Path Integral of Charged Particle in Black Cavity

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Abstract. We solve the forward–backward path integral for a point particle in a bath of photons and derive from it a master equation for the density matrix with electromagnetic dissipation, as well as the associated Langevin equation. The path integral approach yields an alternative access to the Wigner-Weisskopf formula for the natural line width of an atomic state at zero temperature and, in addition, the temperature broadening caused by decoherence.

1. Introduction

The time evolution of a quantum-mechanical density matrix $\rho(x_+, x_-; t_a)$ of a particle coupled to an external electromagnetic vector potential $A(x, t)$ is determined by a forward–backward path integral [1, 2, 3]

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

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

$$
\rho(x_{+b}, x_{-b}; t_b) = \int dx_+ dx_- U(x_{+b}, x_{-b}, t_b|x_{+a}, x_{-a}, t_a)\rho(x_{+a}, x_{-a}; t_a).
$$

The vector potential $A(x, t)$, appearing in the electromagnetic action $A_{\text{em}} = \int d^4x(E^2 - B^2)/2c$ in the radiation gauge via $E = \dot{A}/c$, $B \equiv \nabla \times A$, is a superposition of oscillators $X_k(t)$ of frequency $\Omega_k = c|k|$ in a volume $V$:

$$
A(x, t) = \sum_k f_k(x)X_k(t), \quad f_k(x) = \frac{e^{ikx}}{\sqrt{2V\Omega_k/c}}, \quad \sum_k \equiv V \int \frac{d^3k}{(2\pi)^3}.
$$

These oscillators are assumed to be in equilibrium at a finite temperature $T$, where we shall write their time-ordered correlation functions as $G^{ij}_{kk}(t, t') = \langle \hat{T}X^i_k(t)\cdots\hat{T}X^j_k(t')\rangle = \delta^{ij}_{kk}G_{0k}(t, t') \delta_{kk}^T$, $G^{ij}_{kk}(t, t') \equiv \delta_{kk}^T(\delta^{ij} - k^i k^j/k^2)G_{0k}(t, t')$, the transverse Kronecker symbol resulting from the sum over the

1 Based on a talk presented at the conference “Progress in Nonequilibrium Green’s Functions III, Kiel, Germany, 22. – 25. August 2005”
two polarization vectors $\sum_{\alpha=\pm} e^\alpha(k,h) e^{j}\alpha(k,h)$ of the vector potential $A(x,t)$. For a single
oscillator of frequency $\Omega$, one has for $t > t'$:
\[
G_\Omega(t,t') = \frac{1}{2} \left[ A_\Omega(t,t') + C_\Omega(t,t') \right] = \frac{\hbar}{2M\Omega} \frac{\cosh \frac{\Omega}{2} [\hbar \beta - i (t - t')]}{\sinh \frac{\hbar \Omega \beta}{2}}, \quad t > t'
\]
which is the analytic continuation of the periodic imaginary-time Green function to $\tau = it$.
The decomposition into $A_\Omega(t,t')$ and $C_\Omega(t,t')$ distinguishes real and imaginary parts, which are
commutator and anticommutator functions of the bath of photons. They are sums of correlation
functions over the bath of the oscillators of frequency $\Omega$.

\[
\langle [\hat{X}(t), \hat{X}(t')]_T \rangle = \langle [\hat{X}(t), \hat{X}(t')]_{T} \rangle, \quad t > t'
\]

where $\exp\{iA_{FV}[x_+,x_-]/\hbar\}$ is the Feynman-Vernon influence functional. The influence action
$A_{FV}[x_+,x_-]$ is the sum of a dissipative and a fluctuating part $A_{D}^{FV}[x_+,x_-]$ and $A_{F}^{FV}[x_+,x_-]$, respectively, whose explicit forms are

\[
A_{D}^{FV}[x_+,x_-] = \frac{i e^2}{2\hbar c^2} \int dt \int dt' \Theta(t-t') \left[ \hat{x}_+ C_b(x_+ t, x'_+ t') \hat{x}'_+ - \hat{x}_- C_b(x_- t, x'_- t') \hat{x}'_- \right.
\]
\[
\left. - \hat{x}_- C_b(x_- t, x'_+ t') \hat{x}'_+ - \hat{x}_- C_b(x_- t, x'_- t') \hat{x}'_- \right].
\]

and

\[
A_{F}^{FV}[x_+,x_-] = \frac{i e^2}{2\hbar c^2} \int dt \int dt' \Theta(t-t') \left[ \hat{x}_+ A_b(x_+ t, x'_+ t') \hat{x}'_+ - \hat{x}_+ A_b(x_+ t, x'_- t') \hat{x}'_- \right.
\]
\[
\left. - \hat{x}_- A_b(x_- t, x'_+ t') \hat{x}'_+ + \hat{x}_- A_b(x_- t, x'_- t') \hat{x}'_- \right].
\]

where $x_\pm, x'_\pm$ are short for $x_\pm(t), x'_\pm(t')$, and $C_b(x_- t, x'_- t'), A_b(x_- t, x'_- t')$ are $3 \times 3$
commutator and anticommutator functions of the bath of photons. They are sums of correlation
functions over the bath of the oscillators of frequency $\Omega_k$, each contributing with a weight
$f_k(x)f_{-k}(x') = e^{ik(x-x')} c/2\Omega_k V$ (the normalization follows from the action $\int d^3x (E^2 - B^2)/2c$).

