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Master and Langevin equations for electromagnetic dissipation and decoherence of density matrices

Z. Haba[a] and H. Kleinert[b]

Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

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Abstract. 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. We also derive the associated Langevin equation. As an application, we recalculate the Wigner-Weisskopf 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. Our master equation also yields the correct Lamb shift of atomic levels. The two equations may have applications to dilute interstellar gases or to few-particle systems in cavities.

PACS. 03.65.-w Quantum mechanics – 03.65.Yz Decoherence; open systems; quantum statistical methods – 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 05.45.-a Nonlinear dynamics and nonlinear dynamical systems

1 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]

$$
\begin{aligned}
&(\mathbf{x}_{+b}, t_b|\mathbf{x}_{+a}, t_a)(\mathbf{x}_{-b}, t_b|\mathbf{x}_{-a}, t_a)^* \equiv \\
&\qquad U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a) \\
&= \int \mathcal{D}\mathbf{x}_+ \mathcal{D}\mathbf{x}_- \, \exp\left\{ \frac{\mathrm{i}}{\hbar} \int_{t_a}^{t_b} \left[\frac{M}{2}\left(\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2\right) - V(\mathbf{x}_+) \right.\right. \\
&\qquad \left.\left. + V(\mathbf{x}_-) - \frac{e}{c}\dot{\mathbf{x}}_+ \mathbf{A}(\mathbf{x}_+, t) + \frac{e}{c}\dot{\mathbf{x}}_- \mathbf{A}(\mathbf{x}_-, t) \right] \right\}, \qquad (1.1)
\end{aligned}
$$

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

$$
\begin{aligned}
\rho(\mathbf{x}_{+b}, \mathbf{x}_{-b}; t_b) &= \int \mathrm{d}\mathbf{x}_{+a}\, \mathrm{d}\mathbf{x}_{-a} \\
&\quad \times U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a)\rho(\mathbf{x}_{+a}, \mathbf{x}_{-a}; t_a). \qquad (1.2)
\end{aligned}
$$

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

$$
\begin{aligned}
\mathbf{A}(\mathbf{x}, t) &= \sum_\mathbf{k} f_\mathbf{k}(\mathbf{x})\mathbf{X}_\mathbf{k}(t), \quad f_\mathbf{k}(\mathbf{x}) = \frac{\mathrm{e}^{\mathrm{i}\mathbf{k}\mathbf{x}}}{\sqrt{2V\Omega_\mathbf{k}/c}}, \\
\sum_\mathbf{k} &\equiv V \int \frac{\mathrm{d}^3k}{(2\pi)^3} \cdot \qquad (1.3)
\end{aligned}
$$

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

$$
\begin{aligned}
G_\Omega(t, t') &= \frac{1}{2}\left[A_\Omega(t, t') + C_\Omega(t, t')\right] \\
&= \frac{\hbar}{2M\Omega} \frac{\cosh \dfrac{\Omega}{2}\left[\hbar\beta - \mathrm{i}(t - t')\right]}{\sinh \dfrac{\hbar\Omega\beta}{2}}, \quad t > t' \qquad (1.4)
\end{aligned}
$$

which is the analytic continuation of the periodic imaginary-time Green function to $\tau = \mathrm{i}t$. The decomposition into $A_\Omega(t, t')$ and $C_\Omega(t, t')$ distinguishes real and imaginary parts, which are commutator and

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[a] On leave from Institute of Theoretical Physics, University of Wroclaw, Poland

[b] e-mail: `kleinert@physik.fu-berlin.de`
URL: `http://www.physik.fu-berlin.de/~kleinert`

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 evolution kernel (1.1) is then given by the forward – backward path integral

$$U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) = \int \mathcal{D}\mathbf{x}_+(t)\int \mathcal{D}\mathbf{x}_-(t) \times \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\left[\frac{M}{2}(\dot{\mathbf{x}}_+^2-\dot{\mathbf{x}}_-^2)-(V(\mathbf{x}_+)-V(\mathbf{x}_-))\right] + \frac{\mathrm{i}}{\hbar}\mathcal{A}^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-]\right\}. \quad (1.5)$$

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

$$\mathcal{A}_D^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-] = \frac{\mathrm{i}e^2}{2\hbar c^2}\int\mathrm{d}t\int\mathrm{d}t'\,\Theta(t-t') \times\Big[\dot{\mathbf{x}}_+\mathbf{C}_\mathrm{b}(\mathbf{x}_+\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}'_+ - \dot{\mathbf{x}}_+\mathbf{C}_\mathrm{b}(\mathbf{x}_+\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}'_- - \dot{\mathbf{x}}_-\mathbf{C}_\mathrm{b}(\mathbf{x}_-\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}'_+ - \dot{\mathbf{x}}_-\mathbf{C}_\mathrm{b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}'_-\Big] \quad (1.6)$$

and

$$\mathbf{A}_F^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-] = \frac{\mathrm{i}e^2}{2\hbar c^2}\int\mathrm{d}t\int\mathrm{d}t'\,\Theta(t-t') \times\Big[\dot{\mathbf{x}}_+\mathbf{A}_\mathrm{b}(\mathbf{x}_+\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}'_+ - \dot{\mathbf{x}}_+\mathbf{A}_\mathrm{b}(\mathbf{x}_+\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}'_- - \dot{\mathbf{x}}_-\mathbf{A}_\mathrm{b}(\mathbf{x}_-\,t,\mathbf{x}'_+\,t')\dot{\mathbf{x}}'_+ + \dot{\mathbf{x}}_-\mathbf{A}_\mathrm{b}(\mathbf{x}_-\,t,\mathbf{x}'_-\,t')\dot{\mathbf{x}}'_-\Big], \quad (1.7)$$

