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THE QUANTUM LANGEVIN EQUATION   DIAS - STP-88-27

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ABSTRACT

The macroscopic description of a quantum particle with
passive dissipation and moving in an arbitrary external potential
is formulated in terms of the generalized Langevin equation. The
coupling with the heat bath corresponds to two terms: a mean force
characterized by a memory function $\mu(t)$ and an operator-valued
random force. Explicit expressions are given for the correlation
and commutator of the random force. The random force is *never*
Markovian. It is shown that $\tilde{\mu}(z)$, the Fourier transform of the
memory function, is a positive real function, analytic in the
upper half plane and with $\mathrm{Re}\{\tilde{\mu}(\omega + i0^{+})\}$ a positive distribution
on the real axis. This form is then derived for the
independent-oscillator (IO) model of a heat bath. It is shown that
the most general quantum Langevin equation can be realized by this
simple model. A critical comparison is made with a number of other
models which have appeared in the literature.

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I. INTRODUCTION

The problem of a quantum particle coupled to a heat bath appears in many fields of physics: statistical mechanics, condensed-matter, quantum optics, atomic physics, etc. Here we formulate the description of such a system in terms of the quantum Langevin equation for a particle in an arbitrary external potential. This description has the advantage that it is complete and can be characterized in a general way. We then show how this description can be realized by a simple independent-oscillator model of the heat bath.

In Section II we describe the quantum Langevin equation. The key point there is that this is a *macroscopic* equation corresponding to a reduced description of the system. Central to this description is the requirement that the bath be *passive*. A passive system is one for which there is a unique thermal equilibrium state. In the present case this physical requirement of passivity is expressed explicitly in the mathematical requirement that the Fourier transform of the memory function be a *positive real function*, analytic in the upper half plane and with real part positive on the real axis. We show that this property of the memory function is a consequence of causality and, in Section III, of the second law of thermodynamics.

In Section IV we discuss the independent-oscillator model of the heat bath. The key result there is that the most general quantum Langevin equation can be realized with such a model. Then, in Section V we show in some detail the relation of this model to various other models which have appeared in the literature.

Before proceeding we should perhaps make something of a disclaimer. Knowing readers will recognize that some of what we have to say is not entirely new. Yet, for example, the general description we give in Section II appears explicitly nowhere in the literature. On the other hand, a famous discussion remark of Kubo at the 1968 conference on Statistical Mechanics[1] makes clear that at least something of the general idea has long been known to many scholars, and the general characterization in terms of positive real functions is straight out of the electrical engineering literature. We have attempted by an eclectic choice of

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references to give credit to earlier authors and to indicate where our ideas have grown out of theirs. At the same time we have supressed references to more recent authors who have, perhaps independently, only rediscovered what has for a long time been in the literature.

II. THE QUANTUM LANGEVIN EQUATION

In this section we describe the quantum Langevin equation, which can be taken as the basis of the macroscopic description of a quantum particle linearly coupled to a passive heat bath. In Section IV we derive this equation from a simple model, the independent oscillator (IO) model. Our reasons for, so to speak, inverting the order and stating the results before describing a basis for their derivation are, first, the description and characterization of the equation is somewhat lengthy and should be clearer as a separate whole, and, second and more important, we claim the description given is more general than the model.

We consider, therefore, a quantum particle of mass m moving in a one-dimensional portential V(x) and linearly coupled to a passive heat bath at temperature T. The macroscopic equation describing the time-development of the particle motion is the quantum Langevin equation:

$$m\ddot{x} + \int_{-\infty}^{t}dt'\,\mu(t - t')\dot{x}(t') + V'(x) = F(t) , \qquad (2.1)$$

where the dot and prime denote, resp., the derivative with respect to t and x. This is the Heisenberg equation of motion for the coordinate operator x. The coupling with the heat bath is described by two terms: an operator-valued random force F(t) with mean zero, and a mean force char⋅cterized by a memory function $\mu(t)$. The (symmetric) autocorrelation of F(t) is

$$\frac{1}{2}\langle F(t)F(t') + F(t')F(t)\rangle$$
$$= \frac{1}{\pi} \int_{0}^{\infty}d\omega\ \text{Re}\{\tilde{\mu}(\omega + i0^{+})\}\ \hbar\omega\ \coth(\hbar\omega/2kT)\ \cos\omega(t - t') , \qquad (2.2)$$

and the nonequal-time commutator of F(t) is

$$[F(t),F(t')] = \frac{2}{i\pi} \int_{0}^{\infty}d\omega\ \text{Re}\{\tilde{\mu}(\omega + i0^{+})\}\ \hbar\omega\ \sin\omega(t - t') . \qquad (2.3)$$

In these expressions

$$\tilde{\mu}(z) = \int_{0}^{\infty}dt\,e^{izt}\mu(t) , \quad \text{Im}\,z > 0 \qquad (2.4)$$

is the Fourier transform of the memory function $\mu(t)$. (By

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convention, the memory function vanishes for negative times.)
Finally, F(t) has the Gaussian property: correlations of an odd
number of factors of F vanish, those of an even number of factors
are equal to the sum of products of pair correlations
(autocorrelations), the sum being over all pairings with the order
of the factors preserved within each pair.

