Langevin Equation for Particle in Thermal Photon Bath

Z. Haba\textsuperscript{*} and H. Kleinert\textsuperscript{†}
Institut für Theoretische Physik,
Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The forward–backward path integral describing a charged particle moving in a thermal bath of photons is expressed in terms of the solution of a Langevin-type of equation. Approximate methods for solving this equation are discussed.

I. INTRODUCTION

The interaction of charged nonrelativistic point particles with radiation is a fundamental problem of atomic physics. The electrons in light atoms move with nonrelativistic speed and may be described by a Schrödinger equation with the Hamilton operator
\begin{equation}
\hat{H}_x = \frac{1}{2M} \left[ \hat{p} - \frac{e}{c} \mathbf{A}(x, t) \right]^2 + V(x),
\end{equation}
where $\mathbf{A}(x, t)$ is the electromagnetic vector potential and $V(x) = Z\alpha/r$ the Coulomb potential of the nucleus. The decay of an atom is governed by dipole radiation, and the matrix elements of the dipole operator between initial and final atomic states allow us to calculate directly the natural line width of a single atom in the vacuum.

In actual physical systems, this simple situation becomes more involved. An atom may lose its energy in a variety of competing processes which lead to an additional broadening of its spectral lines. In this note we want to set up a theoretical framework for studying the broadening due to the interaction of the atom with a grand-canonical ensemble of photons in thermal equilibrium at high and moderately high temperatures. This will be referred to as a thermal bath of photons. Our work is a physically more realistic version of the well-known treatment of a particle in contact with a thermal bath of oscillators [1–4].

II. DERIVATION OF THE LANGEVIN EQUATION

The time evolution of the density matrix $\rho(x_+; x_-, t)$ of the system described by (1.1) follows a quantum Liouville equation
\begin{equation}
\frac{i\hbar}{\hbar} \partial_t \rho = \hat{H}_x \rho - \hat{H}_x \rho.
\end{equation}
This corresponds to a global time evolution equation
\begin{equation}
\rho(x_+; x_-, t_b) = \int d\mathbf{x}_+ d\mathbf{x}_- U(x_+, x_-, t_b | x_+, x_-, t_a) \rho(x_+, x_-, t_a).
\end{equation}

The evolution kernel may be expressed as a forward–backward path integral due to Feynman and Vernon [1–3]:

\begin{equation}
U(x_+, x_-, t_b | x_+, x_-, t_a) = \int D\mathbf{x}_+ D\mathbf{x}_- \delta(x_+ - x_+ \delta(x_- - x_- \delta(x_+ - x_+) \delta(x_- - x_-)
\times \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} \left[ \frac{M}{2} \left( \dot{x}_+^2 - \dot{x}_-^2 \right) - V(x_+) + V(x_-) - \frac{e}{c} \mathbf{x}_+ \mathbf{A}(x_+) + \frac{e}{c} \mathbf{x}_- \mathbf{A}(x_-) \right] \right\}. \quad (2.3)
\end{equation}

To describe a particle in a bath of photons, we perform a thermal average over the fluctuating vector potential $\mathbf{A}(x, t)$. This is done with the help of Wick’s theorem, according to which the result can be expressed completely in terms of the time-ordered correlation functions at temperature $T$:

\textsuperscript{*}On leave from Institute of Theoretical Physics, University of Wroclaw, Poland; e-mail: zhab@ift.uni.wroc.pl

\textsuperscript{†}Email: kleinert@physik.fu-berlin.de URL: http://www.physik.fu-berlin.de/~kleinert
where we rewrite the evolution kernel in the form (see [5] for more details)

\[
\langle \tilde{T} \tilde{A}^i(x, t) \tilde{A}^j(x', t') \rangle = G^{ij}(x, x') = \hbar c^2 \int \frac{d^3k}{2\Omega_k(2\pi)^3} \tilde{\delta}_{kk}^{\alpha \beta} \cos k(x - x') \left[ \cos \Omega_k(t - t') \coth \frac{\hbar \Omega_k}{2k_B T} - i \sin \Omega_k(t - t') \right] (2.4)
\]

where \( \Omega_k \equiv |k| \) are the frequencies of wave vector \( k \), \( k_B \) is the Boltzmann constant, and \( \tilde{\delta}_{kk}^{\alpha \beta} \equiv \delta_{ij} - k_i k_j / k^2 \) the transverse \( \delta \)-function. We have used the four-vector notation \( x \equiv (x, t) \) for space and time. The operator \( \tilde{T} \) is the time-ordering operator.