Thus we may write

\[
C_{b}^{ij}(x t, x' t') = \sum_k f_{-k}(x)f_k(x') \left\langle \left[ \hat{X}^i_{-k}(t), \hat{X}^j_{k}(t') \right] \right\rangle_T
\]
\[
= -i e^2 \hbar \int \frac{d\omega d^3k}{(2\pi)^3} \sigma_k(\omega') \delta_{ki}^{\text{tr}} \exp i k(x-x') \sin \omega'(t-t'),
\]

\[
A_{b}^{ij}(x t, x' t') = \sum_k f_{-k}(x)f_k(x') \left\langle \left\{ \hat{X}^i_{-k}(t), \hat{X}^j_{k}(t') \right\} \right\rangle_T
\]
\[
= \delta^2 \hbar \int \frac{d\omega d^3k}{(2\pi)^3} \sigma_k(\omega') \delta_{ki}^{\text{tr}} \coth \frac{\hbar \omega'}{2k_B T} \exp i k(x-x') \cos \omega'(t-t'),
\]

where $\sigma_k(\omega')$ is the spectral density contributed by the oscillator of momentum $k$:

\[
\sigma_k(\omega') = \frac{2\pi}{2\Omega_k} \delta(\omega' - \Omega_k) - \delta(\omega' + \Omega_k).
\]
At zero temperature, we recognize in (8) and (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

\[
G(x, x') = \frac{1}{2} \left[ A(x, x') + C(x, x') \right] = \int \frac{d\omega d^4k}{(2\pi)^4} \frac{ie^2\hbar}{\omega^2 - \Omega_k^2 + i\eta} e^{-i[\omega(t-t') - \mathbf{k}(\mathbf{x}-\mathbf{x}')}}.
\]

(11)

where \( \eta \) is an infinitesimally small number > 0.

We shall now focus attention upon systems which are so small that the effects of retardation can be neglected. Then we can ignore the \( x \)-dependence in (8) and (9) and find

\[
C_{ij}^{(x)}(x, x') \approx C_{ij}^{(x)}(t, t') = i\frac{\hbar}{2\pi^2} \delta^{ij} \delta(t - t').
\]

(12)

Inserting this into (6) and integrating by parts, we obtain two contributions. The first is a diverging term

\[
\Delta A_{loc}[x_+, x_-] = \frac{\Delta M}{2} \int_{t_a}^{t_b} dt \left( \dddot{x}_+^2 - \dddot{x}_-^2 \right)(t),
\]

(13)

where

\[
\Delta M = \frac{e^2}{c^2} \int \frac{d\omega' d^3k \sigma_k(\omega')}{(2\pi)^4} \frac{\delta^{ij}}{\omega' \omega^2} \delta_{kk} = \frac{e^2}{3\pi^2 c^3} \int_0^\infty dk.
\]

(14)

diverges linearly. This simply renormalizes the kinetic terms in the path integral (5), renormalizing them to

\[
\frac{i}{\hbar} \int_{t_a}^{t_b} dt \frac{M_{ren}}{2} \left( \dddot{x}_+^2 - \dddot{x}_-^2 \right).
\]

(15)

By identifying \( M \) with \( M_{ren} \) this renormalization may be ignored.

The second term has the form

\[
A_{DV}^{U}[x_+, x_-] = -\frac{\gamma M}{2} \int_{t_a}^{t_b} dt \left( \dddot{x}_+ - \dddot{x}_- \right)(t)(\dddot{x}_+ + \dddot{x}_-)^R(t),
\]

(16)

with the friction constant

\[
\gamma \equiv \frac{e^2}{6\pi c^3 M} = \frac{2}{3} \frac{\alpha}{\omega_M},
\]

(17)

where \( \alpha \equiv e^2/\hbar c \approx 1/137 \) is the fine-structure 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.

Note that the retardation enforced by the Heaviside function in the exponent of (6) removes the left-hand half of the \( \delta \)-function. It expresses the causality of the dissipation forces, which is crucial for producing a probability conserving time evolution of the probability distribution [4]. The superscript \( R \) in (16) accounts for this by indicating that the acceleration \((\dddot{x}_+ + \dddot{x}_-)(t)\) is slightly shifted with respect to the velocity factor \((\dddot{x}_+ - \dddot{x}_-)(t)\) towards an earlier time.

We now turn to the anticommutator function. Inserting (10) and the friction constant \( \gamma \) from (17), it becomes

\[
\frac{e^2}{c^2} A_0(\mathbf{x}, \mathbf{x}') \equiv 2\gamma k_B TK(t, t'),
\]

(18)
where

\[ K(t, t') = K(t - t') = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} K(\omega') e^{-i\omega'(t-t')}, \quad (19) \]

with a Fourier transform

\[ K(\omega') = \frac{\hbar \omega'}{2k_B T} \coth \frac{\hbar \omega'}{2k_B T}, \quad (20) \]

whose high-temperature expansion starts out like

\[ K(\omega') \approx K^{HT}(\omega') \equiv 1 + \frac{1}{3} \left( \frac{\hbar \omega'}{2k_B T} \right)^2. \quad (21) \]

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

\[ \int_{-\infty}^{\infty} dt \ K(t-t') = 1. \quad (22) \]

Thus \( K(t-t') \) may be viewed as a \( \delta \)-function broadened by quantum fluctuations.

