissipation and decoherence. As an application, we recalculate the Weisskopf-Wigner formula for the natural line width of an atomic state at zero temperature and find, in addition, the temperature broadening caused by the decoherence term.

### I. INTRODUCTION

The time evolution of a quantum-mechanical density matrix  $\rho(\mathbf{x}_{+a}, \mathbf{x}_{-a}; t_a)$  of a particle coupled to an external electromagnetic vector potential  $\mathbf{A}(\mathbf{x}, t)$  is determined by a forward-backward path integral [1]

$$(\mathbf{x}_{+b}, t_b | \mathbf{x}_{+a}, t_a)(\mathbf{x}_{-b}, t_b | \mathbf{x}_{-a}, t_a)^* \equiv U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a)$$

$$= \int \mathcal{D}\mathbf{x}_{+} \mathcal{D}\mathbf{x}_{-} \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} \left[ \frac{M}{2} \left( \dot{\mathbf{x}}_{+}^2 - \dot{\mathbf{x}}_{-}^2 \right) - V(\mathbf{x}_{+}) + V(\mathbf{x}_{-}) - \frac{e}{c} \dot{\mathbf{x}}_{+} \mathbf{A}(\mathbf{x}_{+}, t) + \frac{e}{c} \dot{\mathbf{x}}_{-} \mathbf{A}(\mathbf{x}_{-}, t) \right] \right\}, \tag{1.1}$$

where  $\mathbf{x}_{+}(t)$  and  $\mathbf{x}_{-}(t)$  are two fluctuating paths connecting the initial and final points  $\mathbf{x}_{+a}$  and  $\mathbf{x}_{-b}$ , and  $\mathbf{x}_{-a}$  and  $\mathbf{x}_{-b}$ , respectively. In terms of this expression, the density matrix  $\rho(\mathbf{x}_{+b}, \mathbf{x}_{-b}; t_b)$  at a time  $t_b$  is found from that at an earlier time  $t_a$  by the integral

$$\rho(\mathbf{x}_{+b}, \mathbf{x}_{-b}; t_b) = \int d\mathbf{x}_{+a} d\mathbf{x}_{-a} U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a) \rho(\mathbf{x}_{+a}, \mathbf{x}_{-a}; t_a). \tag{1.2}$$

The vector potential  $\mathbf{A}(\mathbf{x},t)$  is a superposition of oscillators  $\mathbf{X}_{\mathbf{k}}(t)$  of frequency  $\Omega_{\mathbf{k}} = c|\mathbf{k}|$  in a volume V:

$$\mathbf{A}(\mathbf{x},t) = \sum_{\mathbf{k}} c_{\mathbf{k}}(\mathbf{x}) \mathbf{X}_{\mathbf{k}}(t), \quad c_{\mathbf{k}} = \frac{e^{i\mathbf{k}\mathbf{x}}}{\sqrt{2\Omega_{\mathbf{k}}V}}, \quad \sum_{\mathbf{k}} = \int \frac{d^3kV}{(2\pi)^3}.$$
 (1.3)

These oscillators are assumed to be in equilibrium at a finite temperature T, where we shall write their time-ordered correlation functions as  $G^{ij}_{\mathbf{k}\mathbf{k}'}(t,t') = \langle \hat{T}\hat{X}^i_{\mathbf{k}}(t), \hat{X}^j_{-\mathbf{k}'}(t') \rangle = \delta^{ij}_{\mathbf{k}\mathbf{k}'}G_{\Omega_{\mathbf{k}}}(t,t') \equiv (\delta^{ij} - k^ik^j/\mathbf{k}^2)G_{\Omega_{\mathbf{k}}}(t,t')$ , the transverse Kronecker symbol resulting from the sum over the two polarization vectors  $\sum_{h=\pm} \epsilon^i(\mathbf{k},h)\epsilon^{j*}(\mathbf{k},h)$  of the vector potential  $\mathbf{A}(\mathbf{x},t)$ . For a single oscillator of frequency  $\Omega$ , one has for t > t':

$$G_{\Omega}(t,t') = \frac{1}{2} \left[ A_{\Omega}(t,t') + C_{\Omega}(t,t') \right] = \frac{\hbar}{2M\Omega} \frac{\cosh\frac{\Omega}{2} \left[ \hbar\beta - i(t-t') \right]}{\sinh\frac{\hbar\Omega\beta}{2}}, \quad t > t'$$

$$(1.4)$$

which is the analytic continuation of the periodic imaginary-time Green function to  $\tau=it$ . The decompostion into  $A_{\Omega}(t,t')$  and  $C_{\Omega}(t,t')$  distinguishes real and imaginary parts, which are commutator and anticommutator functions of the oscillator at temperature  $T: C_{\Omega}(t,t') \equiv \langle [\hat{X}(t),\hat{X}(t')] \rangle_T$  and  $A_{\Omega}(t,t') \equiv \langle [\hat{X}(t),\hat{X}(t')] \rangle_T$ , respectively. The thermal average of the probability (1.1) is then given by the forward–backward path integral

$$U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a) = \int \mathcal{D}\mathbf{x}_{+}(t) \int \mathcal{D}\mathbf{x}_{-}(t)$$

$$\times \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{M}{2} (\dot{\mathbf{x}}_{+}^2 - \dot{\mathbf{x}}_{-}^2) - (V(\mathbf{x}_{+}) - V(\mathbf{x}_{-}))\right] + \frac{i}{\hbar} \mathcal{A}^{\text{FV}}[\mathbf{x}_{+}, \mathbf{x}_{-}]\right\}. \tag{1.5}$$