At high temperature and for particle systems small in comparison to the mean wave length \( 1 / |k| \), we may neglect the \( x \)-dependence in \( G(x, x') \). Then \( G(x, x') \) can be approximated by

\[
G(x, x') \approx \frac{2}{3 \pi} \left( \frac{2 \hbar c}{k_B T} \right)^{3/2} \left( \delta(t - t') - \frac{\hbar^2}{12(k_B T)^2} \delta(t - t') - \cdots \right) - i \delta(t - t') \quad (2.5)
\]

the brackets being the Fourier transform of the Taylor expansion of \( (\hbar \Omega_k/2k_B T) \coth \hbar \Omega_k/2k_B T \) in (2.4). Moreover, the fluctuations around the average path \( x(t) \equiv [x_+(t) + x_-(t)] / 2 \) are small, so that we can approximate

\[
V(x_+) - V(x_-) \approx y \cdot \nabla V(x), \quad (2.6)
\]

where \( y(t) \equiv x_+(t) - x_-(t) \) is the difference between forward and backward paths. Then the path integral (2.3) takes the form (see [5] for more details)

\[
U(x_{+b}, x_{-b}, t_b | x_{+a}, x_{-a}, t_a) = \int \mathcal{D}x \mathcal{D}y \delta (x(t_b) - x_b) \delta (y(t_b) - y_b)
\times \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[ y \left( M \dot{x} - M \gamma \dot{x} + \frac{y}{2\hbar} \dot{y} - \frac{w}{24(k_B T)^2} \dot{y} + \cdots \right) - y \nabla V(x) \right] \right\}, \quad (2.7)
\]

where we have abbreviated

\[
\gamma \equiv \frac{e^2}{3\pi c M}, \quad w \equiv 2M \gamma k_B T \quad (2.8)
\]

At \( t_a \), the paths \( x(t) \) and \( y(t) \) start from \( x_a \equiv (x_{+a} + x_{-a}) / 2 \) and \( y_a \equiv x_{+a} - x_{-a} \), respectively. Representing the \( \delta \)-function \( \delta (y(t_b) - y_b) \) in (2.7) as a Fourier integral, and inserting for \( y(t_b) \) the equation

\[
y(t_b) = \int_{t_a}^{t_b} dt' \dot{y}(t') + y_a, \quad (2.9)
\]

we rewrite the evolution kernel in the form

\[
U(x_{+b}, x_{-b}, t_b | x_{+a}, x_{-a}, t_a) = \int \mathcal{D}p \int \mathcal{D}x \mathcal{D}y \exp \left\{ \frac{i}{\hbar} \int_{t_a}^{t_b} dt \left[ y - \frac{w}{2\hbar} \dot{y} + \cdots \right) - y_b \nabla V(x) \right] \right\} \delta (x(t_b) - x_b), \quad (2.10)
\]

where we introduced the new variable

\[
\eta(t) \equiv M \dot{x}(t) - M \gamma \dot{x}(t) + \int_{t_a}^{t} dt' \nabla V(x(t')) - p. \quad (2.11)
\]