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 3×3 commutator and anticommutator functions of the bath of photons. They are sums of correlation functions over the bath of the oscillators of frequency $\Omega_\mathbf{k}|$, each contributing with a weight $f_\mathbf{k}(\mathbf{x})f_{-\mathbf{k}}(\mathbf{x}') = \mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{x}-\mathbf{x}')}\,c/2\Omega_\mathbf{k}V$ (the normalization following from the action $\int\mathrm{d}^4x(\mathbf{E}^2-\mathbf{B}^2)/2c$). Thus we may write

$$C_\mathrm{b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') = \sum_\mathbf{k} f_{-\mathbf{k}}(\mathbf{x})f_\mathbf{k}(\mathbf{x}')\left\langle[\hat{X}^i_{-\mathbf{k}}(t),\hat{X}^j_\mathbf{k}(t')]\right\rangle_T = -\mathrm{i}c^2\hbar\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\sigma_\mathbf{k}(\omega')\delta^{ij\,\mathrm{tr}}_{\mathbf{kk}}\mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{x}-\mathbf{x}')}\sin\omega'(t-t'), \quad (1.8)$$

$$A_\mathrm{b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') = \sum_\mathbf{k} f_{-\mathbf{k}}(\mathbf{x})f_\mathbf{k}(\mathbf{x}')\left\langle\left\{\hat{X}^i_{-\mathbf{k}}(t),\hat{X}^j_\mathbf{k}(t')\right\}\right\rangle_T = c^2\hbar\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\sigma_\mathbf{k}(\omega')\delta^{ij\mathrm{tr}}_{\mathbf{kk}}\coth\frac{\hbar\omega'}{2k_\mathrm{B}T}\mathrm{e}^{\mathrm{i}\mathbf{k}(\mathbf{x}-\mathbf{x}')}\cos\omega'(t-t'), \quad (1.9)$$

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

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

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

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

where η 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 $\mathbf{x}$-dependence in (1.8) and (1.9) and find

$$C_\mathrm{b}^{ij}(\mathbf{x}\,t,\mathbf{x}'\,t') \approx C_\mathrm{b}^{ij}(t,t') = \mathrm{i}\frac{\hbar}{2\pi c}\frac{2}{3}\delta^{ij}\partial_t\delta(t-t'). \quad (1.12)$$

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

$$\Delta\mathcal{A}_\mathrm{loc}[\mathbf{x}_+,\mathbf{x}_-] = \frac{\Delta M}{2}\int_{t_a}^{t_b}\mathrm{d}t\,(\dot{\mathbf{x}}_+^2-\dot{\mathbf{x}}_-^2)(t), \quad (1.13)$$

where

$$\Delta M \equiv -\frac{e^2}{c^2}\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\frac{\sigma_\mathbf{k}(\omega')}{\omega'}\delta^{ij\,\mathrm{tr}}_{\mathbf{kk}} = -\frac{e^2}{3\pi^2c^3}\int_0^\infty\mathrm{d}k. \quad (1.14)$$

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

$$\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\frac{M_\mathrm{ren}}{2}\left(\dot{\mathbf{x}}_+^2-\dot{\mathbf{x}}_-^2\right). \quad (1.15)$$

By identifying M with M_ren this renormalization may be ignored.

The second term has the form

$$\mathcal{A}_D^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-] = -\gamma\frac{M}{2}\int_{t_a}^{t_b}\mathrm{d}t\,(\dot{\mathbf{x}}_+-\dot{\mathbf{x}}_-)(t)(\ddot{\mathbf{x}}_++\ddot{\mathbf{x}}_-)^R(t), \quad (1.16)$$

with the friction constant

$$\gamma \equiv \frac{e^2}{6\pi c^3M} = \frac{2}{3}\frac{\alpha}{\omega_M}, \quad (1.17)$$

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 (1.6) removes the left-hand half of the δ-function. It expresses the *causality* of the dissipation forces, which is crucial for producing a probability conserving time evolution of the probability distribution [2]. The superscript R in (1.16) accounts for this by indicating that 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.

We now turn to the anticommutator function. Inserting (1.10) and the friction constant γ from (1.17), it becomes

$$\frac{e^2}{c^2}A_{\mathrm{b}}(\mathbf{x}\,t, \mathbf{x}'\,t') \approx 2\gamma k_{\mathrm{B}}TK(t,t'), \tag{1.18}$$

where

$$K(t,t') = K(t-t') \equiv \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega'}{2\pi}K(\omega')\mathrm{e}^{-\mathrm{i}\omega'(t-t')}, \tag{1.19}$$

with a Fourier transform

$$K(\omega') \equiv \frac{\hbar\omega'}{2k_{\mathrm{B}}T}\coth\frac{\hbar\omega'}{2k_{\mathrm{B}}T}, \tag{1.20}$$

whose high-temperature expansion starts out like

$$K(\omega') \approx K^{\mathrm{HT}}(\omega') \equiv 1 + \frac{1}{3}\left(\frac{\hbar\omega'}{2k_{\mathrm{B}}T}\right)^2. \tag{1.21}$$

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

$$\int_{-\infty}^{\infty}\mathrm{d}t\,K(t-t') = 1. \tag{1.22}$$

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

With the function $K(t,t')$, the fluctuation part of the influence functional in (1.5–1.7) becomes

$$\mathcal{A}_F^{\mathrm{FV}}[\mathbf{x}_+,\mathbf{x}_-] = \mathrm{i}\frac{w}{2\hbar}\int_{t_a}^{t_b}\mathrm{d}t \times \int_{t_a}^{t_b}\mathrm{d}t'\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t)\,K(t,t')\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(t'). \tag{1.23}$$

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

$$w \equiv 2Mk_{\mathrm{B}}T\gamma, \tag{1.24}$$

for brevity.