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where  $\exp\{i\mathcal{A}^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-]/\hbar\}$  is the Feynman-Vernon influence functional. The inluence action  $i\mathcal{A}^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-]$  is the sum of a dissipative and a fluctuating part  $\mathcal{A}^{\mathrm{FV}}_D[\mathbf{x}_+,\mathbf{x}_-]$  and  $\mathcal{A}^{\mathrm{FV}}_F[\mathbf{x}_+,\mathbf{x}_-]$ , respectively, whose explicit forms are

$$\mathcal{A}_{D}^{\text{FV}}[\mathbf{x}_{+}, \mathbf{x}_{-}] = \frac{ie^{2}}{2\hbar c^{2}} \int dt \int dt' \,\Theta(t - t') \Big[ \dot{\mathbf{x}}_{+} \mathbf{C}_{\text{b}}(\mathbf{x}_{+} t, \mathbf{x}'_{+} t') \dot{\mathbf{x}}'_{+} - \dot{\mathbf{x}}_{+} \mathbf{C}_{\text{b}}(\mathbf{x}_{+} t, \mathbf{x}'_{-} t') \dot{\mathbf{x}}'_{-}$$

$$- \dot{\mathbf{x}}_{-} \mathbf{C}_{\text{b}}(\mathbf{x}_{-} t, \mathbf{x}'_{+} t') \dot{\mathbf{x}}'_{+} - \dot{\mathbf{x}}_{-} \mathbf{C}_{\text{b}}(\mathbf{x}_{-} t, \mathbf{x}'_{-} t') \dot{\mathbf{x}}'_{-} \Big].$$

$$(1.6)$$

and

$$\mathbf{A}_{F}^{\text{FV}}[\mathbf{x}_{+}, \mathbf{x}_{-}] = \frac{ie^{2}}{2\hbar c^{2}} \int dt \int dt' \,\Theta(t - t') \Big[ \dot{\mathbf{x}}_{+} \mathbf{A}_{\text{b}}(\mathbf{x}_{+} t, \mathbf{x}_{+}' t') \dot{\mathbf{x}}_{+}' - \dot{\mathbf{x}}_{+} \mathbf{A}_{\text{b}}(\mathbf{x}_{+} t, \mathbf{x}_{-}' t') \dot{\mathbf{x}}_{-}' \\ - \dot{\mathbf{x}}_{-} \mathbf{A}_{\text{b}}(\mathbf{x}_{-} t, \mathbf{x}_{+}' t') \dot{\mathbf{x}}_{+}' + \dot{\mathbf{x}}_{-} \mathbf{A}_{\text{b}}(\mathbf{x}_{-} t, \mathbf{x}_{-}' t') \dot{\mathbf{x}}_{-}' \Big].$$

$$(1.7)$$

where  $\mathbf{x}_{\pm}$ ,  $\mathbf{x}'_{\pm}$  are short for  $\mathbf{x}_{\pm}(t)$ ,  $\mathbf{x}_{\pm}(t')$ , and  $\mathbf{C}_{\mathrm{b}}(\mathbf{x}_{-}t,\mathbf{x}'_{-}t')$ ,  $\mathbf{A}_{\mathrm{b}}(\mathbf{x}_{-}t,\mathbf{x}'_{-}t')$  are  $3\times3$  commutator and anticommutator functions of the bath of photons. They are sums of correlation functions over the bath of the oscillators of frequency  $\Omega_{\mathbf{k}}$ , each contributing with a weight  $c_{\mathbf{k}}(\mathbf{x})c_{-\mathbf{k}}(\mathbf{x}')=e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')}/2\Omega_{\mathbf{k}}V$ . Thus we may write

$$C_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') = \sum_{\mathbf{k}} c_{-\mathbf{k}}(\mathbf{x})c_{\mathbf{k}}(\mathbf{x}') \left\langle \left[\hat{X}_{-\mathbf{k}}^{i}(t),\hat{X}_{\mathbf{k}}^{j}(t')\right]\right\rangle_{T} = -i\hbar \int \frac{d\omega' d^{3}k}{(2\pi)^{4}} \sigma_{\mathbf{k}}(\omega') \delta_{\mathbf{k}\mathbf{k}}^{ij\,\mathrm{tr}} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \sin\omega'(t-t'), \tag{1.8}$$

$$A_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') = \sum_{\mathbf{k}} c_{-\mathbf{k}}(\mathbf{x})c_{\mathbf{k}}(\mathbf{x}') \left\langle \left\{ \hat{X}_{-\mathbf{k}}^{i}(t), \hat{X}_{\mathbf{k}}^{j}(t') \right\} \right\rangle_{T} = \hbar \int \frac{d\omega' d^{3}k}{(2\pi)^{4}} \sigma_{\mathbf{k}}(\omega') \delta_{\mathbf{k}\mathbf{k}}^{ij\,\text{tr}} \coth \frac{\hbar\omega'}{2k_{B}T} e^{i\mathbf{k}(\mathbf{x}-\mathbf{x}')} \cos \omega'(t-t'), \quad (1.9)$$

where  $\sigma_{\mathbf{k}}(\omega')$  is the spectral density contributed by the oscillator of momentum  $\mathbf{k}$ :

$$\sigma_{\mathbf{k}}(\omega') \equiv \frac{2\pi}{2\Omega_{\mathbf{k}}} [\delta(\omega' - \Omega_{\mathbf{k}}) - \delta(\omega' + \Omega_{\mathbf{k}})]. \tag{1.10}$$