In Eq. (2.10), the variables \( \dot{y}(t) \) at different points \( t_a < t < t_b \) are independent of each other, and we choose at the end points \( \dot{y}(t_a) = \dot{y}(t_b) = 0 \). This may be justified in a time sliced formulation, where the integrations over the variables next to the end points give only a trivial factor with respect to the product of integrals in which these variables are held fixed at the endpoint values. Furthermore, the path integral (2.10) does not depend on \( \eta(t) \) outside the interval \( t \in (t_a, t_b) \), and is independent of \( \eta(t_b) \) and \( \eta(t_a) \). Hence we may choose \( \eta(t_a) = \eta(t_b) = 0 \), for convenience, and Eq. (2.11) can be solved as a differential equation on the interval \( t_a \leq t \leq t_b \)

\[
M \ddot{x} - M \gamma \dot{x} + \nabla V(x) = \eta(t), \quad (2.12)
\]

with the initial conditions

\[
x(t_a) = x_a, \quad M \dot{x}(t_a) - M \gamma \dot{x}(t_a) = p. \quad (2.13)
\]
We now perform the integral over \( \dot{y} \) in Eq. (2.10). We shall, from now on, neglect the expansion terms indicated by the dots, and obtain the path integral
\[
U(x_{+b}, x_{-b}, t_b; x_{+a}, x_{-a}, t_a) = \int \frac{d^3p}{(2\pi)^3} \int Dx \exp \left[ -\frac{1}{2w} \int_{t_a}^{t_b} dt \eta^2(t) \right] \exp \left\{ -\frac{i}{\hbar} \left[ y_b \int_{t_a}^{t_b} dt \nabla V(x) + p(y_b - y_a) \right] \right\} \delta(x(t_b) - x_b) \tag{2.14}
\]
where \( \eta(t) \) depends on \( x(t) \) via (2.11). There are some virtues of this representation in comparison with the path integral (2.10), in particular, if forward and backward paths start out and end at the same points, such that \( y_a = y_b = 0 \); the oscillatory integral in (2.10) is transformed into a Gaussian integral (2.14) which converges exponentially fast. Such a representation is obviously more suitable for numerical simulations.

For convenience, let us express the evolution of the density matrix (2.2) in terms of the Wigner function defined by the Fourier transform
\[
W(x, p; t) = \left( \frac{1}{2\pi\hbar} \right)^3 \int d^3y e^{ipy/\hbar} \rho(x, y; t). \tag{2.15}
\]
Here and in the sequel, we omit subscripts \( b \) from \( t \) for brevity. Then Eq. (2.14) yields the time evolution equation for the Wigner function as a functional integral
\[
W(x, p; t) = \int Dx \exp \left[ -\frac{1}{2w} \int_{t_a}^{t_b} dt' \eta^2(t') \right] W(x(t), p - \int_{t_a}^{t_b} dt' \nabla V(x(t')); t_a) \tag{2.16}
\]
This equation has a simple physical interpretation. In the limit \( T \to 0 \), the functional integral (2.16) is concentrated around \( \eta(t') = 0 \), corresponding to a deterministic solution of Eq. (2.11) with \( \eta(t') = 0 \). In this limit, we obtain from Eq. (2.16) the Wigner function
\[
W(x, p; t) = W \left( x(t), p - \int_{t_a}^{t_b} dt' \nabla V(x(t')); t_a \right) \tag{2.17}
\]
If the particle is decoupled from the bath, \( \gamma = 0 \), we have \( p = M\dot{x}(t_a) \) and \( M\dot{x}(t) = p - \int_{t_a}^{t_b} dt \nabla V(x(t)), \) and we see that the time evolution of the Wigner function is given by the Liouville equation
\[
\partial_t W + \frac{1}{M} p \cdot \nabla_x W - \nabla_x V \cdot \nabla_p W = 0. \tag{2.18}
\]
The time evolution kernel can also be expressed as a path integral over the noise variable \( \eta(t) \). For this simply change the integration variable in (2.16) from \( x(t) \) to \( \eta(t) \). To find the functional determinant, we integrate Eq. (2.11) once more and write the result as
\[
\partial_t^{-2} \delta \eta(t) = M[x(t) - x_a] - M\gamma[x(t) - \dot{x}(t_a)] + \int_{t_a}^{t_b} ds \int_{t_a}^{s} ds' \nabla V(x(s')) \delta(s' - t') - p(t - t_a). \tag{2.19}
\]
Differentiating this we obtain
\[
\frac{\delta \eta(t)}{\delta x_j(t')} = M\partial_t^2 \left[ \delta_{ij} \delta(t - t') - \gamma \delta_{ij} \delta(t - t') + \frac{1}{M} \int_{t_a}^{t_b} ds \int_{t_a}^{s} ds' \nabla_i \nabla_j V(x(s')) \delta(s' - t') \right]. \tag{2.20}
\]
Applying the product formula \( \text{Det} AB = \text{Det} A \text{Det} B \), the identity \( \text{Det} (1 + K) = \exp \left( \text{Tr} K - \frac{1}{2} \text{Tr} K^2 \ldots \right) \), and the property \( \text{Tr} K^n = 0 \), we see that the Jacobian for the transformation \( x(t) \to \eta(t) \) is a constant, so that we can rewrite Eq. (2.16) as
\[
W(x, p; t) = \left\langle W \left( x(t), p - \int_{t_a}^{t_b} dt' \nabla V(x(t')), t_a \right) \right\rangle_{\eta}, \tag{2.21}
\]
where the average with respect to \( \eta(t) \) fluctuations is performed with the functional integral
\[
\left\langle \ldots \right\rangle_{\eta} = \int D\eta \ldots \exp \left[ -\frac{1}{2w} \int_{t_a}^{t_b} dt \eta^2(t) \right]. \tag{2.22}
\]
The calculation of (2.21) proceeds by solving first the Langevin equation (2.12) with the boundary conditions (2.13) to obtain the solution $x(t)$, and subsequently take the expectation value with respect to the white noise with the correlation function
\[ \langle \eta^i(t) \eta^i(t') \rangle = w \delta^{ij} \delta(t - t'). \quad (2.23) \]