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

$$\begin{aligned}U(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) &= \int\mathcal{D}\mathbf{x}_+(t)\int\mathcal{D}\mathbf{x}_-(t)\\ &\times\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\left[\frac{M}{2}(\dot{\mathbf{x}}_+^2 - \dot{\mathbf{x}}_-^2) - (V(\mathbf{x}_+) - V(\mathbf{x}_-))\right]\right\}\\ &\times\exp\left\{-\frac{\mathrm{i}}{2\hbar}M\gamma\int_{t_a}^{t_b}\mathrm{d}t\ (\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)(\ddot{\mathbf{x}}_+ + \ddot{\mathbf{x}}_-)^R\right.\\ &\left.\qquad -\frac{w}{2\hbar^2}\int_{t_a}^{t_b}\mathrm{d}t\,(\dot{\mathbf{x}}_+ - \dot{\mathbf{x}}_-)^2\right\},\end{aligned} \tag{1.25}$$

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 (1.21) which adds to the exponent an additional term

$$-\frac{w}{24(k_{\mathrm{B}}T)^2}\int_{t_a}^{t_b}\mathrm{d}t(\ddot{\mathbf{x}}_+ - \ddot{\mathbf{x}}_-)^2. \tag{1.26}$$

In the classical limit, the last term in (1.25) squeezes the forward and backward paths together. The density matrix (1.25) becomes diagonal, and the γ-term describes classical radiation damping.

2 Master equation for time evolution of density matrix

We now derive a Schrödinger-like differential equation describing the evolution of the density matrix $\rho(x_{+a}, x_{-a}; t_a)$ in equation (1.2). In the standard derivation of such an equation [3] one first makes the last term local *via* a quadratic completion involving a fluctuating noise variable $\eta(t)$. Then one goes over to a canonical formulation of the path integral (1.25), by rewriting it as a path integral

$$\begin{aligned}U_\eta(\mathbf{x}_{+b},\mathbf{x}_{-b},t_b|\mathbf{x}_{+a},\mathbf{x}_{-a},t_a) &= \int\mathcal{D}\mathbf{x}_+(t)\int\mathcal{D}\mathbf{x}_-(t)\int\frac{\mathcal{D}\mathbf{p}_+}{(2\pi)^3}\int\frac{\mathcal{D}\mathbf{p}_-}{(2\pi)^3}\\ &\times\exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\ \left[\mathbf{p}_+\dot{\mathbf{x}}_+ - \mathbf{p}_-\dot{\mathbf{x}}_- - \mathcal{H}_\eta(\mathbf{p}_+,\mathbf{p}_-,\mathbf{x}_+,\mathbf{x}_-)\right]\right\}.\end{aligned} \tag{2.1}$$

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

$$\mathrm{i}\hbar\partial_t U_\eta(\mathbf{x}\,,\mathbf{y}\,,t|\mathbf{x}_a,\mathbf{y}_a,t_a) = \hat{\mathcal{H}}_\eta\,U_\eta(\mathbf{x}\,,\mathbf{y}\,,t|\mathbf{x}_a,\mathbf{y}_a,t_a). \tag{2.2}$$

The same equation is obeyed by the density matrix $\rho(\mathbf{x}_+,\mathbf{x}_-;t_a)$.

At high temperatures where the action in the path integral (1.25) is local, we can set up directly a Hamiltonian without the noise-averaging procedure. However, the standard procedure of going to a canonical formulation is not applicable because of the high time derivatives of $\mathbf{x}(t)$ in the action of (1.25). They can be transformed into canonical momentum variables only by introducing several auxiliary independent variables $\mathbf{v} \equiv \dot{\mathbf{x}}$, $\mathbf{b} \equiv \ddot{\mathbf{x}}, \ldots$ [4,5]. 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 electromagnetism, and include the effect of the latter recursively. For simplicity, we shall treat only the local limiting form of the last term in (1.25). In this limit, we define a Hamilton-like operator as follows:

$$\hat{\mathcal{H}} \equiv \frac{1}{2M}\left(\hat{\mathbf{p}}_+^2 - \hat{\mathbf{p}}_-^2\right) + V(\mathbf{x}_+) - V(\mathbf{x}_-) + \frac{M\gamma}{2}\,(\hat{\dot{\mathbf{x}}}_+ - \hat{\dot{\mathbf{x}}}_-)(\hat{\ddot{\mathbf{x}}}_+ + \hat{\ddot{\mathbf{x}}}_-)^R - \mathrm{i}\frac{w}{2\hbar}(\hat{\dot{\mathbf{x}}}_+ - \hat{\dot{\mathbf{x}}}_-)^2. \tag{2.3}$$

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

$$\hat{\dot{\mathbf{x}}} \equiv \frac{\mathrm{i}}{\hbar}[\hat{\mathcal{H}}, \hat{\mathbf{x}}], \qquad \hat{\ddot{\mathbf{x}}} \equiv \frac{\mathrm{i}}{\hbar}[\hat{\mathcal{H}}, \hat{\dot{\mathbf{x}}}]. \tag{2.4}$$

A direct differentiation of equation (1.25) over time leads to the conclusion that the density matrix $\rho(x_+, x_-; t_a)$ satisfies the time evolution equation

$$\mathrm{i}\hbar\partial_t\rho(x_+, x_-; t_a) = \hat{\mathcal{H}}\rho(x_+, x_-; t_a). \tag{2.5}$$

At moderately high temperatures, we also include a term coming from (1.26)

$$\mathcal{H}_1 \equiv \mathrm{i}\frac{w\hbar}{24(k_{\mathrm{B}}T)^2}(\hat{\ddot{\mathbf{x}}}_+ - \hat{\ddot{\mathbf{x}}}_-)^2. \tag{2.6}$$

For systems with friction caused by a conventional heat bath of harmonic oscillators as discussed by Caldeira and Leggett [6], the analogous extra term was shown by Diosi [7] to bring the Master equation to the general Lindblad form [8] which ensures positivity of the probabilities resulting from the solutions of (2.5).