At zero temperature, we recognize in (1.8) and (1.9) twice the imaginary and real parts of the Feynman propagator of a massless particle for t > t', which in four-vector notation with  $k = (\omega/c, \mathbf{k})$  and  $x = (ct, \mathbf{x})$  reads

$$G(x,x') = \frac{1}{2} \left[ A(x,x') + C(x,x') \right] = \int \frac{d^4k}{(2\pi)^4} e^{ik(x-x')} \frac{i\hbar}{k^2 + i\eta} = \int \frac{d\omega}{(2\pi)^4} \frac{d^3k}{\omega^2 - \Omega_{\mathbf{k}}^2 + i\eta} e^{-i[\omega(t-t') - \mathbf{k}(\mathbf{x} - \mathbf{x}')]}, \quad (1.11)$$

where  $\eta$  is an infinitesimally small number > 0.

We shall now focus attention upon nonrelativistic systems which are so small that the effects of retardation can be neglected. Then we can ignore the **x**-dependence in (1.8) and (1.9) and find

$$C_{\rm b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') \approx C_{\rm b}^{ij}(t,t') = -i\frac{\hbar}{6\pi^2}\delta^{ij}\partial_t\delta^R(t-t'). \tag{1.12}$$

The superscript R indicate that the  $\delta$ -function is a right-sided one, with the property

$$\int dt \,\Theta(t)\delta^R(t) = 1. \tag{1.13}$$

The retarded nature of the  $\delta$ -function expresses the *causality* of the dissipation forces, which is crucial for producing a probability conserving time evolution of the probability distribution [6].

Inserting this into (1.6) and integrating by parts, we obtain two contributions. The first is a diverging term

$$\Delta \mathcal{A}_{loc}[\mathbf{x}_+, \mathbf{x}_-] = \frac{\Delta M}{2} \int_{t_a}^{t_b} dt \, (\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2)(t), \tag{1.14}$$

where

$$\Delta M \equiv -\frac{e^2}{c^2} \int \frac{d\omega' d^3k}{(2\pi)^4} \frac{\sigma_{\mathbf{k}}(\omega')}{\omega'} \delta_{\mathbf{k}\mathbf{k}}^{ij \text{ tr}} = -\frac{e^2}{6\pi^2 c^3} \int_{-\infty}^{\infty} dk.$$
 (1.15)

diverges linearly. This simply renormalizes the kinetic terms in the path integral (1.5), renormalizing them to

$$\frac{i}{\hbar} \int_{t_a}^{t_b} dt \, \frac{M_{\text{ren}}}{2} \left( \dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2 \right). \tag{1.16}$$

By identifying M with  $M_{\rm ren}$  this renormalization may be ignored.

The second term has the form

$$\mathcal{A}_D^{\text{FV}}[\mathbf{x}_+, \mathbf{x}_-] = -\gamma \frac{M}{2} \int_{t_a}^{t_b} dt \, (\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t) (\ddot{\mathbf{x}}_+ + \ddot{\mathbf{x}}_-)^R(t), \tag{1.17}$$

with the friction constant

$$\gamma \equiv \frac{e^2}{6\pi c^3 M} = \frac{2}{3} \frac{\alpha}{\omega_M},\tag{1.18}$$

where  $\alpha \equiv e^2/\hbar c \approx 1/137$  is the feinstructure constant and  $\omega_M \equiv Mc^2/\hbar$  the Compton frequency associated with the mass M. In contrast to the ordinary friction constant, this has the dimension 1/frequency. A dependence of the mass renormalization on the potential V (the Lamb shift) will be discussed in Sec. IV.

The superscript R in (1.17) indicates that the the acceleration  $(\ddot{\mathbf{x}}_+ + \ddot{\mathbf{x}}_-)(t)$  is slightly shifted with respect to the velocity factor  $(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t)$  towards an earlier time. This accounts for the fact that a physical friction force is always retarded, due to the Heaviside function in (1.6). The retardation expresses the *causality* of the dissipation forces, which is crucial for producing a probability conserving time evolution of the probability distribution [6].

We now turn to the anticommutator function. Inserting (1.10) and the friction constant  $\gamma$  from (1.18), it becomes

$$\frac{e^2}{c^2} A_{\rm b}(\mathbf{x} t, \mathbf{x}' t') \approx 2\gamma k_B T K(t, t'), \tag{1.19}$$

where

$$K(t,t') = K(t-t') \equiv \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} K(\omega') e^{-i\omega'(t-t')},$$
(1.20)

with a Fourier transform

$$K(\omega') \equiv \frac{\hbar \omega'}{2k_B T} \coth \frac{\hbar \omega'}{2k_B T},\tag{1.21}$$

whose high-temperature expansion starts out like

$$K(\omega') \approx K^{\rm HT}(\omega') \equiv 1 - \frac{1}{3} \left(\frac{\hbar \omega'}{2k_B T}\right)^2.$$
 (1.22)