It is clear from the above description that, as in the
classical case,[2] the coupling to the heat bath is characterized by
the function $\tilde{\mu}(z)$. Now this function has three important
mathematical properties which follow in turn from three
corresponding general physical principles. The first of these, as
we see from (2.4), is that $\tilde{\mu}(z)$ is analytic in the upper
half-plane Im z > 0. This is a consequence of causality; the mean
force exerted by the heat bath on the particle depends only upon
the *past* motion of the particle. The second property is that the
boundary value of $\tilde{\mu}(z)$ on the real axis has everywhere a positive
real part:

$$\text{Re}\{\tilde{\mu}(\omega + i0^+)\} \geq 0 \qquad , \quad -\infty < \omega < \infty \ . \tag{2.5}$$

This, as we show in Section III, is a consequence of the second
law of thermodynamics. The third property is the reality
condition:

$$\tilde{\mu}(\omega + i0^+) = \tilde{\mu}(-\omega + i0^+)^* \ , \tag{2.6}$$

which follows from the fact that x is a Hermitian operator. Thus
$\text{Re}\{\tilde{\mu}(\omega + i0^+)\}$ is an even function of ω. Such functions of a
complex variable, analytic in the upper half-plane and with real
part a positive, even distribution on the real axis, are termed
positive real functions. They form a very restricted class of
functions of a complex variable. Among their properties are the
following.[3,4]

1° The most general positive real function has the
representation in the upper half-plane (the Stieltjes inversion
theorem):[5]

$$\tilde{\mu}(z) = -icz + \frac{2iz}{\pi} \int_0^\infty d\omega \ \frac{\text{Re}\{\tilde{\mu}(\omega + i0^+)\}}{z^2 - \omega^2} \ . \tag{2.7}$$

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where c is a positive constant. Thus the real positive *distribution* $\text{Re}\{\tilde{\mu}(\omega + i0^{+})\}$ characterizes the function, except for the constant c, which in our case can be absorbed into the particle mass (beware, this is not mass renormalization). With some hesitation in introducing a new terminology in an old subject, we shall call this the spectral distribution of the memory function.

2° The real part of a positive real function is positive in the upper half-plane:

$$\text{Re}\{\tilde{\mu}(z)\} > 0 \qquad , \quad \text{Im } z > 0 \ . \tag{2.8}$$

Thus there are neither poles nor zeros in the upper half-plane.

3° The reciprocal of a positive real function is a positive real function.

4° The sum of two positive real functions is a positive real function.

5° On the real axis, a positive real function can have only simple zeros, each with negative imaginary coefficient, and simple poles, each with positive imaginary residue.

Before we conclude this section, we make a number of general remarks about this description of a quantum stochastic process by the generalized Langevin equation.

The quantum Langevin equation (2.1) is a *macroscopic* equation. What we mean by this is that it is a *contracted* description of the system; the dynamical variables of the heat bath do not appear. It is also a *phenomenological* equation. By this we mean that the interaction with the heat bath is uniquely characterized by the spectral distribution $\text{Re}\{\tilde{\mu}(\omega + i0^{+})\}$, which in principle could be determined experimentally, although in most applications it is derived on the basis of some microscopic model of the bath. As with all macroscopic descriptions, this one has the subtle difficulty that, although we believe that it is appropriate to the description of a wide variety of systems (e.g., a Brownian particle in a dense fluid, or the electrons in a metal, or a Josephson junction), we can only derive it for simple microscopic models (e.g., systems of coupled oscillators).[6] In this regard perhaps it is worth quoting the

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remark of Benguria and Kac,[7] "It follows that either the Langevin equation here is a fluke of the special FKM model which led to it or that there is no general valid quantum Langevin equation."

If this is a general macroscopic phenomenological description, then some general constraints are set by our physical intuition about the systems to which it applies. One of these is that the mean force exerted by the heat bath (sometimes called the radiation reaction force) is linear in the particle motion. Another is that this force is the result of a *given* motion of the particle and is independent of how that motion arose. This last implies that the memory function $\mu(t)$ should be independent of the potential $V(x)$ and the particle mass m, depending only upon the parameters describing the coupling to the heat bath.

The classical Langevin equation corresponds to a constant spectral distribution: $\tilde{\mu}(\omega + i0^+) = \zeta$, where ζ is the friction constant. The equation (2.1) then takes the form:

$$m\ddot{x} + \zeta\dot{x} + V'(x) = F(t) \ . \tag{2.9}$$

In this case, since the past motion does not appear, one says there is no memory. On the other hand, the expression (2.2) for the autocorrelation of the quantum mechanical random force takes the form:

$$\frac{1}{2}\langle F(t)F(t') + F(t')F(t)\rangle$$

$$= \frac{\zeta}{\pi} \int_0^\infty d\omega \ \hbar\omega \ \coth(\hbar\omega/2kT) \ \cos\omega(t - t')$$

$$= kT\zeta \ \frac{d}{dt} \coth[\pi kT(t-t')/\hbar] \ , \tag{2.10}$$

which is not proportional to a delta function in time. Thus we have the situation that, although there is no memory, the quantum mechanical process is not Markovian in the customary sense of the term. In the classical mechanical case, taking the limit $\hbar \rightarrow 0$, we see from (2.3) that the commutator vanishes and the autocorrelation (2.10) of the random force becomes

$$\langle F(t)F(t')\rangle \xrightarrow[\hbar \rightarrow 0]{} 2kT\zeta\delta(t-t') \ , \tag{2.11}$$

which is the familiar form of the (Markovian) classical theory.[8] Note that this limit is not uniform. The time scale is $\hbar/kT$,

independent of the friction constant ζ, and becomes longer the lower the temperature.

As a final remark, we draw attention to the fact that the lower limit on the time integration in the memory term in (2.1) is $t = -\infty$. This is first of all a clear indication that time reversal invariance is broken, since the distant past is singled out over the distant future. On the other hand the equation is invariant under time translations: $t \rightarrow t + t_o$, which means that the solutions $x(t)$ correspond to a *stationary* quantum stochastic process.