With the function \( K(t, t') \), the fluctuation part of the influence functional in (7), (6), (5) becomes

\[ \mathcal{A}^{FV}_F[x_+, x_-] = i \frac{w}{2\hbar} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' (\dot{x}_+ - \dot{x}_-)(t) K(t, t') (\ddot{x}_+ - \ddot{x}_-)(t'). \quad (23) \]

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 also have introduced the constant

\[ w \equiv 2Mk_B T\gamma, \quad (24) \]

for brevity.

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

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

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 (21) which adds to the exponent an additional term

\[ -\frac{w}{24(k_B T)^2} \int_{t_a}^{t_b} dt (\ddot{x}_+ - \ddot{x}_-)^2. \quad (26) \]

In the classical limit, the last squeezes the forward and backward paths together. The density matrix (25) becomes diagonal. The \( \gamma \)-term, however, remains and describes classical radiation damping.
we define a Hamilton-like operator as follows:

$$\hat{U}$$

For simplicity, we shall treat only the local limiting form of the last term in (25). In this limit, the quantum system without electromagnetism, and include the effect of the latter recursively. Consider, it is preferable to proceed in another way by going first to a canonical formulation of

$$\rho$$

of (25). They can be transformed into canonical momentum variables only by introducing several

$$\eta(t)$$

a canonical formulation is not applicable because of the high time derivatives of

$$\hat{H}$$

The same equation is obeyed by the density matrix

$$\rho(x, x'; t_a)$$

Then (25) becomes

$$U(x_b, x_a, t_b | x_a, x_a, t_a) = \int D\gamma(t) \int D\gamma(t) \int \frac{D\gamma_+}{(2\pi)^3} \int \frac{D\gamma_-}{(2\pi)^3} \exp \left\{ -\frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[ M \left( -\dot{y}_x + \gamma \ddot{y}_x R \right) + V \left( x + \frac{y}{2} \right) - V \left( x - \frac{y}{2} \right) - \frac{w}{2} \int_{t_a}^{t_b} dt \int_{t_a}^{t_b} dt' \dot{y}(t) K(t, t') \dot{y}(t') \right] \right\}. \tag{28}$$

2. Master Equation for Time Evolution of Density Matrix

We now derive a Schrödinger-like differential equation describing the evolution of the density matrix \( \rho(x_{+}, x_{-}; t_{a}) \) in Eq. (2). In the standard derivation of such an equation \([3]\) 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 (25), by rewriting it as a path integral

$$U_{\eta}(x_{+}, x_{-}; t_{b} | x_{+}, x_{-}, t_{a}) = \int D\gamma_{+}(t) \int D\gamma_{-}(t) \int \frac{D\gamma_{+}}{(2\pi)^3} \int \frac{D\gamma_{-}}{(2\pi)^3} \times \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[ \gamma \ddot{y}_x \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \r...
At moderately high temperatures, we also include a term coming from (26)

$$\mathcal{H}_1 \equiv i \frac{\hbar}{24(k_B T)^2} (\hat{x}_+ - i \hat{x}_-)^2.$$  \hspace{1cm} (34)

For systems with friction 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 (33).

It is useful to re-express (33) 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) by $\hat{H} = \hat{p}^2/2M + V$, then Eq. (33) with the term (34) takes the operator form

$$i\hbar \partial_t \hat{\rho} = \hat{H} \hat{\rho} \equiv [\hat{H}, \hat{\rho}] + \frac{M \gamma}{2} \left( \hat{x} \hat{\rho} - \hat{\rho} \hat{x} + \hat{x} \hat{\rho} \hat{x} - \hat{x} \hat{\rho} \hat{x} \right) - \frac{iw \hbar}{2\hbar} [\hat{x}, [\hat{x}, \hat{\rho}]] - \frac{i \hbar}{24(k_B T)^2} [\hat{x}, [\hat{x}, \hat{\rho}]].$$  \hspace{1cm} (35)

The retardation of $\hat{x}_\pm$ in (31) leads to the specific operator order in the second term, with $\hat{x}$ standing next to $\hat{\rho}$ on both sides. This ensures that Eqs. (31) and (35) preserve the total probability.