It is useful to re-express (2.5) 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 equation (2.5) with the term (2.6) takes the operator form

$$\mathrm{i}\hbar\partial_t\hat{\rho} = \hat{\mathcal{H}}\,\hat{\rho} \equiv [\hat{H}, \hat{\rho}] + \frac{M\gamma}{2}\left(\hat{\dot{\mathbf{x}}}\hat{\ddot{\mathbf{x}}}\hat{\rho} - \hat{\rho}\hat{\ddot{\mathbf{x}}}\hat{\dot{\mathbf{x}}} + \hat{\dot{\mathbf{x}}}\,\hat{\rho}\,\hat{\ddot{\mathbf{x}}} - \hat{\ddot{\mathbf{x}}}\,\hat{\rho}\,\hat{\dot{\mathbf{x}}}\right) - \frac{\mathrm{i}w}{2\hbar}[\hat{\dot{\mathbf{x}}}, [\hat{\dot{\mathbf{x}}}, \hat{\rho}]] - \frac{\mathrm{i}w\hbar}{24(k_{\mathrm{B}}T)^2}[\hat{\ddot{\mathbf{x}}}, [\hat{\ddot{\mathbf{x}}}, \hat{\rho}]]. \tag{2.7}$$

The operator order in the terms in parentheses need explanation. It is fixed by the retardation of $\ddot{\mathbf{x}}_\pm$ with respect to $\dot{\mathbf{x}}_\pm$ in (2.3), which implies that the associated operator $\hat{\ddot{\mathbf{x}}}(t)$ has a time argument which lies slightly *before* that of $\hat{\dot{\mathbf{x}}}_\pm$, thus acting upon $\hat{\rho}$ before the operator of velocity $\hat{\dot{\mathbf{x}}}$. This puts it to the right of $\hat{\dot{\mathbf{x}}}$, *i.e.*, next to $\hat{\rho}$. On the right-hand side of $\hat{\rho}$, the time runs in the opposite direction such that $\hat{\ddot{\mathbf{x}}}$ must lie left of $\hat{\dot{\mathbf{x}}}$, again next to $\hat{\rho}$. In this way we obtain an operator order which ensures that equation (2.7) conserves the total probability.

This property and the positivity of $\hat{\rho}$ are guaranteed by the observation, that equation (2.7) can be written in the extended *Lindblad form* [8]

$$\partial_t\hat{\rho} = -\frac{\mathrm{i}}{\hbar}[\hat{H}, \hat{\rho}] - \sum_{n=1}^{2}\left(\frac{1}{2}\hat{L}_n\hat{L}_n^\dagger\hat{\rho} + \frac{1}{2}\hat{\rho}\hat{L}_n\hat{L}_n^\dagger - \hat{L}_n^\dagger\hat{\rho}\hat{L}_n\right). \tag{2.8}$$

with the two Lindblad operators

$$\hat{L}_1 \equiv \frac{\sqrt{w}}{2\hbar}\hat{\dot{\mathbf{x}}}, \qquad \hat{L}_2 \equiv \frac{\sqrt{3w}}{2\hbar}\left(\hat{\dot{\mathbf{x}}} - \mathrm{i}\frac{\hbar}{3k_{\mathrm{B}}T}\hat{\ddot{\mathbf{x}}}\right). \tag{2.9}$$

Note that the operator order prevents the term $\hat{\dot{\mathbf{x}}}\hat{\ddot{\mathbf{x}}}\hat{\rho}$ from being a pure divergence. If we rewrite it as a sum of a commutator and an anticommutator, $[\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}]/2 + \{\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}\}/2$, then the latter term is a pure divergence, and we can think of the first two γ-terms in (2.7) as being due to an additional anti-Hermitian term in the Hamilton operator $\hat{H}$, the *dissipation operator*

$$\hat{H}_\gamma = \frac{\gamma M}{4}\,[\hat{\dot{\mathbf{x}}}, \hat{\ddot{\mathbf{x}}}]. \tag{2.10}$$

For a free particle with $V(\mathbf{x}) \equiv 0$ and $[\hat{H}, \hat{\mathbf{p}}] = 0$, one has $\hat{\dot{\mathbf{x}}}_\pm = \hat{\mathbf{p}}_\pm/M$ to all orders in γ, such that the time evolution equation (2.7) becomes

$$\mathrm{i}\hbar\partial_t\hat{\rho} = [\hat{H}, \hat{\rho}] - \frac{\mathrm{i}w}{2M^2\hbar}[\hat{\mathbf{p}}, [\hat{\mathbf{p}}, \hat{\rho}]]. \tag{2.11}$$

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 $-\mathrm{i}\Gamma \equiv -\mathrm{i}w(\mathbf{p}-\mathbf{p}')^2/2M^2\hbar^2$ 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 Γ.

In general, equation (2.3) 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 $\hat{\dot{\mathbf{x}}}$ by $\hat{\mathbf{p}}/M$ and $\hat{\ddot{\mathbf{x}}} = -\boldsymbol{\nabla}V/M$ in equation (2.7).