The function  $K(\omega')$  has the normalization K(0) = 1, giving K(t - t') a unit temporal area:

$$\int_{-\infty}^{\infty} dt \, K(t - t') = 1. \tag{1.23}$$

Thus K(t-t') may be viewed as a  $\delta$ -function broadened by quantum fluctuations and relaxation effects. With the function K(t,t'), the fluctuation part of the influence functional in (1.7), (1.6), (1.5) becomes

$$\mathcal{A}_{F}^{\text{FV}}[\mathbf{x}_{+}, \mathbf{x}_{-}] = i \frac{w}{2\hbar} \int_{t_{a}}^{t_{b}} dt \int_{t_{a}}^{t_{b}} dt' \left(\dot{\mathbf{x}}_{+} - \dot{\mathbf{x}}_{-}\right)(t) K(t, t') \left(\dot{\mathbf{x}}_{+} - \dot{\mathbf{x}}_{-}\right)(t'). \tag{1.24}$$

Here we have used the symmetry of the function K(t, t') to remove the Heaviside function  $\Theta(t-t')$  from the integrand, extending the range of t'-integration to the entire interval  $(t_a, t_b)$ . We have also introduced the constant

$$w \equiv 2M\gamma k_B T,\tag{1.25}$$

for brevity.

At very high temperatures, the time evolution amplitude for the density matrix is given by the path integral

$$U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a) = \int \mathcal{D}\mathbf{x}_{+}(t) \int \mathcal{D}\mathbf{x}_{-}(t) \exp\left\{\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[\frac{M}{2} (\dot{\mathbf{x}}_{+}^2 - \dot{\mathbf{x}}_{-}^2) - (V(\mathbf{x}_{+}) - V(\mathbf{x}_{-}))\right]\right\}$$

$$\times \exp\left\{-\frac{i}{2\hbar} M \gamma \int_{t_a}^{t_b} dt \left(\dot{\mathbf{x}}_{+} - \dot{\mathbf{x}}_{-}\right) (\ddot{\mathbf{x}}_{+} + \ddot{\mathbf{x}}_{-})^R - \frac{w}{2\hbar^2} \int_{t_a}^{t_b} dt \left(\dot{\mathbf{x}}_{+} - \dot{\mathbf{x}}_{-}\right)^2\right\}, \quad (1.26)$$

where the last term becomes local for high temperatures, since  $K(t,t') \to \delta(t-t')$ . This is the *closed-time path integral* of a particle in contact with a thermal reservoir. For moderately high temperature, we should include also the first correction term in (1.22) which adds to the exponent an additional term.

$$\frac{w}{24(k_BT)^2} \int_{t_a}^{t_b} dt \, (\ddot{\mathbf{x}}_+ - \ddot{\mathbf{x}}_-)^2. \tag{1.27}$$

In the classical limit, the last squeeses the forward and backward paths together. The density matrix (1.26) becomes diagonal. The  $\gamma$ -term, however, remains and describes classical radiation damping.

# II. LANGEVIN EQUATIONS

For high  $\gamma T$ , the last term in the forward–backward path integral (1.26) makes the size of the fluctuations in the difference between the paths  $\mathbf{y}(t) \equiv \mathbf{x}_+(t) - \mathbf{x}_-(t)$  very small. It is then convenient to introduce the average of the two paths as  $\mathbf{x}(t) \equiv [\mathbf{x}_+(t) + \mathbf{x}_-(t)]/2$ , and expand

$$V\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) - V\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \sim \mathbf{y} \cdot \nabla V(\mathbf{x}) + \mathcal{O}(\mathbf{y}^3) \dots$$
, (2.1)

keeping only the first term. We further introduce an auxiliary quantity  $\eta(t)$  by

$$\dot{\boldsymbol{\eta}}(t) \equiv M\ddot{\mathbf{x}}(t) - M\gamma \ddot{\mathbf{x}}(t) + \nabla V(\mathbf{x}(t)). \tag{2.2}$$

With this, the exponential function in (1.26) becomes

$$\exp\left[-\frac{i}{\hbar} \int_{t}^{t_{b}} dt \,\dot{\mathbf{y}} \boldsymbol{\eta} - \frac{w}{2\hbar^{2}} \int_{t}^{t_{b}} dt \,\dot{\mathbf{y}}^{2}(t)\right],\tag{2.3}$$

where w is the constant (1.25).

Consider now the diagonal part of the amplitude (2.1) with  $\mathbf{x}_{+b} = \mathbf{x}_{-b} \equiv \mathbf{x}_b$  and  $\mathbf{x}_{+a} = \mathbf{x}_{-a} \equiv \mathbf{x}_a$ , implying that  $\mathbf{y}_b = \mathbf{y}_a = 0$ . It represents a probability distribution

$$P(\mathbf{x}_b t_b | \mathbf{x}_a t_a) \equiv |(\mathbf{x}_b, t_b | \mathbf{x}_a, t_a)|^2 \equiv U(\mathbf{x}_b, \mathbf{x}_b, t_b | \mathbf{x}_a, \mathbf{x}_a, t_a). \tag{2.4}$$

Now the variable y can simply be integrated out in (2.3), and we find the probability distribution

$$P[\eta] \propto \exp\left[-\frac{1}{2w} \int_{t_a}^{t_b} dt \, \eta^2(t)\right].$$
 (2.5)