The positivity of $\hat{\rho}$ is ensured by the observation, that Eq. (35) can be written in the extended Lindblad form [9]

$$\partial_t \hat{\rho} = -\frac{i}{\hbar} [H_\gamma, \hat{\rho}] - \sum_{n=1}^2 \left( \frac{1}{2} \hat{L}_n \hat{L}_n^\dagger \hat{\rho} + \frac{1}{2} \hat{\rho} \hat{L}_n \hat{L}_n^\dagger - \frac{\hbar}{2} \right) \hat{L}_n^\dagger \hat{\rho} \hat{L}_n \right).$$  \hspace{1cm} (36)

where

$$H_\gamma = \frac{\mathbf{p}^2}{2M} + V + \frac{M \gamma}{4} (\hat{x} \hat{x} + \hat{x} \hat{x})$$

Here, the two Lindblad operators are of the form

$$L_1 = a_1 \hat{x} + ib_1 \hat{x}, \quad L_2 = a_2 \hat{x} + ib_2 \hat{x}$$

where $a$ and $b$ satisfy the equations

$$-\frac{M \gamma}{2\hbar} = b_1 a_1 + a_2 b_2, \quad \frac{w}{\hbar^2} = a_1^2 + a_2^2, \quad \frac{w \beta^2}{12} = b_1^2 + b_2^2$$

The solution is not unique. For $b_1 = 0$ we find

$$\hat{L}_1 = \sqrt{\frac{w}{2\hbar}} \hat{x}, \quad \hat{L}_2 = \sqrt{\frac{w}{2\hbar}} \left( \hat{x} - i \frac{\hbar}{6k_B T} \hat{x} \right).$$  \hspace{1cm} (37)

Another interesting choices is $b_1 = a_1 \mu$ and $b_2 = a_2 \mu$ with

$$\mu = \frac{\hbar \beta}{2\sqrt{3}}$$

In this case we have $L_1 = a_1 A$ and $L_2 = a_2 A^\dagger$ with

$$A = \frac{\hat{x} + i \mu \hat{x}}, \quad a_1^2 = \frac{1}{2\hbar^2} w \left( 1 - \sqrt{3}/2 \right), \quad a_2^2 = \frac{1}{2\hbar^2} w \left( 1 + \sqrt{3}/2 \right).$$
For small $\gamma$ we may set $\hat{x} = -\frac{i}{\hbar}\hbar \nabla$ and $\hat{x} = -\frac{i}{\hbar}\hbar \nabla \hat{x}$, and obtain a proper Lindblad equation which for a harmonic oscillator is an intermediate-temperature master equation describing an exchange of quanta with the heat bath. The solution tends to an equilibrium state which is the Gibbs state.

Note that the operator order prevents the term $\hat{x}\hat{x}\hat{\rho}$ from being a pure divergence. If we rewrite it as a sum of a commutator and an anticommutator, $[\hat{x}, \hat{x}] / 2 \{ \hat{x}, \hat{x} \} / 2$, then the latter term contributes to a hermitian modification $\hat{H} \to \hat{H}_s$ of the Hamilton operator, and we can think of the first two $\gamma$-terms in (35) as being due to an additional antihermitian term in the Hamilton operator $\hat{H}$, the dissipation operator

$$\hat{H}_d = \frac{\gamma M}{4} [\hat{x}, \hat{x}].$$  

For a free particle with $V(x) \equiv 0$ and $[\hat{H}, \hat{p}] = 0$, one has $\hat{x} = \hat{p}_x / M$ to all orders in $\gamma$, such that the time evolution equation (35) becomes

$$i\hbar \partial_t \hat{\rho} = [\hat{H}, \hat{\rho}] - \frac{i\omega}{2M^2\hbar} [\hat{p}, [\hat{p}, \hat{\rho}]].$$  

In the momentum representation of the density matrix $\hat{\rho} = \sum_{pp'} \rho_{pp'} |p\rangle \langle p'|$, where the last term simplifies to $-i\Gamma \equiv -i\omega (p - p')^2 / 2M^2\hbar^2$ multiplying $\hat{\rho}$, which shows 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. (31) is an implicit equation for the Hamilton operator $\hat{\mathcal{H}}$. For small $\epsilon^2$ it can be solved approximately in a single iteration step, replacing $\hat{x}$ by $\hat{p} / M$ and $\hat{x} = -\nabla V / M$ in Eq. (35).

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

$$U(x_{+b}, x_{-b}, t_b | x_{+a}, x_{-a}, t_b - \epsilon) = \int \frac{dp_+ (t_b)}{(2\pi)^3} \int \frac{dp_- (t_b)}{(2\pi)^3} e^{i(p_+ (t_b)[x_+ (t_b) - x_+ (t_b - \epsilon)] - p_- x_- - \mathcal{H}(t_b))/\hbar}. \tag{40}$$

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

$$\epsilon^{-1} [F_+(x_+ (t_b)) U - U F_+(x_+ (t_b - \epsilon))] F_- (x_- (t_b)). \tag{41}$$

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

$$i \frac{\hbar}{\hbar} \left[ \hat{\mathcal{H}}, \hat{F}_+(x_+) \right] F_- (x_-) \tag{42}$$

in the differential operator for the time evolution.

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

Let us apply the master equation (35) to atoms, where $V(x)$ is the Coulomb potential, assuming it to be initially in an eigenstate $|i\rangle$ of $H$, with a density matrix $\hat{\rho}(0) = |i\rangle\langle i|$. Since atoms decay rather slowly, we may treat the $\gamma$-term in (35) perturbatively. It leads to a time derivative of the density matrix

$$\partial_t \langle i|\hat{\rho}(t)|i\rangle = -\frac{\gamma}{\hbar M} \langle i|[\hat{H}, \hat{p}]\hat{p}\rangle|i\rangle = \frac{\gamma}{M} \sum_{f \neq i} \omega_{if} \langle i|\hat{p}|f\rangle \langle f|\hat{p}|i\rangle = -M \gamma \sum_{f} \omega_{if}^2 |x_{fi}|^2, \quad (43)$$

where $\hbar \omega_{if} \equiv E_i - E_f$, and $x_{fi} \equiv \langle f|x|i\rangle$ are the matrix elements of the dipole operator.