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

$$U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_b - \epsilon) = \int\frac{\mathrm{d}\mathbf{p}_+(t_b)}{(2\pi)^3} \times \int\frac{\mathrm{d}\mathbf{p}_-(t_b)}{(2\pi)^3}\mathrm{e}^{\mathrm{i}\{\mathbf{p}_+(t_b)[\mathbf{x}_+(t_b)-\mathbf{x}_+(t_b-\epsilon)]-\mathbf{p}_-\dot{\mathbf{x}}_--\mathcal{H}(t_b)\}/\hbar}. \tag{2.12}$$

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 $\epsilon^{-1}\left[F_+(\mathbf{x}_+(t_b)) - F_+(\mathbf{x}_+(t_b - \epsilon))\right]F_-(\mathbf{x}_-(t_b))$. It it can be taken out of the integral, yielding

$$\epsilon^{-1}\left[F_+(\mathbf{x}_+(t_b))U - UF_+(\mathbf{x}_+(t_b - \epsilon))\right]F_-(\mathbf{x}_-(t_b)). \tag{2.13}$$

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

$$\frac{\mathrm{i}}{\hbar}\left[\hat{\mathcal{H}}, \hat{F}_+(\mathbf{x}_+)\right]F_-(x_-) \tag{2.14}$$

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.

3 Line width

Let us apply the master equation (2.7) 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 $\hat{\rho}(0) = |i\rangle\langle i|$. Since atoms decay rather slowly, we may treat the γ-term in (2.7) perturbatively. It leads to a time derivative of the density matrix

$$\begin{aligned}\partial_t\langle i|\hat{\rho}(t)|i\rangle &= -\frac{\gamma}{\hbar M}\langle i|[\hat{H},\hat{\mathbf{p}}]\,\hat{\mathbf{p}}\,\hat{\rho}(0)|i\rangle\\ &= \frac{\gamma}{M}\sum_{f\neq i}\omega_{if}\langle i|\mathbf{p}|f\rangle\langle f|\mathbf{p}|i\rangle\\ &= -M\gamma\sum_f \omega_{if}^3\,|\mathbf{x}_{fi}|^2, \qquad (3.1)\end{aligned}$$

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

An extra width, which we have not seen discussed in the literature so far, comes from the last two terms in (2.7):

$$\begin{aligned}\partial_t\langle i|\hat{\rho}(t)|i\rangle &= -\frac{w}{M^2\hbar^2}\langle i|\mathbf{p}^2|i\rangle - \frac{w}{12M^2(k_{\rm B}T)^2}\langle i|\dot{\mathbf{p}}^2|i\rangle\\ &= -w\sum_n \omega_{if}^2\left[1+\frac{\hbar^2\omega_{if}^2}{12(k_{\rm B}T)^2}\right]|\mathbf{x}_{fi}|^2. \qquad (3.2)\end{aligned}$$

This time dependence is caused by spontaneous emission and induced emission and absorption. To identify the different contributions, we rewrite the spectral decompositions (1.8) and (1.9) in the $\mathbf{x}$-independent approximation as

$$\begin{aligned}C_b(t,t') + A_b(t,t') &= \frac{4\pi}{3}\hbar\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\\ &\times\left\{1+\coth\frac{\hbar\omega'}{2k_{\rm B}T}\right\}[\delta(\omega'-\Omega_{\mathbf{k}})-\delta(\omega'+\Omega_{\mathbf{k}})]\,\mathrm{e}^{-\mathrm{i}\omega'(t-t')}, \qquad (3.3)\end{aligned}$$

as

$$\begin{aligned}C_b(t,t') + A_b(t,t') &= \frac{4\pi}{3}\hbar\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\\ &\times\left\{2\delta(\omega'-\Omega_{\mathbf{k}})+\frac{2}{\mathrm{e}^{\hbar\Omega_{\mathbf{k}}/k_{\rm B}T}-1}\right.\\ &\left.\times[\delta(\omega'-\Omega_{\mathbf{k}})+\delta(\omega'+\Omega_{\mathbf{k}})]\right\}\mathrm{e}^{-\mathrm{i}\omega'(t-t')}. \qquad (3.4)\end{aligned}$$

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, (3.4) has the expansion

$$\begin{aligned}&\frac{4\pi}{3}\hbar\int\frac{\mathrm{d}\omega'\mathrm{d}^3k}{(2\pi)^4}\frac{\pi}{2M\Omega_{\mathbf{k}}}\left\{2\delta(\omega'-\Omega_{\mathbf{k}})+\left(\frac{2k_{\rm B}T}{\hbar\Omega_{\mathbf{k}}}-1\right.\right.\\ &\left.\left.+\frac{1}{6}\frac{\hbar\Omega_{\mathbf{k}}}{k_{\rm B}T}\right)[\delta(\omega'-\Omega_{\mathbf{k}})+\delta(\omega'+\Omega_{\mathbf{k}})]\right\}\mathrm{e}^{-\mathrm{i}\omega'(t-t')}. \qquad (3.5)\end{aligned}$$

The first term in curly brackets is due to spontaneous emission. It contributes a term $-2M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2$ to the rate of change $\partial_t\langle i|\hat{\rho}(t)|i\rangle$. This differs from the right-hand side of equation (3.1) in two important respects. First, the sum is restricted to the lower states $f<i$ with $\omega_{if}>0$, since the δ-function allows only for decays. Second, there is an extra factor 2. Indeed, by comparing (3.3) with (3.5) we see that the spontaneous emission receives equal contributions from the 1 and the $\coth(\hbar\omega'/2k_{\rm B}T)$ in the curly brackets of (3.3), *i.e.*, from dissipation and fluctuation terms $C_{\rm b}(t,t')$ and $A_{\rm b}(t,t')$.