The expectation value of an arbitrary functional of F[x] can be calculated from the path integral

$$\langle F[\mathbf{x}] \rangle_{\eta} \equiv \mathcal{N} \int \mathcal{D}\mathbf{x} P[\boldsymbol{\eta}] F[\mathbf{x}],$$
 (2.6)

where the normalization factor  $\mathcal{N}$  is fixed by the condition  $\langle 1 \rangle = 1$ . By a change of integration variables from x(t) to  $\eta(t)$ , the expectation value (2.6) can be rewritten as a functional integral

$$\langle F[\mathbf{x}] \rangle_{\eta} \equiv \mathcal{N} \int \mathcal{D} \boldsymbol{\eta} P[\boldsymbol{\eta}] F[\mathbf{x}],$$
 (2.7)

Note that the probability distribution (2.5) is  $\hbar$ -independent. Hence in the approximation (2.1) we obtain the classical Langevin equation. In principle, the integrand contains a factor  $J^{-1}[x]$ , where J[x] is the functional Jacobian

$$J[\mathbf{x}] \equiv \text{Det}\left[\delta \eta^{i}(t)/\delta x^{j}(t')\right] = \det\left[\left(M\partial_{t}^{2} - M\gamma \partial_{t}^{3R}\right)\delta_{ij} + \nabla_{i}\nabla_{j}V(\mathbf{x}(t))\right]. \tag{2.8}$$

It can be shown that the determinant is unity, due to the retardation of the friction term [6], thus justifying its omission in (2.7).

The path integral (2.7) may be interpreted as an expectation value with respect to the solutions of a *stochastic* differential equation (2.2) driven by a Gaussian random noise variable  $\eta(t)$  with a correlation function

$$\langle \eta^i(t)\eta^j(t')\rangle_T = \delta^{ij}w\,\delta(t-t'). \tag{2.9}$$

Since the dissipation carries a third time derivative, the treatment of the initial conditions is nontrivial and will be discussed elsewhere. In most physical applications  $\gamma$  leads to slow decay rates. In this case the simplest procedure to solve (2.2) is to write the stochastic equation as

$$M\ddot{\mathbf{x}}(t) + \nabla V(\mathbf{x}(t)) = \dot{\boldsymbol{\eta}}(t) + M\gamma \ddot{\mathbf{x}}(t), \tag{2.10}$$

and solve it iteratively, first without the  $\gamma$ -term, inserting the solution on the right-hand side, and such a procedure is equivalent to a perturbative expansion in  $\gamma$  in Eq. (1.26).

# III. MASTER EQUATION FOR TIME EVOLUTION OF DENSITY MATRIX

We now derive a Schrödinger-like differential equation describing the evolution of the density matrix  $\rho(x_{+a}, x_{-a}; t_a)$  in Eq. (1.2). In the standard derivation of such an equation [4] one first localizes the last term via a quadratic completion involving a fluctuating noise variable  $\eta(t)$ . Then one goes over to a canonical formulation of the path integral (1.26), by rewriting it as a path integral

$$U_{\eta}(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_{b} | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_{a}) = \int \mathcal{D}\mathbf{x}_{+}(t) \int \mathcal{D}\mathbf{x}_{-}(t) \int \frac{\mathcal{D}\mathbf{p}_{+}}{(2\pi)^{3}} \int \frac{\mathcal{D}\mathbf{p}_{-}}{(2\pi)^{3}}$$

$$\times \exp \left\{ \frac{i}{\hbar} \int_{t_{a}}^{t_{b}} dt \left[ \mathbf{p}_{+} \dot{\mathbf{x}}_{+} - \mathbf{p}_{-} \dot{\mathbf{x}}_{-} - \mathcal{H}_{\eta}(\mathbf{p}_{+}, \mathbf{p}_{-}, \mathbf{x}_{+}, \mathbf{x}_{-}) \right] \right\}. \tag{3.1}$$

Then  $U_{\eta}(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a)$  satisfies the differential equation

$$i\hbar \partial_t U_{\eta}(x, y, t | x_a, y_a, t_a) = \hat{\mathcal{H}}_{\eta} U_{\eta}(x, y, t | x_a, y_a, t_a). \tag{3.2}$$

The same equation is obeyed by the density matrix  $\rho(x_+, x_-; t_a)$ .

At high temperatures where the action in the path integral (1.26) is local, we can find directly a Hamiltonian without the noise-averaging procedure. However, the standard procedure of finding a canonical formulation is not applicable because of the high time derivatives of  $\mathbf{x}(t)$  in the action of (1.26). They can be transformed into canonical momentum variables only by introducing several auxiliary independent variables  $\mathbf{v} \equiv \dot{\mathbf{x}}$ ,  $\mathbf{b} \equiv \ddot{\mathbf{x}}$ , ... [2,3]. For small dissipation, which we shall consider, it is preferable to proceed in another way by going first to a canonical formulation of the quantum system without the effect of electromagnetism, and include the effect of the latter recursively. For simplicity, we shall treat only the local limiting form of the last term in (1.26). In this limit, we define a Hamilton-like operator as follows:

$$\hat{\mathcal{H}} = \frac{1}{2M} \left( \hat{\mathbf{p}}_{+}^{2} - \hat{\mathbf{p}}_{-}^{2} \right) + V(\mathbf{x}_{+}) - V(\mathbf{x}_{-}) + \frac{M\gamma}{2} \left( \hat{\mathbf{x}}_{+} - \hat{\mathbf{x}}_{-} \right) \left( \hat{\mathbf{x}}_{+} + \hat{\mathbf{x}}_{-} \right)^{R} - i \frac{w}{2\hbar} (\hat{\mathbf{x}}_{+} - \hat{\mathbf{x}}_{-})^{2}.$$
(3.3)