An extra width comes from the last two terms in (35):

$$\partial_t \langle i|\hat{\rho}(t)|i\rangle = -\frac{w}{M^2 \hbar^2} \langle i|\hat{p}^2|i\rangle - \frac{w}{12M^2(k_B T)^2} \langle i|\hat{p}^2|i\rangle = -w \sum_{n} \omega_{if}^2 \left[ 1 + \frac{\hbar^2 \omega_{if}^2}{12(k_B T)^2} \right] |x_{fi}|^2. \quad (44)$$

This time dependence is caused by spontaneous emission and induced emission and absorption. To identify the different contributions, we rewrite the spectral decompositions (8) and (9) in the $x$-independent approximation as

$$C_b(t, t') + A_b(t, t') = \frac{4\pi}{3} \hbar \int \frac{d\omega' d^3k}{(2\pi)^4} \frac{\pi}{2M \Omega_k} \left\{ 1 + \coth \frac{\hbar \omega'}{2k_B T} \right\} \times \left[ \delta(\omega' - \Omega_k) - \delta(\omega' + \Omega_k) \right] e^{-i\omega'(t-t')} \quad (45)$$

or

$$C_b(t, t') + A_b(t, t') = \frac{4\pi}{3} \hbar \int \frac{d\omega' d^3k}{(2\pi)^4} \frac{\pi}{2M \Omega_k} \left\{ 2\delta(\omega' - \Omega_k) + \frac{2}{e^{\hbar \Omega_k/k_B T} - 1} \delta(\omega' + \Omega_k) \right\} e^{-i\omega'(t-t')} \quad (46)$$

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. For high and intermediate temperatures, (46) has the expansion

$$\frac{4\pi}{3} \hbar \int \frac{d\omega' d^3k}{(2\pi)^4} \frac{\pi}{2M \Omega_k} \times \left\{ 2\delta(\omega' - \Omega_k) + \left( \frac{2k_B T}{\hbar \Omega_k} - 1 + \frac{1}{6} \frac{\hbar \Omega_k}{k_B T} \right) \delta(\omega' + \Omega_k) \right\} e^{-i\omega'(t-t')} \quad (47)$$

The first term in curly brackets corresponds to the spontaneous emission. It contributes to the rate of change $\partial_t \langle i|\hat{\rho}(t)|i\rangle$ a term $-2M \gamma \sum_{f < i} \omega_{if}^3 |x_{fi}|^2$. This differs from the right-hand side of Eq. (43) in two important respects. First, the sum is restricted to the lower states $f < i$ with $\omega_{if} > 0$, since the $\delta$-function allows only for decays. Second, there is an extra factor 2. Indeed, by comparing (45) with (47) we see that the spontaneous emission receives equal contributions from the 1 and the coth($\hbar \omega'/2k_B T$) in the curly brackets of (45), i.e., from dissipation and fluctuation terms $C_b(t, t')$ and $A_b(t, t')$.

Thus our master equation yields for the natural line width of atomic levels the equation

$$\Gamma = 2M \gamma \sum_{f < i} \omega_{if}^3 |x_{fi}|^2, \quad (48)$$

in agreement with the historic Wigner-Weisskopf formula.
In terms of $\Gamma$, the rate (43) can therefore be written as
\[
\partial_t \langle i| \hat{\rho}(t) |i\rangle = -\Gamma + M_\gamma \sum_{f < i} \omega_{if}^3 |x_{f,i}|^2 + M_\gamma \sum_{f > i} \omega_{if}^3 |x_{f,i}|^2. \tag{49}
\]
The second and third terms do not contribute to the total rate of change of $\langle i| \hat{\rho}(t) |i\rangle$ since they are canceled by the induced emission and absorption terms associated with the $-1$ in the big parentheses of the fluctuation part of (47). The finite lifetime changes the time dependence of the state $|i, t\rangle$ from $|i, t\rangle = |i, 0\rangle e^{-iEt}$ to $|i, 0\rangle e^{-iEt - \Gamma t/2}$.

Note that due to the restriction to $f < i$ in (48), there is no operator local in time whose expectation value is $\Gamma$. Only the combination of spontaneous and induced emissions and absorptions in (49) can be obtained from a local operator, which is in fact the dissipation operator (38).

For all temperatures, the spontaneous and induced transitions together lead to the rate of change of $\langle i| \hat{\rho}(t) |i\rangle$:
\[
\partial_t \langle i| \hat{\rho}(t) |i\rangle = -2M_\gamma \left( \sum_{f < i} \omega_{if}^3 + \sum_{f} \omega_{if}^3 \frac{1}{e^{\hbar\omega_{if}/k_B T} - 1} \right) |x_{f,i}|^2. \tag{50}
\]
For a state with principal quantum number $n$ the temperature effects become detectable only if $T$ becomes larger than $-1/(n+1)^2 + 1/n^2 \approx 2/n^3$ times the Rydberg temperature $T_{\text{Ry}} = 157886.601K$. Thus we have to go to $n \gtrsim 20$ to have observable effects at room temperature.