III. THE POSITIVITY CONDITION

Here we show that the positivity condition (2.5) is a consequence of the second law of thermodynamics, which in the Kelvin-Planck form states: "It is impossible to construct an engine which will work in a complete cycle, and produce no effect excepting the raising of a weight and the cooling of a heat reservoir".[14] In our case we choose the heat reservoir to be the system of a quantum particle coupled to the heat bath. We then consider the effect of an applied c-number force f(t) that acts on the particle. We suppose that this applied force vanishes in the distant future and past, but is otherwise arbitrary. Its effect, therefore, is to carry the reservoir (particle coupled to the heat bath) from a state of equilibrium, through a (continuous) sequence of intermediate states, and back to a state of equilibrium. Thus, the external force works in a complete cycle on an otherwise isolated reservoir. The second law requires that the net work done by this force be positive.

In this cycle, the instantaneous power supplied by the force f(t) is

$$P = f(t)<v(t)> , \tag{3.1}$$

where $v = \dot{x}$ is the particle velocity operator. The net work done on the system in the cycle is, therefore,

$$W = \int_{-\infty}^{\infty} dt f(t)<v(t)> . \tag{3.2}$$

The mean or expectation value of the velocity appears in these expressions because the second law addresses mean values, fluctuations are another matter. The work (3.2) is therefore the thermodynamic work and must be positive.

If we introduce Fourier transforms, the Parseval formula allows us to write:

$$W = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{f}(\omega)<\tilde{v}(-\omega)> > 0 , \tag{3.3}$$

where, as in (2.4), we denote the Fourier transform by a superposed tilde, e.g.,

$$\tilde{v}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} v(t) . \tag{3.4}$$

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Now, since the memory function is independent of the external potential, it is sufficient to consider the case of a free particle, for which the Langevin equation (2.1) takes the form:

$$m\dot{v} + \int_{-\infty}^{t} dt'\, \mu(t - t')v(t') = F(t) + f(t) .$$

(3.5)

Forming the mean and taking the Fourier transform, we get

$$[-i\omega m + \tilde{\mu}(\omega + 0^{+})]\langle\tilde{v}(\omega)\rangle = \tilde{f}(\omega) ,$$

(3.6)

where we have used the fact that F(t) has mean zero. Putting this in (3.3), we find

$$W = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, [-i\omega m + \tilde{\mu}(\omega + i0^{+})]\langle\tilde{v}(\omega)\rangle\langle\tilde{v}(-\omega)\rangle .$$

(3.7)

Replacing in the integration $\omega \rightarrow -\omega$ and using the reality condition (2.6), we see that within the square bracket only $\mathrm{Re}\{\tilde{\mu}(\omega + i0^{+})\}$ contributes to the integral. If we then use the reality condition on the velocity: $\tilde{v}(-\omega) = \tilde{v}(\omega)^{*}$, we obtain the following expression for the net work done by the force f(t).

$$W = \frac{1}{\pi} \int_{0}^{\infty} d\omega\, \mathrm{Re}\{\tilde{\mu}(\omega + i0^{+})\}|\langle\tilde{v}(\omega)\rangle|^{2}.$$

(3.8)

The second law requires that this be positive for any f(t) which vanishes at $t = \pm\infty$. Since $\tilde{f}(\omega)$ and, through (3.6), $\langle\tilde{v}(\omega)\rangle$ are therefore arbitrary, the integrand in this expression must be positive for all ω. We thus obtain the positivity condition (2.5).

We conclude this section with a pair of remarks about this deceptively simple proof.

Clearly it is important that the operator x be a displacement operator, so that $f(t)\langle v(t)\rangle$ is the instantaneous power supplied by f. Another way of saying this is that a term $V(x,t) = -xf(t)$ added to the Hamiltonian of the *system* of particle plus heat bath must result in a term f(t) added to the right hand side of (2.1). One must therefore be cautious in applying the description in Section II to an equation which is formally similar to the Langevin equation but in which the physical meaning of x is different.

In the proof we have assumed that when f(t) = 0 the system will in the course of time relax to a unique thermal equilibrium

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state. This is the passivity condition. In practice this requires that the number of degrees of freedom in the heat bath must be infinite and that the memory function must vanish for long times,[5]

$$\mu(t) \xrightarrow[t\to\infty]{} 0 \ . \tag{3.8}$$

Indeed, when these conditions are not met there is in our opinion no macroscopic description of the form (2.1).

IV. THE INDEPENDENT OSCILLATOR MODEL OF A HEAT BATH

The IO model is the very simple model in which the quantum particle is surrounded by a large (eventually infinite) number of heat bath particles, each attached to it by a spring. The Hamiltonian of the system is then

$$H = \frac{p^2}{2m} + V(x) + \sum_j \left[\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2(q_j - x)^2 \right] . \tag{4.1}$$

We of course have the usual commutation rules:

$$[x,p] = i\hbar , \quad [q_j, p_k] = i\hbar\delta_{jk} , \tag{4.2}$$

and all other commutators vanish. This model is not original with us, yet it appears rarely in the literature.[9,10,11] Much more frequently appearing is the superficially similar linear coupling model in which the bath particles are attached to a fixed origin (i.e., in the sum in (4.1) x is set equal to zero) and the coupling is represented by adding a term of the form: $x\sum_j \lambda_j q_j$. We shall have more to say about such models in Section IV. Here we only stress that for any potential V(x) for which the uncoupled particle Hamiltonian,

$$H_o = \frac{p^2}{2m} + V(x) , \tag{4.3}$$

has a spectrum with a lower bound, i.e., has a ground state, the same will be true of our Hamiltonian (4.1). It will not be true in general for these other models.