Here  $\hat{\mathbf{x}}$ ,  $\hat{\mathbf{x}}$  are abbreviations for the commutators

$$\hat{\mathbf{x}} \equiv \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{\mathbf{x}}], \quad \hat{\mathbf{x}} \equiv \frac{i}{\hbar} [\hat{\mathcal{H}}, \hat{\dot{\mathbf{x}}}]. \tag{3.4}$$

A direct differentiation of Eq. (1.26) over time leads to the conclusion that the density matrix  $\rho(x_+, x_-; t_a)$  satisfies the time evolution equation

$$i\hbar\partial_t \rho(x_+, x_-; t_a) = \hat{\mathcal{H}}\rho(x_+, x_-; t_a). \tag{3.5}$$

At moderately high temperatures, we also include a term coming from (1.27)

$$\mathcal{H}_1 \equiv i \frac{w}{24(k_B T)^2} (\hat{\mathbf{x}}_+ - \hat{\mathbf{x}}_-)^2. \tag{3.6}$$

For systems with fricition caused by a conventional heat bath of harmonic oscillators as discussed by Caldeira and Leggett [7], the analogous extra term was shown by Diosi [8] to bring the Master equation to the general Lindblad form [9] which ensures positivity of the probabilities resulting from the solutions of (3.5).

It is useful to re-express (3.5) in the standard quantum-mechanical operator form where the density matrix has a bra-ket representation  $\hat{\rho}(t) = \sum_{mn} \rho_{nm}(t) |m\rangle\langle n|$ . Let us denote the initial Hamilton operator of the system in (1.1) by  $\hat{H} = \hat{\mathbf{p}}^2/2M + \hat{V}$ , then Eq. (3.5) with the term (3.6) takes the operator form

$$i\hbar\partial_t\hat{\rho} = \hat{\mathcal{H}}\,\hat{\rho} \equiv [\hat{H},\hat{\rho}] + \frac{M\gamma}{2}\left(\hat{\mathbf{x}}\hat{\mathbf{x}}\hat{\rho} + \hat{\rho}\hat{\mathbf{x}}\hat{\mathbf{x}} - \hat{\mathbf{x}}\,\hat{\rho}\,\hat{\mathbf{x}} - \hat{\mathbf{x}}\,\hat{\rho}\,\hat{\mathbf{x}}\right) - \frac{iw}{2}[\hat{\mathbf{x}},[\hat{\mathbf{x}},\hat{\rho}]] + \frac{iw\hbar^2}{24(k_BT)^2}[\hat{\mathbf{x}},[\hat{\mathbf{x}},\hat{\rho}]]. \tag{3.7}$$

The retardation of  $\ddot{\mathbf{x}}_{\pm}$  in (3.3) leads to the specific operator order in the second term, which ensures that Eqs. (3.3) and (3.7) preserve the total probability.

For a free particle with V=0 and  $[\mathcal{H}, \mathbf{p}]=0$ , one has  $\hat{\mathbf{x}}_{\pm}=\hat{\mathbf{p}}_{\pm}/M$  to all orders in  $\gamma$ , such that the time evolution equation (3.7) becomes

$$i\hbar\partial_t\hat{\rho} = [\hat{H},\hat{\rho}] - \frac{iw}{2M^2}[\hat{\mathbf{p}},[\hat{\mathbf{p}},\hat{\rho}]].$$
 (3.8)

In the momentum representation of the density matrix  $\hat{\rho} = \sum_{\mathbf{p}\mathbf{p}'} \rho_{\mathbf{p}\mathbf{p}'} |\mathbf{p}\rangle\langle\mathbf{p}'|$ , the last term simplifies to  $-i\Gamma \equiv -iw(\mathbf{p} - \mathbf{p}')^2/2M^2$  showing that a free particle does not dissipate energy by radiation, and that the off-diagonal matrix elements decay with the rate  $\Gamma$ .

In general, Eq. (3.3) is an implicit equation for the Hamilton operator  $\hat{\mathcal{H}}$ . For small  $e^2$  it can be solved approximately in a single iteration step, replacing  $\hat{\mathbf{x}}$  by  $\hat{\mathbf{p}}/M$  and  $\hat{\mathbf{x}} = -\nabla V/M$  in Eq. (3.7).

The validity of this iterative procedure is most easily proven in the time-sliced path integral. The final slice of infinitesimal width  $\epsilon$  reads

$$U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b | \mathbf{x}_{+a}, \mathbf{x}_{-a}, t_b - \epsilon) = \int \frac{d\mathbf{p}_+(t_b)}{(2\pi)^3} \int \frac{d\mathbf{p}_-(t_b)}{(2\pi)^3} e^{\frac{i}{\hbar} \{\mathbf{p}_+(t_b)[\mathbf{x}_+(t_b) - \mathbf{x}_+(t_b - \epsilon)] - \mathbf{p}_-\dot{\mathbf{x}}_- - \mathcal{H}(t_b)\}}.$$
(3.9)