3.1. Lamb shift

For atoms, the Feynman influence functional (5) allows us to calculate the celebrated Lamb shift. Being interested in the time behavior of the pure-state density matrix $\rho = |i\rangle \langle i|$, we may calculate the effect of the actions (6) and (7) perturbatively. For this, consider the dissipative part of the influence action (6), and in it the first term involving $x_+ (t)$ and $x_+ (t')$, and integrate the external positions in the path integral (5) over the initial wave functions, forming
\[
U_{i i', t_{i'}; i i', t_a} = \int d\mathbf{x}_{+b} d\mathbf{x}_{-b} \int d\mathbf{x}_{+a} d\mathbf{x}_{-a} \langle i| \mathbf{x}_{+b} \langle i| \mathbf{x}_{-b} \rangle \times U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a) \langle \mathbf{x}_{+b}| i\rangle \langle \mathbf{x}_{-b}| i\rangle. \tag{51}
\]
To lowest order in $\gamma$, the effect of the $\mathbf{C}_b$-term in (6) can be evaluated in the local approximation (12) as follows. We take the linear approximation to the exponential $\exp[\int dt dt' \mathcal{O}(t, t')] \approx 1 + \int dt dt' \mathcal{O}(t, t')$ and propagate the initial state with the help of the amplitude $U_{i i', t_{i'}; i i', t_a}$ to the first time $t'$, then with $U_{f_i, t_i; f_i, t_i'}$ to the later time $t_i$, and finally with $U_{i i, t_i; i i, t_a}$ to the final time $t_a$. The intermediate state between the times $t$ and $t'$ are arbitrary and must be summed. In this way we find
\[
\Delta C_U_{i i', t_{i'}; i i', t_a} = \frac{i e^2}{2 \hbar^2 c^2} \int_{t_a}^{t_b} dt dt' \sum_f \int d\mathbf{x}_+ \int d\mathbf{x}'_+ \sum_{i i', t_i, t_i', t_i'} \langle i| \mathbf{x}_+ \rangle \langle \mathbf{x}_+ | i\rangle \times [\partial_t \partial_{\mathbf{C}_b} (t, t')] U_{f_i, t_i; f_i, t_i'} \langle f| \mathbf{x}'_+ \rangle \langle \mathbf{x}'_+ | f\rangle U_{i i, t_i; i i, t_a}.
\]
Inserting $U_{i i, t_i; i i, t_a} = e^{-iE_i (t_a - t_i)/h}$ etc., this becomes
\[
\Delta C_U_{i i', t_{i'}; i i', t_a} = -\frac{e^2}{2 \hbar^2 c^2} \int_{t_a}^{t_b} dt dt' \langle i| \hat{\mathbf{x}}(t) \hat{\mathbf{x}}(t') | i\rangle U_{f_i, t_i; f_i, t_i'} \langle f| \mathbf{x}'_+ \rangle \langle \mathbf{x}'_+ | f\rangle \mathbf{C}_b(b, t, t') \langle f| \hat{\mathbf{x}} | i\rangle.
\]

\[
\Delta C_U_{i i', t_{i'}; i i', t_a} = -\frac{e^2}{2 \hbar^2 c^2} \int_{t_a}^{t_b} dt dt' e^{i\omega_{if}(t-t')} \langle i| \hat{\mathbf{x}}(t) \hat{\mathbf{x}}(t') | i\rangle \mathbf{C}_b(b, t, t') \langle f| \mathbf{x}'_+ \rangle \langle \mathbf{x}'_+ | f\rangle. \tag{53}
\]
Expressing $C_{ij}^b(t, t')$ of Eq. (12) in the form

$$C_{ij}^b(t, t') = \frac{\hbar}{2 \pi c^3} 2 \delta^{ij} \int \frac{d\omega}{2\pi} \omega e^{-i\omega(t-t')},$$

the integration over $t$ and $t'$ yields

$$\Delta C_{Uii,tii,t_a} = -i e^2 \frac{2}{4\pi \hbar c^3} \int_{t_a}^{t_b} dt \int \frac{d\omega}{2\pi} \sum_f \frac{\omega}{\omega - \omega_i + i\eta} |\hat{x}_fi|^2.$$

The same treatment is applied to the $A_b$ in the action (7), where the first term involving $x_+(t)$ and $x_+(t')$ changes (56) to

$$\Delta U_{ii,tii,t_a} = -i e^2 \frac{2}{4\pi \hbar c^3} \int_{t_a}^{t_b} dt \int \frac{d\omega}{2\pi} \sum_f \frac{\omega}{\omega - \omega_i + i\eta} \left(1 + \coth \frac{\hbar \omega}{2k_B T}\right) |\hat{x}_fi|^2.$$