The derivation of the generalized Langevin equation from this model takes but a few steps. The Heisenberg equations of motion from (4.1) are

$$\dot{x} = [x,H]/i\hbar = p/m$$

$$\dot{p} = [p,H]/i\hbar = -V'(x) + \sum_j m_j\omega_j^2(q_j - x)$$

$$\dot{q}_j = [q_j,H]/i\hbar = p_j/m_j \tag{4.4}$$

$$\dot{p}_j = [p_j,H]/i\hbar = -m_j\omega_j^2(q_j - x) ,$$

where dot and prime represent, respectively, differentiation with respect to t and x. Eliminating the the momentum variables, we can

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write these in the form:

$$m\ddot{x} + V'(x) = \sum_j m_j\omega_j^2(q_j - x) ,$$ (4.5)

$$\ddot{q}_j + \omega_j^2 q_j = \omega_j^2 x .$$ (4.6)

The equations (4.6) are inhomogeneous differential equations for the q_j, whose general solution is

$$q_j(t) = q_j^h(t) + x(t) - \int_{-\infty}^{t} dt' \cos\omega_j(t - t') \dot{x}(t') ,$$ (4.7)

where $q_j^h(t)$ is the general solution of the homogeneous equation ($x \equiv 0$). This is given by

$$q_j^h(t) = q_j \cos w_j t + p_j \frac{\sin\omega_j t}{m_j\omega_j} ,$$ (4.8)

where q_j and p_j are time independent operators satisfying the same commutation rules (4.2).

The seemingly straightforward step leading to (4.7) is in fact profound, since in choosing the retarded solution of the inhomogeneous equation we have broken the time reversal invariance of the original equations. The picture we have is that in the distant past the quantum particle is held fixed at x = 0, say, by fastening it to a large mass. The oscillators are then allowed to come to equilibrium at temperature T, say, by a weak coupling with still another bath. Then, still in the distant past, the system is released and the subsequent motion is governed by the Hamiltonian (4.1). This is typical of the way time reversal invariance is broken in macroscopic equations: they describe only the time development of a class of solutions of the microscopic equations.

The remaining steps are indeed straightforward. We put (4.7) in (4.5) to get the Langevin eqution (2.1) with

$$\mu(t) = \sum_j m_j\omega_j^2 \cos\omega_j t \; \theta(t) ,$$ (4.9)

where $\theta(t)$ is the Heaviside step function, and with

$$F(t) = \sum_j m_j\omega_j^2 q_j^h(t) .$$ (4.10)

To find expressions for the autocorrelation and commutator of F(t), we recall the expression (4.8) for $q_j^h(t)$ and that in the distant past the oscillators are in equilibrium at temperature T

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and with respect to the Hamiltonian:

$$H_B = \sum_j \left(\frac{1}{2m_j} p_j^2 + \frac{1}{2} m_j \omega_j^2 q_j^2 \right) , \qquad (4.11)$$

corresponding to fixing $x = 0$ in (4.1). This means that

$$\langle q_j q_k \rangle \equiv \text{Tr}\left\{ q_j q_k \exp\left(-H_B/kT \right) \right\} \Big/ \text{Tr}\left\{ \exp\left(-H_B/kT \right) \right\}$$

$$= \frac{\hbar}{2m_j \omega_j} \coth(\hbar\omega_j/2kT) \, \delta_{jk} , \qquad (4.12)$$

$$\langle p_j p_k \rangle = \frac{\hbar m_j \omega_j}{2} \coth(\hbar\omega_j/2kT) \, \delta_{jk} ,$$

$$\langle q_j p_k \rangle = -\langle p_j q_k \rangle = \frac{1}{2} i\hbar \, \delta_{jk} .$$

With these, using (4.8) and (4.10), we find

$$\frac{1}{2}\langle F(t)F(t') + F(t')F(t) \rangle$$

$$= \frac{1}{2} \sum_j \hbar m_j \omega_j^3 \coth(\hbar\omega_j/2kT) \cos\omega_j(t - t') . \qquad (4.13)$$

In a similar way, using the commutation relations (4.2), we find

$$[F(t), F(t')] = -i \sum_j \hbar m_j \omega_j^3 \sin\omega_j(t-t') . \qquad (4.14)$$

The final step is to form

$$\tilde{\mu}(z) = \int_0^\infty dt \, e^{izt} \sum_j m_j \omega_j^2 \cos\omega_j t$$

$$= \frac{i}{2} \sum_j m_j \omega_j^2 \left(\frac{1}{z - \omega_j} + \frac{1}{z + \omega_j} \right) . \qquad (4.15)$$

Using the well known result: $1/(x \mp i0^+) = P(1/x) - i\pi\delta(x)$, we see that the spectral distribution is given by

$$\text{Re}\{\tilde{\mu}(\omega + i0^+)\} = \frac{\pi}{2} \sum_j m_j \omega_j^2 \left[\delta(\omega - \omega_j) + \delta(\omega + \omega_j) \right] . \qquad (4.16)$$

With this it is clear that (4.13) is equivalent with (2.2) and that (4.14) is equivalent with (2.3). (Note that this is a positive, even distribution.) Finally, we have the Gaussian property of $F(t)$, which follows from the same property of the q_j and p_j. We won't discuss this Gaussian property further here since it is adequately treated in the literature.[12]

It is clear that, by suitably choosing the distribution of the frequencies and force constants for the independent oscillators, one can with (4.16) represent the most general real,

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positive, even distribution, i.e., the most general spectral distribution. This in turn means that, with the Stieltjes inversion theorem (2.7), one can represent the most general positive real function, and through it the most general quantum Langevin equation. We stress that this does not mean that in every physical situation in which this equation arises the actual bath is an IO bath, but rather that from a study of the equation and its solutions (i.e.,from the macroscopic description) one cannot tell the difference. It is remarkable that such a naive and simple model has such generality.

V RELATION WITH OTHER MODELS

In this section we consider a number of other heat bath models and their relation with the IO model.