Consider now a term of the generic form  $\dot{F}_{+}(\mathbf{x}_{+})F_{-}(\mathbf{x}_{-})$  in  $\mathcal{H}$ . When differentiating  $U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_{b}|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_{b} - \epsilon)$  with respect to the final time  $t_{b}$ , the integrand receives a factor  $-\mathcal{H}(t_{b})$ . The term  $\dot{F}_{+}(\mathbf{x}_{+})F_{-}(\mathbf{x}_{-})$  in  $\mathcal{H}$  has the explicit form  $\epsilon^{-1}[F_{+}(\mathbf{x}_{+}(t_{b})) - F_{+}(\mathbf{x}_{+}(t_{b} - \epsilon))]F_{-}(\mathbf{x}_{-}(t_{b}))$ . It it can be taken out of the integral, yielding

$$\epsilon^{-1} \left[ F_{+}(\mathbf{x}_{+}(t_b))U - UF_{+}(\mathbf{x}_{+}(t_b - \epsilon)) \right] F_{-}(\mathbf{x}_{-}(t_b)). \tag{3.10}$$

In operator language, the amplitude U is equal to  $\hat{U} \approx 1 - i\epsilon \hat{\mathcal{H}}/\hbar$ , such the term  $\dot{F}_{+}(\mathbf{x}_{+})F_{-}(\mathbf{x}_{-})$  in  $\mathcal{H}$  yields an operator

$$\frac{i}{\hbar} \left[ \hat{\mathcal{H}}, \hat{F}_{+}(\mathbf{x}_{+}) \right] F_{-}(x_{-}) \tag{3.11}$$

in the differential operator for the time evolution.

For functions of the second derivative  $\ddot{\mathbf{x}}$  we have to split off the last two time slices and convert the two intermediate integrals over  $\mathbf{x}$  into operator expressions, which obviously leads to the repeated commutator of  $\hat{\mathcal{H}}$  with  $\hat{\mathbf{x}}$ , and so on.

## IV. LINE WIDTH

Let us apply the master equation (3.7) to atoms, where  $V(\mathbf{x})$  is the Coulomb potential, assuming it to be initially in an eigenstate  $|i\rangle$  of H, with a density matrix  $\rho = |i\rangle\langle i|$ . Since atoms decay rather slowly, we may treat the  $\gamma$ -term in (3.7) perturbatively. It leads to a time derivative of the density matrix

$$\partial_t \langle i|\hat{\rho}(t)|i\rangle = -\frac{\gamma}{\hbar M} \langle i|[\hat{H}, \hat{\mathbf{p}}] \hat{\mathbf{p}} \hat{\rho}(0)|i\rangle = \frac{\gamma}{M} \sum_{f \neq i} \omega_{fi} \langle i|\mathbf{p}|f\rangle \langle f|\mathbf{p}|i\rangle = -M\gamma \sum_f \omega_{fi}^3 |\mathbf{x}_{fi}|^2. \tag{4.1}$$

where  $\hbar\omega_{fi} \equiv E_i - E_f$  and  $\mathbf{x}_{fi} \equiv \langle f|\mathbf{x}|i\rangle$  are the matrix elements of the dipole operator. A further contribution comes the last two terms in (3.7):

$$\partial_t \langle i | \rho | i \rangle = -\frac{w}{M^2 \hbar^2} \langle i | \mathbf{p}^2 | i \rangle + \frac{w}{12M^2 (k_B T)^2} \langle i | \dot{\mathbf{p}}^2 | i \rangle = -w \sum_n \omega_{fi}^2 \left[ 1 - \frac{\hbar^2 \omega_{fi}^2}{12(k_B T)^2} \right] |\mathbf{x}_{fi}|^2. \tag{4.2}$$

This time dependence is caused by spontaneous emission and induced emission and absorption. To identify these terms we rewrite the spectral content of a single oscillator of frequency  $\Omega$  in the local approximation  $A_{\rm b}^{ij}(t,t') + C_{\rm b}^{ij}(t,t')$  to the correlation functions in (1.8) and (1.9) in the **x**-independent approximation as

$$C_b(t,t') + A_b(t,t') = \frac{4\pi}{3}\pi\hbar \int \frac{d\omega d^3k}{(2\pi)^4} \frac{\pi}{2M\Omega_{\mathbf{k}}} \left(\coth\frac{\omega'}{2k_BT} + 1\right) \left[\delta(\omega' - \Omega_{\mathbf{k}}) - \delta(\omega' + \Omega_{\mathbf{k}})\right] e^{-i\omega'(t-t')},\tag{4.3}$$

as

$$C_b(t,t') + A_b(t,t') = \frac{4\pi}{3}\hbar \int \frac{d\omega d^3k}{(2\pi)^4} \frac{\pi}{M\Omega} \left\{ \delta(\omega' - \Omega_{\mathbf{k}}) + \frac{1}{e^{\Omega_{\mathbf{k}}/k_BT} - 1} [\delta(\omega' - \Omega_{\mathbf{k}}) + \delta(\omega' + \Omega_{\mathbf{k}})] \right\} e^{-i\omega'(t-t')}. \tag{4.4}$$

Following Einstein's intuitive interpretation, the first term in curly brackets is due to spontaneous emission, the other two terms accompanied by the Bose occupation function account for induced emission and absorption. In the large-T expressions (4.1) and (4.2), the first term in (4.4) leads to part of the sum with  $\omega_{fi} > 0$  only. This is the famous Wigner-Weisskopf formula for the natural line width of atomic levels.

The rest of the time dependence is due to induced absorption and emission.