The $\omega$-integral is conveniently split into a zero-temperature part and a finite-temperature correction

$$I(\omega_i, 0) \equiv \int_0^\infty \frac{d\omega}{\pi} \sum_f \frac{\omega}{\omega - \omega_i + i\eta},$$

and

$$\Delta I_T(\omega_i, T) \equiv 2 \int_0^\infty \frac{d\omega}{\pi} \sum_f \frac{\omega}{\omega - \omega_i + i\eta} \frac{1}{e^{\hbar \omega/k_B T} - 1}.$$

Decomposing $1/(\omega_i - \omega + i\eta) = P/(\omega - \omega_i) - i\pi \delta(\omega_i - \omega)$, the imaginary part of the $\omega$-integral yields half of the natural line width in (43). The other half comes from the part of the integral (6) involving $x_-(t)$ and $x_-(t')$. The principal-value part of the zero-temperature integral diverges linearly, the divergence yielding again the mass renormalization (14). Subtracting this divergence from $I(\omega_i, 0)$, the remaining integral has the same form as $I(\omega_i, 0)$, but with $\omega$ in the numerator replaced by $\omega_i = 0$. This integral diverges logarithmically like $(\omega_i/\pi) \log(\Lambda - \omega_i/|\omega_i|)$, where $\Lambda$ is Bethe’s cutoff.[10] For $\Lambda \gg |\omega_i|$, the result (56) implies an energy shift of the atomic level $|i\rangle$:

$$\Delta E_i = \frac{e^2}{4\pi c^3} \frac{2}{3\pi} \sum_f \omega_i^3 |\hat{x}_fi|^2 \log \frac{\Lambda}{|\omega_i|},$$

which is the Lamb shift.

Usually, the weakly varying logarithm is approximated by a weighted average $L = \log(|\Lambda/|\omega_i||)$ over energy levels and taken out of the integral. Then contribution of the term (56) can be attributed to an extra term

$$\hat{H}_{LS} \approx -\frac{i}{\pi} \gamma M \frac{1}{4} [\hat{x}, \hat{x}]$$

in the Hamiltonian (35). In this form, the Lamb shift appears as a Hermitian logarithmically divergent correction to the operator (38) governing the spontaneous emission of photons.

To lowest order in $\gamma$, the commutator is for a Coulomb potential $V(x) = -e^2/r$ equal to

$$-\frac{i}{M^2} [\hat{p}, \hat{p}] = \frac{\hbar}{M^2} \nabla^2 V(x) = \frac{\hbar^2 c \alpha}{M^2} 4\pi \delta^{(3)}(x),$$

where

$$\delta^{(3)}(x) = \int d^3x \delta(x - x') \delta^{(3)}(x - x')$$

is the 3D Dirac delta function.
leading to
\[ \Delta E_i = \frac{4\alpha^2\hbar^3}{3M^2c^2} (i|\delta^{(3)}(x)|i). \] (62)

For an atomic state of principal quantum number \( n \) with a wave function \( \psi_n(x) \), this becomes
\[ \Delta E_n = \frac{4\alpha\hbar^3}{3M^2c^2} aL |\psi_n(0)|^2. \] (63)

Only atomic \( s \)-states can contribute, since the wave functions of all other angular momenta vanish at the origin. Explicitly, the \( s \)-states of the hydrogen atom have the value at the origin
\[ \psi_n(0) = \frac{1}{\sqrt{n^3\pi}} \left( \frac{1}{a_H} \right)^{3/2} \] (64)

where \( a_H = \hbar/Mc\alpha \) is the Bohr radius. If the nuclear charge is \( Z \), then \( a_B \), is diminished by this factor. Thus we obtain the energy shift
\[ \Delta E_n = \frac{4\alpha^2\hbar^3}{3M^2c^2} \left( \frac{M\alpha}{\hbar} \right)^3 \frac{L}{n^3\pi}. \] (65)

For a hydrogen atom with \( n = 2 \), this becomes
\[ \Delta E_2 = \frac{\alpha^3}{6\pi} \alpha^2 M c^2 L. \] (66)

The quantity \( Mc^2\alpha^2 \) is the unit energy of atomic physics determining the hydrogen spectrum to be \( E_n = -Mc^2\alpha^2/2n^2 \). Thus
\[ M\alpha^2 = 4.36 \times 10^{-11} \text{erg} = 27.21 \text{eV} = 2 \cdot 3.288 \times 10^{15} \text{Hz}. \] (67)

Inserting this together with \( \alpha \approx 1/137.036 \) into (66) yields
\[ \Delta E_2 \approx 135.6 \text{MHz} \times L. \] (68)

The constant \( L \) can be calculated approximately as
\[ L \approx 9.3, \] (69)

leading to the estimate
\[ \Delta E_2 \approx 1261 \text{MHz}. \] (70)

The experimental Lamb shift
\[ \Delta E_{\text{Lamb shift}} \approx 1057 \text{MHz} \] (71)

is indeed contained in this range. In this calculation, two effects have been ignored: the vacuum polarization of the photon and the form factor of the electron caused by radiative corrections. They reduce the frequency (70) by \((27.3 + 51)\text{MHz}\) bringing the theoretical number closer to experiment.