A. Velocity coupling model.

This model is a version of the IO model but in which the coupling is through the particle momentum. With sufficient generality it corresponds to the Hamiltonian:

$$H_{VC} = \frac{1}{2m}\Big(p + \sum_j m_j\omega_j q_j\Big)^2 + V(x) + \sum_j \Big[\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 q_j^2 \Big] . \qquad (5.1)$$

This model has a number of attractive features, e.g., the translation invariance for the free particle (V = 0) is immediately obvious. It is however identical with the IO model, which we can see as follows. We first make a unitary transformation corresponding to the operator:

$$U = \exp\Big(- \frac{i}{\hbar} x \sum_j m_j\omega_j q_j \Big) . \qquad (5.2)$$

It is a simple matter to show that under this transformation,

$$p \rightarrow U^\dagger p U = p - \sum_j m_j\omega_j q_j \quad , \quad x \rightarrow x$$

$$p_j \rightarrow p_j - m_j\omega_j x \qquad , \quad q_j \rightarrow q_j \qquad (5.3)$$

$$H \rightarrow U^\dagger H U = \frac{p^2}{2m} + V(x) + \sum_j \Big[\frac{1}{2m_j}(p_j - m_j\omega_j x)^2 + \frac{1}{2}m_j\omega_j^2 q_j^2 \Big] .$$

Next we make a second unitary transformation of the bath variables alone, corresponding to the unitary operator:

$$U_1 = \exp\Big[\frac{i\pi}{2\hbar} \sum_j \Big(\frac{1}{2m_j\omega_j}p_j^2 + \frac{1}{2}m_j\omega_j q_j^2 \Big) \Big] . \qquad (5.4)$$

Again, it is straightforward to show that

$$q_j \rightarrow U_1^\dagger q_j U_1 = - \frac{1}{m_j\omega_j}p_j \quad , \quad p_j \rightarrow m_j\omega_j q_j$$

$$\qquad (5.5)$$

$$H_{VC} \rightarrow U_1^\dagger H_{VC} U_1 = \frac{p^2}{2m} + V(x) + \sum_j \Big[\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2(q_j - x)^2 \Big] .$$

But this is exactly the Hamiltonian (4.1) of the IO model. Therefore, the velocity coupling model is equivalent with the IO model, and leads to the identical form (4.16) for the spectral distribution $\mathrm{Re}\{\tilde{\mu}(\omega + i0^+)\}$ characterizing the quantum Langevin

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equation. We should perhaps stress the fact that in making this conclusion it is important that the unitary transformations (5.2) and (5.4) do not change the coordinate operator x.

B. The blackbody radiation field.

A one-electron atom interacting with the radiation field in the dipole approximation corresponds to the Hamiltonian:

$$H_{QED} = \frac{1}{2m}(\vec{p} + \frac{e}{c}\vec{A})^2 + V(\vec{r}) + \sum_{\vec{k},s} \hbar\omega_k(a^\dagger_{\vec{k},s}a_{\vec{k},s} + \frac{1}{2}) , \qquad (5.6)$$

where the vector potential is given by

$$\vec{A} = \sum_{\vec{k},s} \left(\frac{2\pi\hbar c^2}{\omega_k V}\right)^{1/2} f_k \hat{e}_{\vec{k},s} \left(a_{\vec{k},s} + a^\dagger_{\vec{k},s} \right) . \qquad (5.7)$$

Here the symbols have their usual meanings.[13] The quantity f_k is the electron form factor (Fourier transform of the electron charge distribution). Without loss of generality we have taken the form factor as well as the polarization vector $\hat{e}_{\vec{k},s}$ to be real. The form factor, which is sometimes called a cut-off factor, must have ths property that it is unity up to some large cut-off frequency Ω after which it falls to zero.

The electrodynamic Hamiltonian (5.6) is a three dimensional version of the velocity coupling Hamiltonian (5.1). To see this more precisely, we introduce

$$m_k = \frac{4\pi e^2 f_k^2}{\omega_k^2 V} , \qquad (5.8)$$

and write

$$a_{\vec{k},s} = \frac{m_k \omega_k q_{\vec{k},s} + i p_{\vec{k},s}}{\sqrt{2m_k \hbar\omega_k}} . \qquad (5.9)$$

The Hamiltonian (5.6) then can be written:

$$H_{QED} = \frac{1}{2m}\left[\vec{p} + \sum_{\vec{k},s} m_k \omega_k q_{\vec{k},s} \hat{e}_{\vec{k},s}\right]^2 + V(\vec{r})$$

$$\qquad (5.10)$$

$$+ \sum_{\vec{k},s} \left(\frac{1}{2m_k} p_{\vec{k},s}^2 + \frac{1}{2}m_k \omega_k^2 q_{\vec{k},s}^2 \right)^2 .$$

This form is clearly equivalent to the velocity coupling model (5.1), excepting only the trivial difference that, because of the

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transversality condition, only two of the three components of $\vec{k}$ contribute to the coupling in each spatial direction. This gives a factor of 2/3, so that for the blackbody radiation heat bath the expression (4.16) for the spectral distribution takes the form:

$$\text{Re}\{\tilde{\mu}(\omega + i0^+) = \frac{\pi}{3} \sum_{\vec{k}} m_k \omega_k^2 \left[\delta(\omega - \omega_k) + \delta(\omega + \omega_k) \right]$$

$$= \frac{4\pi^2 e^2}{3V} \sum_{\vec{k}} f_k^2 \left[\delta(\omega - \omega_k) + \delta(\omega + \omega_k) \right] .$$

(5.11)

Although with this expression we have shown the equivalence of the blackbody field to an IO heat bath and have in principle completely characterized the quantum Langevin equation for the blackbody field, it is perhaps useful to exhibit some more explicit formulas. Thus, the (three dimensional) random force is

$$\vec{F} = \frac{e}{c} \frac{\partial \vec{A}}{\partial t} .$$

(5.12)