The quantum corrections to the Langevin equation are taken into account by replacing (2.23) by the colored-noise correlation function
\[ \langle \eta^i(t) \eta^j(t') \rangle = w \delta^{ij} \coth \left( \frac{i \hbar}{2 k_B T} \frac{d}{dt} \right) \frac{i \hbar}{2 k_B T} \delta(t - t') \]
\[ = w \delta^{ij} \left[ 1 - \frac{\hbar^2}{12(k_B T)^2} \frac{d^2}{dt^2} - \cdots \right] \delta(t - t'). \quad (2.24) \]

### III. APPROXIMATIONS TO LIOUVILLE EQUATION

From Eq. (2.24) we see that the average size of $\eta$ is $\sqrt{2M\gamma k_B T}$ and thus proportional to $\sqrt{T}$. Let us therefore set $\eta = \sqrt{T/T_H} \tilde{\eta}$ with the characteristic Bohr temperature $T_H \equiv \alpha^2 Mc^2/k_B$ ($\alpha \equiv e^2/\hbar c$). Restricting ourselves now to one-dimensional systems, we search a solution of Eq. (2.12) in the form
\[ x(t) = e^{-\gamma B(t)} \left[ x_{cl}(t) + \sqrt{T/T_H} Q(t) \right], \quad (3.1) \]

where the first term on the right-hand side describes small dissipative correction to the classical equation
\[ M \ddot{x}_{cl} + V'(x_{cl}) = 0. \quad (3.2) \]

The second term on the right-hand side depends on the noise $\tilde{\eta}$. Then, comparing terms of first order in $\gamma$ or $\sqrt{T/T_H}$, and considering terms $\gamma \sqrt{T/T_H}$ as being of higher order, we obtain the following equations
\[ x_{cl} \ddot{B} + 2 \dot{B} \dot{x}_{cl} + B \left[ \ddot{x}_{cl} + \frac{1}{M} V''(x_{cl}) x_{cl} \right] - \frac{1}{M} V''(x_{cl}) \dot{x}_{cl} = 0, \quad (3.3) \]
\[ M \ddot{Q} + V''(x_{cl}) Q = \ddot{\tilde{\eta}}. \quad (3.4) \]

The solution $x_{cl}(t)$ depends on the boundary condition (2.13), in which we set $\gamma = 0$ in the present lowest-order approximation.