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

$$\Gamma = 2M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2, \qquad (3.6)$$

which is the historic *Wigner-Weisskopf formula.*

In terms of Γ, the rate (3.1) can therefore be written as

$$\begin{aligned}\partial_t\langle i|\hat{\rho}(t)|i\rangle = -\Gamma &+ M\gamma\sum_{f<i}\omega_{if}^3\,|\mathbf{x}_{fi}|^2\\ &+ M\gamma\sum_{f>i}|\omega_{if}|^3\,|\mathbf{x}_{fi}|^2. \qquad (3.7)\end{aligned}$$

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 (3.5). The finite lifetime changes the time dependence of the state $|i,t\rangle$ from $|i,t\rangle = |i,0\rangle\mathrm{e}^{-\mathrm{i}Et}$ to $|i,0\rangle\mathrm{e}^{-\mathrm{i}Et-\Gamma t/2}$.

Note that due to the restriction to $f<i$ in (3.6), there is no operator local in time whose expectation value is Γ. Only the combination of spontaneous and induced emissions and absorptions in (3.7) can be obtained from a local operator, which is in fact the dissipation operator (2.10).

For all temperatures, the spontaneous and induced transitions together lead to the rate of change:

$$\begin{aligned}\partial_t\langle i|\hat{\rho}(t)|i\rangle &= -2M\gamma\\ &\times\left(\sum_{f<i}\omega_{if}^3+\sum_f\omega_{if}^3\frac{1}{\mathrm{e}^{\hbar\omega_{if}/k_{\rm B}T}-1}\right)|\mathbf{x}_{fi}|^2. \qquad (3.8)\end{aligned}$$

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 $T_{\rm Ry} = 157886.601$ K. Thus we must go to $n\gtrsim 20$ to have observable effects at room temperature.

4 Lamb shift

For atoms, the Feynman influence functional (1.5) 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 (1.6) and (1.7) perturbatively as follows: Consider the action (1.6), and in it the first term involving $\mathbf{x}_+(t)$ and $\mathbf{x}_+(t')$, and integrate the external positions in the path integral (1.5) over the initial wave functions, forming

$$U_{ii,t_b;ii,t_a} = \int \mathrm{d}\mathbf{x}_{+b}\,\mathrm{d}\mathbf{x}_{-b} \int \mathrm{d}\mathbf{x}_{+a}\,\mathrm{d}\mathbf{x}_{-a} \langle i|\mathbf{x}_{+b}\rangle\langle i|\mathbf{x}_{-b}\rangle \\ \times U(\mathbf{x}_{+b}, \mathbf{x}_{-b}, t_b|\mathbf{x}_{+a}, \mathbf{x}_{-a}, t_a)\langle \mathbf{x}_{+b}|i\rangle\langle \mathbf{x}_{-b}|i\rangle. \tag{4.1}$$

To lowest order in γ, the effect of the $\mathbf{C}_\mathrm{b}$-term in (1.6) can be evaluated in the local approximation (1.12) as follows. We take the linear approximation to the exponential $\exp[\int \mathrm{d}t\mathrm{d}t'\mathcal{O}(t,t')] \approx 1 + \int \mathrm{d}t\mathrm{d}t'\mathcal{O}(t,t')$ and propagate the initial state with the help of the amplitude $U_{ii,t';ii,t_a}$ to the first time t', then with $U_{fi,t;fi,t'}$ to the later time t, and finally with $U_{ii,t_a;ii,t}$ to the final time t_b. The intermediate state between the times t and t' are arbitrary and must be summed. Details of how to do such a perturbation expansion are given in Section 3.10 of the textbook [3]. Thus we find

$$\Delta_C U_{ii,t_b;ii,t_a} = \mathrm{i}\frac{e^2}{2\hbar^2 c^2}\int_{t_a}^{t_b}\mathrm{d}t\mathrm{d}t' \sum_f \int \mathrm{d}\mathbf{x}_+ \\ \times \int \mathrm{d}\mathbf{x}'_+\, U_{ii,t_a;ii,t}\langle i|\mathbf{x}_+\rangle \mathbf{x}_+ \langle \mathbf{x}_+|f\rangle \\ \times [\partial_t\partial_{t'}\mathbf{C}_\mathrm{b}(t,t')]U_{fi,t;fi,t'}\langle f|\mathbf{x}'_+\rangle\mathbf{x}'_+\langle\mathbf{x}'_+|i\rangle U_{ii,t';ii,t_a}. \tag{4.2}$$

Inserting $U_{ii,t_a;ii,t} = \mathrm{e}^{-\mathrm{i}E_i(t_a-t)/\hbar}$ etc., this becomes

$$\Delta_C U_{ii,t_b;ii,t_a} = \\ -\frac{e^2}{2\hbar^2c^2}\int_{t_a}^{t_b}\mathrm{d}t\mathrm{d}t'\,\langle i|\hat{\mathbf{x}}(t)\,[\partial_t\partial_{t'}\mathbf{C}_\mathrm{b}(t,t')]\,\hat{\mathbf{x}}(t')|i\rangle \\ = -\frac{e^2}{2\hbar^2c^2}\sum_f\int_{t_a}^{t_b}\mathrm{d}t\mathrm{d}t'\mathrm{e}^{\mathrm{i}\omega_{if}(t-t')}\langle i|\hat{\dot{\mathbf{x}}}|f\rangle\mathbf{C}_\mathrm{b}(t,t')\langle f|\hat{\dot{\mathbf{x}}}|i\rangle. \tag{4.3}$$