In the limit of large volume for the blackbody cavity, we can use the familiar prescription:

$$\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3} \int d\vec{k} ,$$

(5.13)

to write the spectral distribution in the form:

$$\text{Re}\{\tilde{\mu}(\omega + i0^+) = \frac{e^2}{6\pi} \int d\vec{k} f_k^2 \delta(\omega - \omega_k) = \frac{2e^2 \omega^2}{3c^3} f_k^2 .$$

(5.14)

The physically significant results for this model should not depend upon details of the electron form factor, subject, of course, to the condition that it be unity up to some large frequency Ω and falls to zero thereafter. A convenient form which satisfies this condition is

$$f_k^2 = \frac{\Omega^2}{\omega^2 + \Omega^2} .$$

(5.15)

Using this in (5.14) the Stieltjes inversion formula (2.7) gives

$$\tilde{\mu}(z) = \frac{2e^2 \Omega^2}{3c^3} \frac{z}{z + i\Omega} .$$

(5.16)

This is the form obtained by direct calculation in an earlier publication.[15] Note, incidentally, that we see here a manifestation of the general feature that the memory function is independent of the external potential and the particle mass.

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C.Linear coupling models.

The linear coupling model appears frequently in the literature and in many guises. It is sometimes called the Ullersma model,[16] although it was discussed by several authors before Ullersma.[17,18,4] Another equivalent version is the Schwabl-Thirring model.[19] These are all oscillator-bath models in which the coupling to the particle is through a term linear in the particle displacement. The Hamiltonian is therefore of the form:

$$H_{LC} = \frac{p^2}{2m} + V(x) + \sum_j \left(\frac{p_j^2}{2M_j} + \frac{1}{2}M_j\omega_j^2 q_j^2 \right) + x\sum_j \lambda_j q_j \ . \qquad (5.17)$$

However, this Hamiltonian has a grave defect: for a free particle, $V(x) = 0$, there is no lower bound on the energy. This means that there is no thermal equilibrium state; the bath is not passive. A separate defect is that, again for the free particle, the Hamiltonian is not invariant under spatial translations. Now, in the papers we have cited, the authors have, at least implicitly, recognized this and repaired the linear coupling Hamiltonian by adding at a later stage a term:

$$\sum_j \frac{\lambda_j^2}{2M_j\omega_j^2} x^2 \ . \qquad (5.18)$$

With this addition the linear coupling Hamiltonian (5.17) becomes

$$H_{LC}' = \frac{p^2}{2m} + V(x) + \sum_j \left(\frac{p_j^2}{2M_j} + \frac{1}{2}M_j\omega_j^2 [q_j + \frac{\lambda_j}{M_j\omega_j^2} x]^2 \right) \ . \qquad (5.19)$$

But this is just the IO model. To see this explicitly, one makes the canonical transformation: $q_j \rightarrow -(\lambda_j/M_j\omega_j)q_j$, $p_j \rightarrow -(M_j\omega_j/\lambda_j)p_j$. Then one obtains the IO Hamiltonian (4.1) with

$$m_j = \lambda_j^2/M_j\omega_j^4 \ . \qquad (5.20)$$

For this repaired model, the spectral distribution (4.16) is

$$Re\{\tilde{\mu}(\omega + i0^+)\} = \frac{\pi}{2} \sum_j \frac{\lambda_j^2}{M_j\omega_j^2} [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)] \ . \qquad (5.21)$$

Thus, when properly repaired, the linear coupling model is equivalent with an IO model. Unfortunately, it is not always

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realized that such a repair is necessary to make a physically consistent model, and this has led to errors in the subsequent literature. Moreover, the repair is not unique. For example, an added term of the form:

$$\frac{1}{2}Kx^2 + \frac{1}{2K}\left(\sum_j \lambda_j q_j\right)^2,$$ (5.22)

where K is a positive constant, will also repair the Hamiltonian. But the result is a *different* model. In the well known work of Ullersma, it was just such a confusion which led to an incorrect form for the Langevin equation for a charged oscillator interacting with the radiation field [Ref.16,Sec.6], a form which misses the important high-temperature T^2 dependence of the oscillator energy.[14]

It would perhaps be useful to give here the relation with a pair of functions which have appeared in the literature in connection with the linear coupling model. The first of these is Ullersma's strength function (in Ullersma's paper $M_j = 1$):[16]

$$\gamma(\omega) = \sum_j \frac{\lambda_j^2}{M_j} [\delta(\omega - \omega_j) + \delta(\omega + \omega_j)] .$$ (5.23)

The second has been called the spectral density,[20] and is given by:

$$J(\omega) = \frac{\pi}{2} \sum_j \frac{\lambda_j^2}{M_j \omega_j} [\delta(\omega - \omega_j) - \delta(\omega + \omega_j)] .$$ (5.24)

The relation with the spectral distribution (5.21) of the repaired model is

$$\frac{\pi}{2}\gamma(\omega)/\omega^2 = J(\omega)/\omega = \text{Re}\{\tilde{\mu}(\omega + i0^+)\} .$$ (5.25)

D. The rotating wave approximation.

This is a version of the linear coupling model. It appears frequently in works on quantum optics, where it is generally applied to the case of the oscillator. We do so here and consider the Hamiltonian (5.17) for the linear coupling model with external potential of the form:

$$V(x) = \frac{1}{2}m\omega_o^2 x^2 .$$ (5.26)