The first equation is closely related to the second as can be seen by introducing $A(t) \equiv x_{cl}(t) B(t)$ which satisfies
\[ M \ddot{A} + V''(x_{cl}) A = V''(x_{cl}) \dot{x}_{cl}. \quad (3.5) \]

Let $G(t, t')$ be the Green function of the operator on the left-hand sides of (3.4) and (3.5), satisfying the harmonic differential equation
\[ \left[ \frac{d^2}{dt^2} + \Omega^2(t) \right] G(t, t') = \delta(t - t'), \quad (3.6) \]

with the time-dependent frequency
\[ \Omega^2(t) \equiv \frac{1}{M} V''(x_{cl}(t)). \quad (3.7) \]

Then, the solutions of Eqs. (3.3) and (3.4) are given by
\[ Q(t) = \int_0^t dt' G(t, t') \tilde{\eta}(t') \quad (3.8) \]

and
\[ B(t) = \frac{1}{Mx_{cl}(t)} \int_{0}^{t} dt' G(t, t') V''(x_{cl}(t')) \dot{x}_{cl}(t'), \]  

(3.9)

respectively. The Green function can be expressed in terms of two independent solutions \( \xi_1(t) \) and \( \xi_2(t) \) of the homogeneous version of the differential equation (3.6) with the initial conditions \( \xi_1(0) = 0 \) and \( \xi_1(0) = 1 \) and \( \xi_2(0) = 1 \) and \( \xi_2(0) = 0 \). These, in turn, can be obtained directly from the classical solution \( x_{cl}(t) \).

If the classical solutions are bounded in all directions of phase space, then the Green function and its derivative are bounded. In such a case it follows from Eq. (3) in Ref. [7] that the random perturbation grows at most linearly in \( t^T/T \). A deviation of magnitude \( D \) from the classical solution appears at the time which is proportional to \( D/T \). However, if the classical system is chaotic, which can happen either in multidimensional systems or in a one-dimensional system with a time-dependent potential, then the classical solutions as well as the Green function can grow exponentially fast in some directions of the phase space. In these directions, the classical solution expressed in terms of \( \sqrt{T/T} Q \) can grow to a size of the order \( D \) in a much shorter time \( \ln(D/T) \). Such an increase of quantum corrections in chaotic systems has recently been discussed by H.Zurek [10]. For the quantum systems in a photon bath under discussion, this result is modified by the damping factor \( e^{-B(t)} \). Now, \( B(t) \) can be bounded, or it can increase linearly in \( t \), as it happens for a linear oscillator. In a chaotic system, \( B(t) \) can also grow exponentially fast. Such a strong friction dampens completely the chaotic growth of quantum corrections, such that there is no need to apply quantum mechanics to large macroscopic systems. It behaves like a strongly damped classical system.

The solution (3.1) may be inserted into the Eq. (2.16) to find the time evolution of the Wigner function.

Our semiclassical expansion can be extended systematically to any order, albeit with increasing complexity. Perturbative as well as full nonperturbative solutions can be found most efficiently on a computer, yielding the full time evolution of the Wigner function and thus of the density matrix.

**IV. HARMONIC POTENTIAL**

The solution of our equations is simple for a harmonic potential

\[ V(x) = \frac{M\omega^2}{2} x^2. \]  

(4.1)

Then Eqs. (3.3) and Eq. (3.4) have the solutions

\[ B(t) = \frac{\omega^2}{2} (t - t_a), \quad Q(t) = \frac{1}{M\omega} \int_{t_a}^{t} dt' \sin \omega (t - t') \dot{\eta}(t'), \]  

(4.2)

and (3.1) yields to lowest order in \( \gamma \) the orbit

\[ x(s) = e^{-\gamma \omega^2 (s-t_a)/2} \left\{ x_a \cos \omega(s-t_a) + \frac{p}{1 + \gamma \omega} \sin \omega (s-t_a) + \frac{1}{M\omega} \int_{t_a}^{s} dt' \sin \omega (s-t') \dot{\eta}(t') \right\} \]  

(4.3)

which determines the Wigner function via Eq. (2.17).