### V. LAMB SHIFT

For atoms, the calculation of the diverging term (1.14) can be done in a more sensitive approximation. Being interested in the time behavior of the pure-state density matrix  $\rho = |i\rangle\langle i|$ , we may calculate the affect of the action (1.6) perturbatively as follows: Consider the first term in the local approximation, and integrate the external positions in the path integral (1.5) over the initial wave functions, forming

$$U_{ii,t_b;ii,t_a} = \int d\mathbf{x}_{+b} d\mathbf{x}_{-b} \int d\mathbf{x}_{+a} d\mathbf{x}_{-a} \langle i|\mathbf{x}_{+b} \rangle \langle i|\mathbf{x}_{-b} \rangle U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) \langle \mathbf{x}_{+b}|i\rangle \langle \mathbf{x}_{-b}|i\rangle$$
(5.1)

To lowest order in  $\gamma$ , the contribution of (1.6) can be evaluated as follows

$$\Delta U_{ii,t_b;ii,t_a} = i \frac{e^2}{\hbar^2 c^2} \int_{t_a}^{t_b} dt dt' \sum_f \int d\mathbf{x}_+ \int d\mathbf{x}_+' U_{ii,t_a;ii,t} \langle i|\mathbf{x}_+ \rangle \mathbf{x}_+ \langle \mathbf{x}_+|f \rangle \partial_t \partial_{t'} C_{\mathbf{b}}^{ij}(t,t') U_{fi,t;fi,t'} \langle f|\mathbf{x}_+' \rangle \mathbf{x}_+' \langle \mathbf{x}_+'|i \rangle U_{ii,t';ii,t_a}$$

$$(5.2)$$

Inserting  $U_{ii,t_a;ii,t} = e^{-iE_i(t_b-t)}$  etc., this becomes

$$\Delta U_{ii,t_b;ii,t_a} = i \frac{e^2}{\hbar^2 c^2} \int_{t_a}^{t_b} dt dt' \, \partial_t \partial_{t'} C_b(t,t') \langle i | \hat{\mathbf{x}}(t) \hat{\mathbf{x}}'(t') | i \rangle = i \frac{e^2}{\hbar^2 c^2} \sum_{\mathbf{f}} \int_{t_a}^{t_b} dt dt' \, C_b(t,t') \langle i | \hat{\mathbf{x}}(t) | f \rangle \langle f | \hat{\mathbf{x}}'(t') | i \rangle. \tag{5.3}$$

The integration over t and t' yields

$$\Delta U_{ii,t_b;ii,t_a} = i \frac{e^2}{\hbar^2 c^2} \int_{t_a}^{t_b} dt \int \frac{d\omega' d^3k}{(2\pi)^4} \sigma_k(\omega') \sum_f \frac{1}{E_i - E_f - \omega' - i\eta} |\hat{\mathbf{x}}_{fi}|^2$$
(5.4)

After subtracting the mass renormalization (1.14), which can be rewritten once more in the same form as in (5.4) with  $E_i - E_f = 0$ , the integral yields  $\ln[(\Lambda + E_i - E_f)/|E_i - E_f|]$  where  $\Lambda$  is Bethe's cutoff [10]. For  $\Lambda \gg |E_i - E_f|$ , the result (5.4) implies an energy shift of the atomic level  $|i\rangle$ :

$$\Delta E_i = \frac{e^2}{\hbar c^3} \frac{2\hbar}{3\pi} \sum_f \omega_{fi}^3 |\hat{\mathbf{x}}_{fi}|^2 \log \frac{\Lambda}{|\omega_{fi}|},\tag{5.5}$$

which is the celebrated Lamb shift. Usually, the logarithm is approximated by a weighted average L over energy levels. Then contribution of the term (5.4) can be attributed to an extra term in the Hamiltonian (3.7)  $H_{LS} = iLM\gamma/2[\hat{x}, \hat{x}]$ .

#### VI. CONCLUSION

We have calculated the master equation for the time evolution of the quantum mechanical density matrix describing dissipation and decoherence of a point particle interacting with the electromagnetic field. The Hamilton-like evolution operator was specified recursively. To lowest order in the electromagnetic coupling strength, we have recovered the known Lamb shift and natural line width of atomic levels. In addition, we have calculated the additional broadening caused by the coupling of the photons to the thermal bath.

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- [1] R.P. Feynman and F.L. Vernon, Ann. Phys. (N. Y.) 24, 118 (1963); see also R.P. Feynman and A.R. Hibbs, Quantum Mechanics and Path Integrals, McGraw-Hill, New York, 1965, Sections 12.8 and 12.9.
  - The hyphen in "forward-backward" is pronounced as minus, to emphasize the opposite signs in the partial actions.
- [2] H. Kleinert, J. Math. Phys. 27, 3003 (1986).
- [3] H. Kleinert, Gauge Fields in Condensed Matter, op. cit., Vol. II, World Scientific, Singapore (1989)
- [4] H. Kleinert, Path Integrals in Quantum Mechanics, Statistics and Polymer Physics, World Scientific, Singapore 1995, (http://www.physik.fu-berlin.de/~kleinert/re0.html#b5)
- [5] U. Weiss, Quantum Dissipative Systems, World Scientific, 1993.
- [6] For more details on the necessity and the consequences of retardation see H. Kleinert, Ann. of Phys. (in press) (quant-ph/0008109).
- [7] A.O. Caldeira and A.J. Leggett, Physica A 121, 587 (1983)
- [8] L. Diosi, Europhys. Lett. 22, 1 (1993)
- [9] G. Lindblad, Comm. Math. Phys. 48, 119 (1976)
- [10] H. A. Bethe, Phys. Rev. **72**, 339 (1947).