If one then introduces the familiar oscillator operators:

$$a = \frac{m\omega_o x + ip}{(2m\hbar\omega_o)^{1/2}} \quad , \quad b_j = \frac{M_j\omega_j q_j + ip_j}{(2M_j\hbar\omega_j)^{1/2}} \quad , \tag{5.27}$$

this linear coupling Hamiltonian becomes

$$H_{LC} = \hbar\omega_o(aa^\dagger + \tfrac{1}{2}) + \sum_j \hbar\omega_j(b_jb_j^\dagger + \tfrac{1}{2})$$

$$+ \sum_j \frac{\hbar\lambda_j}{2(mM_j\omega_o\omega_j)^{1/2}} (ab_j + ab_j^\dagger + a^\dagger b_j + a^\dagger b_j^\dagger). \tag{5.28}$$

The rotating wave approximation consists in discarding the terms ab_j and $a^\dagger b_j^\dagger$ in the second sum, to get

$$H_{RWA} = \hbar\omega_o(a^\dagger a + \tfrac{1}{2}) + \sum_j \hbar\omega_j(b_j^\dagger b_j + \tfrac{1}{2})$$

$$+ \sum_j \frac{\hbar\lambda_j}{2(mM_j\omega_o\omega_j)^{1/2}} (ab_j^\dagger + a^\dagger b_j). \tag{5.29}$$

This is the rotating wave approximation Hamiltonian.[21]

If we return to the original operators, using the expressions (5.27) for the oscillator operators, the rotating wave approximation Hamiltontian takes the form:

$$H_{RWA} = \frac{p^2}{2m} + \tfrac{1}{2}m\omega_o^2 x^2 + \sum_j \left(\frac{p_j^2}{2M_j} + \tfrac{1}{2}M_j\omega_j^2 q_j^2 \right)$$

$$+ \tfrac{1}{2}x\sum_j \lambda_j q_j + \frac{p}{2m\omega_o}\sum_j \frac{\lambda_j}{M_j\omega_j} p_j . \tag{5.30}$$

Here we see that the rotating wave approximation consists in replacing in the linear coupling model half of the coordinate-coordinate interaction term with a corresponding momentum-momentum interaction term. Like the linear coupling Hamiltonian this one is defective in that the bath is not passive. [In the language of quantum optics and the form (5.29) of the Hamiltonian, for ω_o sufficiently small the lowest normal mode frequency of the system is negative. There will then be an associated ladder of energy eigenvalues stretching down to $-\infty$.] The Hamiltonian must therefore be repaired and, again as with the

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linear coupling Hamiltonian, this repair is not unique. One obvious possibility is to add the terms (in the language of quantum optics these would be called self-interaction terms):

$$\sum_j \frac{\lambda_j^2}{8M_j\omega_j^2}x^2 + \frac{1}{8m\omega_o^2}\left(\sum_j \frac{\lambda_j}{M_j\omega_j}p_j\right)^2 , \tag{5.31}$$

which results in the Hamiltonian:

$$H_{RWA} = \frac{1}{2m}\left(p + \sum_j \frac{\lambda_j}{2M_j\omega_j\omega_o}p_j\right)^2 + \frac{1}{2}m\omega_o^2 x^2$$

$$+ \sum_j \left[\frac{p_j^2}{2M_j} + \frac{1}{2}M_j\omega_j^2\left(q_j + \frac{\lambda_j}{2M_j\omega_j^2}x\right)^2\right] . \tag{5.32}$$

This repaired Hamiltonian is equivalent with an IO Hamiltonian. To see this we first make a unitary transformation with the operator:

$$U_2 = \exp\left(-ix\sum_j \frac{\lambda_j p_j}{2\hbar\omega_o M_j\omega_j}\right) . \tag{5.33}$$

Under this transformation,

$$p \rightarrow U_2^\dagger p U_2 = p - \sum_j \frac{\lambda_j}{2M_j\omega_j\omega_o}p_j \quad , \quad x \rightarrow x$$

$$p_j \rightarrow p_j \quad , \quad q_j \rightarrow q_j + \frac{\lambda_j}{2M_j\omega_j\omega_o}x \tag{5.34}$$

and the Hamiltonian (5.32) takes the form:

$$H_{RWA} \rightarrow U_2^\dagger H_{RWA} U_2 . \tag{5.35}$$

$$= \frac{p^2}{2m} + \frac{1}{2}m\omega_o^2 x^2 + \sum_j\left\{\frac{p_j^2}{2M_j} + \frac{1}{2}M_j\omega_j^2\left[q_j + \frac{\lambda_j(\omega_j + \omega_o)}{2M_j\omega_j^2\omega_o}x\right]^2\right\}.$$

Finally a canonical scale transformation:

$$q_j \rightarrow -\frac{\lambda_j(\omega_j + \omega_o)}{2M_j\omega_j^2\omega_o}q_j \quad , \quad p_j \rightarrow -\frac{2M_j\omega_j^2\omega_o}{\lambda_j(\omega_j + \omega_o)}p_j , \tag{5.36}$$

puts this Hamiltonian in the IO form (4.1) with

$$m_j = \frac{\lambda_j^2(\omega_o + \omega_j)^2}{4m_j\omega_j^4\omega_o^2} . \tag{5.37}$$

Thus, the result of all these shenanigans is again an IO model.

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This means that the rotating wave approximation is *to no purpose whatever*. That is, it is only a variant of the seriously flawed linear coupling model, and when the flaw is repaired one gets an IO model. It would be much simpler to start from the beginning with the IO model, which is exactly solvable, with no need for any approximation. It is surprising that this does not seem to have been recognized in the many papers in which this approximation has been applied. Lest we be misunderstood, we hasten to say that this remark does not apply to the use of the rotating wave approximation in discussing spin motion as in the nuclear magnetic resonance problem.

Before we leave these linear coupling models we want to stress again that they all correspond to a bath which is not passive. This means that they must be repaired and the repair is not unique. We have just seen how, starting from the same linear coupling model, one is lead by what seems only a trivial change of formalism to make different repairs which seem "natural" but which give quite different forms for the Langevin equation.