Expressing $C_\mathrm{b}^{ij}(t,t')$ of equation (1.12) in the form

$$C_\mathrm{b}^{ij}(t,t') = \frac{\hbar}{2\pi c}\frac{2}{3}\delta^{ij}\int\frac{\mathrm{d}\omega}{2\pi}\,\omega\,\mathrm{e}^{-\mathrm{i}\omega(t-t')}, \tag{4.4}$$

the integration over t and t' yields

$$\Delta_C U_{ii,t_b;ii,t_a} = \\ -\mathrm{i}\frac{e^2}{4\pi\hbar c^3}\frac{2}{3}\int_{t_a}^{t_b}\mathrm{d}t\int\frac{\mathrm{d}\omega}{2\pi}\sum_f\frac{\omega}{\omega-\omega_{if}-\mathrm{i}\eta}|\hat{\dot{\mathbf{x}}}_{fi}|^2. \tag{4.5}$$

The same treatment is applied to the A_b in the action (1.7), where the first term involving $\mathbf{x}_+(t)$ and $\mathbf{x}_+(t')$ changes (4.5) to

$$\Delta U_{ii,t_b;ii,t_a} = \\ -\mathrm{i}\frac{e^2}{4\pi\hbar c^3}\frac{2}{3}\int_{t_a}^{t_b}\mathrm{d}t\int\frac{\mathrm{d}\omega}{2\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+\mathrm{i}\eta} \\ \times\left(1+\coth\frac{\hbar\omega}{2k_\mathrm{B}T}\right)|\hat{\dot{\mathbf{x}}}_{fi}|^2. \tag{4.6}$$

The ω-integral is conveniently split into a zero-temperature part and a finite-temperature correction

$$I(\omega_{if},0) \equiv \int_0^\infty\frac{\mathrm{d}\omega}{\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+\mathrm{i}\eta}, \tag{4.7}$$

and

$$\Delta I_T(\omega_{if},T) \equiv 2\int_0^\infty\frac{\mathrm{d}\omega}{\pi}\sum_f\frac{\omega}{\omega-\omega_{if}+\mathrm{i}\eta}\frac{1}{\mathrm{e}^{\hbar\omega/k_\mathrm{B}T}-1}\,. \tag{4.8}$$

Decomposing as usual $1/(\omega_{if}-\omega+\mathrm{i}\eta) = \mathcal{P}/(\omega-\omega_{if}) - \mathrm{i}\pi\delta(\omega_{if}-\omega)$, the imaginary part of the ω-integral yields half of the natural line width in (3.1). The other half comes from the part of the integral (1.6) involving $\mathbf{x}_-(t)$ and $\mathbf{x}_-(t')$. The principal-value part of the zero-temperature integral diverges linearly, the divergence yielding again the mass renormalization (1.13). Subtracting this divergence from $I(\omega_{if},0)$, the remaining integral has the same form as $I(\omega_{if},0)$, but with ω in the numerator replaced by $\omega_{if}=0$. This integral diverges logarithmically like $(\omega_{if}/\pi)\log[(\varLambda-\omega_{if})/|\omega_{if}|]$, where $\varLambda$ is Bethe's cutoff [9]. For $\varLambda \gg |\omega_{if}|$, the result (4.5) implies an energy shift of the atomic level $|i\rangle$:

$$\Delta E_i = \frac{e^2}{4\pi c^3}\frac{2}{3\pi}\sum_f\omega_{if}^3|\hat{\dot{\mathbf{x}}}_{fi}|^2\log\frac{\varLambda}{|\omega_{if}|}, \tag{4.9}$$

which is the *Lamb shift*. Usually, the weakly varying logarithm is approximated by a weighted average $L = \log[\varLambda/\langle|\omega_{if}|\rangle]$ over energy levels and taken out of the integral [10]. Then the energy (4.9) can be attributed to an extra term

$$\hat{H}_\mathrm{LS} \approx -\mathrm{i}\frac{L}{\pi}\frac{M\gamma}{2}[\hat{\dot{\mathbf{x}}},\hat{\ddot{\mathbf{x}}}] \tag{4.10}$$

in the Hamiltonian (2.7). In this form, the Lamb shift appears as a Hermitian logarithmically divergent correction to the operator (2.10) governing the spontaneous emission of photons.

To lowest order in γ, the commutator becomes, for $V(\mathbf{x}) = -\hbar c\,\alpha/r$, equal to $-\mathrm{i}\,[\hat{\mathbf{p}},\hat{\dot{\mathbf{p}}}]\,/\,M^2 = \hbar\boldsymbol{\nabla}^2V(\mathbf{x})/M^2 = (\hbar^2c\,\alpha/M^2)\,4\pi\delta^{(3)}(\mathbf{x})$, leading to $\Delta E_i = (4\alpha^2\hbar^3L/3M^2c)\langle i|\delta^{(3)}(\mathbf{x})|i\rangle$. For hydrogen with principal quantum number n one has $\langle n|\delta^{(3)}(\mathbf{x})|n\rangle = \alpha^3M^3c^3/\hbar^3\pi n^3$.

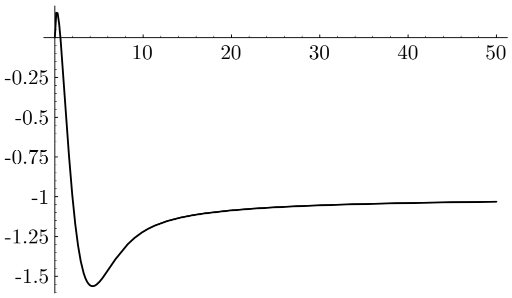

Fig. 1. Behavior of function $6J(z)/\pi^2$.