At finite temperature, (59) changes to
\[ \Delta E_i = \frac{e^2}{4\pi c^2} \frac{2}{3\pi} \sum_f \omega_{ij}^3 |x_{fi}|^2 \left[ \log \frac{\Lambda}{\omega_{ij}} + \left( \frac{k_B T}{\hbar \omega_{ij}} \right)^2 J \left( \frac{\hbar \omega_{ij}}{k_B T} \right) \right], \] (72)

\[ ^2 \text{The precise value of the Lamb constant } \alpha^2 M/6\pi \text{ is } 135.641 \pm 0.004 \text{ MHz}. \]
where \( J(z) \) denotes the integral

\[
J(z) \equiv z \int_0^\infty dz' \frac{z'}{z' - z} e^{z'} - 1,
\]

which has the low-temperature (large-\( z \)) expansion \( J(z) = -\pi^2/6 - 2\zeta(3)/z + \ldots \), and goes to zero for high temperature (small \( z \)) like \(-z \log z\), as shown in Fig. 1.

\[4. \text{Langevin Equations}\]

For high \( \gamma T \), the last term in the forward–backward path integral (25) makes the size of the fluctuations in the difference between the paths \( y(t) = x_+(t) - x_-(t) \) very small. It is then convenient to introduce the average of the two paths as \( x(t) \equiv [x_+(t) + x_-(t)]/2 \), and expand

\[V\left(x + \frac{y}{2}\right) - V\left(x - \frac{y}{2}\right) \sim y \cdot \nabla V(x) + O(y^3) \ldots,\]

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

\[
\dot{\eta}(t) = M\ddot{x}(t) - M\gamma \dddot{x}(t) + \nabla V(x(t)).
\]

With this, the exponential function in (25) becomes

\[
\exp \left[ -\frac{i}{\hbar} \int_a^b dt \dot{y} \eta - \frac{w}{2\hbar^2} \int_a^b dt \dot{y}^2(t) \right],
\]

where \( w \) is the constant (24).

Consider now the diagonal part of the amplitude (74) with \( x_{+b} = x_{-b} \equiv x_b \) and \( x_{+a} = x_{-a} \equiv x_a \), implying that \( y_b = y_a = 0 \). It represents a probability distribution

\[
P(x_b t_b | x_a t_a) \equiv |(x_b, t_b | x_a, t_a)|^2 \equiv U(x_b, x_b, t_b | x_a, x_a, t_a).
\]

Now the variable \( y \) can simply be integrated out in (76), and we find the probability distribution

\[
P[\eta] \propto \exp \left[ -\frac{1}{2w} \int_a^b dt \eta^2(t) \right].
\]
The expectation value of an arbitrary functional of \( F[x] \) can be calculated from the path integral

\[
\langle F[x] \rangle_\eta \equiv \mathcal{N} \int Dx \, P[\eta] \, F[x],
\]

(79)

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 (79) can be rewritten as a functional integral

\[
\langle F[x] \rangle_\eta \equiv \mathcal{N} \int D\eta \, P[\eta] \, F[x],
\]

(80)

Note that the probability distribution (78) is \( \hbar \)-independent. Hence in the approximation (74) we obtain the classical Langevin equation. In principle, the integrand contains a factor \( J^{-1}[x] \), where \( J[x] \) is the functional Jacobian

\[
J[x] \equiv \text{det} \left[ \frac{\delta \eta^i(t)}{\delta x^j(t')} \right] = \text{det} \left[ \left( \frac{\partial^2}{\partial t^2} - M \gamma \frac{\partial^2}{\partial t^2} \right) \delta_{ij} + \nabla_i \nabla_j V(x(t)) \right].
\]

(81)

It can be shown that the determinant is unity, due to the retardation of the friction term [4], thus justifying its omission in (80).

The path integral (80) may be interpreted as an expectation value with respect to the solutions of a stochastic differential equation (75) driven by a Gaussian random noise variable \( \eta(t) \) with a correlation function

\[
\langle \eta^i(t) \eta^j(t') \rangle_T = \delta^{ij} \delta(t - t').
\]

(82)

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 (75) is to write the stochastic equation as

\[
M\ddot{x}(t) + \nabla V(x(t)) = \dot{\eta}(t) + M\gamma \dot{x}(t),
\]

(83)

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. (25).

Note that the lowest iteration of Eq. (83) with \( \eta \equiv 0 \) can be multiplied by \( \dot{x} \) and leads to the equation for the energy change of the particle

\[
\frac{d}{dt} \left[ \frac{1}{2} \dot{x}^2 + V(x) - M\gamma \dot{x} \ddot{x} \right] = -M\gamma \ddot{x}^2.
\]

(84)

The right-hand side is the classical electromagnetic power radiate by an accelerated particle. The extra term in the brackets is known as Schott term [11].

5. 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. Our equation may have applications to dilute interstellar gases or, after a reformulation in a finite volume, to few-particle systems contained in cavities. So far, a master equation has been set up only for a finite number of modes [12].

The results presented here can be found in papers published in collaboration with Z. Haba [13, 14] and in the textbook [3]. Results similar to those in Section 3 have also been derived using conventional quantum-mechanical methods by other authors [15].
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