The fluctuation width is

\[ \langle (x(t) - \langle x(t) \rangle)^2 \rangle = \frac{w}{2M^2 \omega^2} f_\gamma(\omega t) \equiv \frac{w}{2M^2} (t - t_a) e^{-\gamma \omega^2 (t-t_a)} \left[ 1 + \frac{\sin 2\omega(t-t_a)}{2\omega(t-t_a)} \right]. \]  

(4.4)

For small times, this shows the same linear growth in time as for the Brownian motion of a free particle with \( \omega = 0 \):

\[ \langle (x(t) - \langle x(t) \rangle)^2 \rangle = \frac{w}{M^2} (t - t_a), \]  

(4.5)

As the time grows, the width oscillates around this behavior with frequency \( 2\omega \). For large times of the order \( 1/\gamma \omega^2 \), on the other hand, the width goes exponentially fast to zero (see Fig. 4).
FIG. 1. Time dependence of fluctuation width in Eq. (4.4) for different values of friction constant $\gamma$. Time is measured in units of $1/\omega$.

In the free-particle limit, the solution (3.1) reduces to

$$x(t) = x + \frac{p}{M} (t - t_a) + \frac{1}{M} \int_{t_a}^t dt' \eta(t').$$

(4.6)

Inserting this into formula (2.16), we obtain the evolution of the Wigner function. For a wave packet with momentum $k$ and position $x$, the result is

$$W(x, p; t_a) = \frac{1}{\pi \hbar} \exp \left[ -\frac{(p - k)^2 \sigma}{\hbar^2} - \frac{(x - \bar{x})^2}{\sigma} \right].$$

(4.7)

Inserting (4.6) into (2.16), we obtain for $W$ the formula (4.7) with the replacements

$$\bar{x} \rightarrow \bar{x}(t) = \bar{x} - \frac{p}{M} (t - t_a) \quad \text{and} \quad \sigma \rightarrow \sigma(t) = \sigma \left[ 1 + \frac{2\omega}{M^2} (t - t_a) \right],$$

(4.8)

i.e., a free evolution with the well-known spreading of the wave packet.

For the oscillator potential, the mean position and the mean momentum of the particle run along the corresponding classical trajectories, and the thermal spread behaves as in (4.4).

The spread in momentum space can be calculated from this using the relation

$$\langle (p(t) - \langle p(t) \rangle)^2 \rangle = M^2 \omega^4 \left\langle \int_{t_a}^t (x(s) - \langle x(s) \rangle)^2 ds \right\rangle.$$

(4.9)

This research is supported by a grant from a governmental German university program HSP III.

[1] R.P. Feynman and F.L. Vernon, Ann. Phys. (N.Y.) 24, 118 (1963)
[2] R.P. Feynman, A.R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw Hill, New York 1965
[3] A.O. Caldeira and A.J. Leggett, Ann. Phys. 149, 374 (1983), 153, 445(E) (1984).
[4] H. Kleinert, *Path Integrals and Quantum Mechanics, Statistics, and Polymer Physics*, 2nd edition, World Scientific, Singapore, 1995.
[5] Z. Haba, H. Kleinert, *Master equation for electromagnet dissipation and decoherence of density matrix*, Berlin preprint 2000
[6] H. Kleinert and A. Chervyakov, Phys. Lett. A 245, 345 (1998) (quant-ph/9803016); J. Math. Phys. B 40, 6044 (1999) (physics/9712048).
For more details see Sections 3.3.1, 3.5, 3.21, and 4.3 in the third edition of Ref. [4] which can be downloaded from http://www.physik.fu-berlin.de/~kleinert/b3.
[7] Z. Haba, Lett. Math. Phys. 47, 321 (1999).
[8] See Eq. (4.99) in the third edition of Ref. [4].
[9] L. Bieberbach, *Einführung in die Theorie der Differentialgleichungen in Reellen Gebieten*, Springer, 1956.
[10] L. Paz and H. Zurek, Phys. Rev. Lett. 82, 5181 (1999); H. Zurek, Annalen der Phys. 7777 (2000), and Lecture delivered at the conference *Hundred Years Quantum Theory* in Berlin, 2000.