At finite temperature, (4.9) changes to

$$\Delta E_i = \frac{e^2}{4\pi c^3}\frac{2}{3\pi}\sum_f \omega_{if}^3 |\hat{\mathbf{x}}_{fi}|^2 \times \left[\log\frac{\Lambda}{|\omega_{if}|} + \left(\frac{k_{\mathrm{B}}T}{\hbar\omega_{ij}}\right)^2 J\left(\frac{\hbar\omega_{if}}{k_{\mathrm{B}}T}\right)\right], \tag{4.11}$$

where $J(z)$ denotes the integral

$$J(z) \equiv z\int_0^\infty \mathrm{d}z\,\frac{\mathcal{P}}{z'-z}\,\frac{z'}{\mathrm{e}^{z'}-1}, \tag{4.12}$$

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

5 Langevin equations

For high γT, the last term in the forward – backward path integral (1.25) 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

$$V\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right) - V\left(\mathbf{x}-\frac{\mathbf{y}}{2}\right) \sim \mathbf{y}\cdot\boldsymbol{\nabla}V(\mathbf{x}) + \mathcal{O}(\mathbf{y}^3)\dots, \tag{5.1}$$

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

$$\dot{\boldsymbol{\eta}}(t) \equiv M\ddot{\mathbf{x}}(t) - M\gamma\,\dddot{\mathbf{x}}(t) + \boldsymbol{\nabla}V(\mathbf{x}(t)). \tag{5.2}$$

With this, the exponential function in (1.25) becomes

$$\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_a}^{t_b}\mathrm{d}t\,\dot{\mathbf{y}}\boldsymbol{\eta} - \frac{w}{2\hbar^2}\int_{t_a}^{t_b}\mathrm{d}t\,\dot{\mathbf{y}}^2(t)\right], \tag{5.3}$$

where w is the constant (1.24).

Consider now the diagonal part of the amplitude (1.25) 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

$$P(\mathbf{x}_b\, t_b|\mathbf{x}_a\, t_a) \equiv |(\mathbf{x}_b, t_b|\mathbf{x}_a, t_a)|^2 \equiv U(\mathbf{x}_b, \mathbf{x}_b, t_b|\mathbf{x}_a, \mathbf{x}_a, t_a). \tag{5.4}$$

Now the variable $\mathbf{y}$ can simply be integrated out in (5.3), and we find the probability distribution

$$P[\boldsymbol{\eta}] \propto \exp\left[-\frac{1}{2w}\int_{t_a}^{t_b}\mathrm{d}t\,\boldsymbol{\eta}^2(t)\right]. \tag{5.5}$$

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

$$\langle F[\mathbf{x}]\rangle_\eta \equiv \mathcal{N}\int\mathcal{D}\mathbf{x}\,P[\boldsymbol{\eta}]F[\mathbf{x}], \tag{5.6}$$

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 (5.6) can be rewritten as a functional integral

$$\langle F[\mathbf{x}]\rangle_\eta \equiv \mathcal{N}\int\mathcal{D}\boldsymbol{\eta}\,P[\boldsymbol{\eta}]\;F[\mathbf{x}]. \tag{5.7}$$

Note that the probability distribution (5.5) is $\hbar$-independent. Hence in the approximation (5.1) we obtain the classical Langevin equation. In principle, the integrand contains a factor $J^{-1}[x]$, where $J[x]$ is the functional Jacobian

$$\begin{aligned} J[\mathbf{x}] &\equiv \mathrm{Det}\,[\delta\eta^i(t)/\delta x^j(t')] \\ &= \det[\left(M\partial_t^2 - M\gamma\partial_t^{3R}\right)\delta_{ij} + \nabla_i\nabla_j V(\mathbf{x}(t))]. \end{aligned} \tag{5.8}$$

It can be shown that the determinant is unity, due to the retardation of the friction term [2], thus justifying its omission in (5.7).

The path integral (5.7) may be interpreted as an expectation value with respect to the solutions of a *stochastic differential equation* (5.2) driven by a Gaussian random *noise* variable $\eta(t)$ with a correlation function

$$\langle\eta^i(t)\eta^j(t')\rangle_T = \delta^{ij}w\,\delta(t-t'). \tag{5.9}$$

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 γ leads to slow decay rates. In this case the simplest procedure to solve (5.2) is to write the stochastic equation as

$$M\ddot{\mathbf{x}}(t) + \boldsymbol{\nabla}V(\mathbf{x}(t)) = \dot{\boldsymbol{\eta}}(t) + M\gamma\,\dddot{\mathbf{x}}(t), \tag{5.10}$$

and solve it iteratively, first without the γ-term, inserting the solution on the right-hand side, and such a procedure is equivalent to a perturbative expansion in γ in equation (1.25).

Note that the lowest iteration of equation (5.10) with $\boldsymbol{\eta} \equiv 0$ can be multiplied by $\dot{\mathbf{x}}$ and leads to the equation for the energy change of the particle

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{M}{2}\dot{\mathbf{x}}^2 + V(\mathbf{x}) - M\gamma\dot{\mathbf{x}}\ddot{\mathbf{x}}\right] = -M\gamma\,\ddot{\mathbf{x}}^2. \tag{5.11}$$

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].

6 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].

Let us finally point out that results similar to those in Sections 3 and 4 have been derived with conventional quantum-mechanical methods by many authors [13]. There has also been a discussion closer in spirit to ours by Diosi [15], Landau [16], who consider, however, only the zero-temperature case and do not find a Lindblad form for the master equation. There is further a paper by Anastopoulos and Zoupas [17], who study the behavior of electron *fields* in a photon bath.

In a sequel paper we shall present a similar treatment of a particle in a thermal bath of gravitons [18].

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