E. The FKM model.

The FKM model is of interest chiefly because the paper in which it appeared was the first in which the correct formulation of the quantum Langevin equation was indicated.[12] The model corresponds to a system of $(2N+1)$ identical coupled oscillators, with the one with index 0 singled out and placed in an external potential V. The Hamiltonian is of the form:

$$H = \frac{1}{2m} \sum_{i=-N}^{N} p_i^2 + \frac{1}{2}m \sum_{i,k=-N}^{N} q_i A_{ik} q_k + V(q_0) ,$$

(5.38)

where the interaction matrix A is a symmetric cyclic matrix whose elements can be written in the form

$$A_{ji} = \frac{1}{2N+1} \sum_{k=-N}^{N} \omega_k^2 \exp\{i2\pi k(j-1)/(2N+1)\} .$$

(5.39)

The eigenvalues of the matrix A are $\omega_k^2 = \omega_{-k}^2$, $k = 1, 2, \cdots, N$, and $\omega_0^2 = 0$. These are therefore the normal mode frequencies of the coupled system in the absence of the external potential V. The

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system is therefore guaranteed to be passive. The eigenvalue zero corresponds to the uniform translation mode. Thus it is possible to write the Hamiltonian in the form:

$$H = \frac{1}{2m} \sum_{i=-N}^{N} p_i^2 + \frac{1}{2}m \sum_{i,k=-N}^{N} (q_i - q_o) A_{ik} (q_k - q_o) + V(q_o) .$$

(5.40)

From this form it is clear that by a canonical coordinate transformation this Hamiltonian can be brought into the IO Hamiltonian. However, the transformation is rather complicated and uninstructive, so we will forgo giving its explicit form. We can however express the relation with the IO model simply in terms of the positive real function:

$$G(z) = -iz \| (A - z^2)^{-1} \|_{oo} = \frac{1}{2N+1} \sum_{k=-N}^{N} \frac{-iz}{\omega_k^2 - z^2} ,$$

(5.41)

where $\| \cdots \|_{oo}$ indicates the 00 element of the matrix within the double bars. The function $\tilde{\mu}$ of the corresponding IO model is given by

$$\tilde{\mu}(z) = m/G(z) + imz .$$

(5.42)

(Note that for large z, $G(z) \sim i/z$.)

If one introduces the normalized spectrum of eigenfrequencies,

$$g(\omega) = \frac{1}{2N+1} \sum_{k=-N}^{N} [\delta(\omega - \omega_k) + \delta(\omega + \omega_k)] ,$$

(5.43)

then one can write

$$G(z) = -iz \int_0^\infty d\omega \frac{g(\omega)}{\omega^2 - z^2} .$$

(5.44)

Here one sees that, by appropriately choosing the spectrum of eigenfrequencies, one can represent the most general positive real function through these last three equations. Thus, the model described by the Hamiltonian (5.38) is completely equivalent with the general IO model. This generality was, however, not made explicit in the original FKM paper, where the interest was in deriving a model with a constant friction constant. Therefore at an early stage the transition to the limit of a continuous distribution of eigenfrequencies was made. The spectrum was then

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chosen to be $g(\omega) = (2f/\pi)\cdot(\omega^2 + f^2)^{-1}$, which leads to the Langevin equation (2.9) with $\tilde{\mu}(\omega + i0^+) = \zeta = mf$. This is the FKM model.

F. The Lamb model

The Lamb model is the simple, physically intuitive, model in which the particle is attached to the center of an infinite stretched string. It was introduced by Horace Lamb in a paper written in 1900,[22] with the purpose of understanding the then new notion of radiation reaction in electrodynamics. It will be convenient for our discussion to generalize the model slightly, and consider the particle attached to the center of the string by a spring with force constant k and placed in an external potential $V(x)$. The Hamiltonian for the system is then

$$H = \frac{p^2}{2m} + V(x) + \int_0^\infty dy\left[\frac{\pi^2}{2\sigma} + \frac{\tau}{2}\left(\frac{\partial u}{\partial y}\right)^2\right] + \frac{K}{2}[x - u(0)]^2. \tag{5.45}$$

Here $u(y)$ is the string displacement and $\pi(y)$ is the corresponding canonical field momentum. The mass per unit length of the string is σ and the tension is τ.

Rather than construct the canonical transformation to an IO model, we think it more instructive to repeat the derivation of the Langevin equation in the field theoretic language appropriate to this Hamiltonian. The equations of motion are[23]

$$\dot{x} = \frac{p}{m} , \quad \dot{p} = -V'(x) - K[x - u(0)]$$

$$\frac{\partial u}{\partial t} = \frac{\pi}{\sigma} , \quad \frac{\partial \pi}{\partial t} = \tau\frac{\partial^2 u}{\partial y^2} + K[x - u(0)]\delta(y) \tag{5.46}$$

Eliminating the momentum variables, the particle equations of motion become

$$m\ddot{x} + V'(x) = -K[x - u(0)] , \tag{5.47}$$

and the field equations of motion for the string become the inhomogeneous wave equation:

$$\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial^2 u}{\partial y^2} = \frac{K}{\sigma}[x - u(0)]\delta(y) , \tag{5.48}$$

where $c = (\tau/\sigma)^{1/2}$ is the wave velocity. The retarded solution of

this equation is

$$u(y,t) = u^h(y,t) + \frac{K}{2\sigma c}\int_{-\infty}^{t-|y|/c} dt'\, [x(t') - u(0,t')].\qquad(5.49)$$

Setting $y = 0$, we can solve for $u(0,t)$ to write:

$$x(t) - u(0,t) = \int_{-\infty}^{t} dt' \exp\{-\frac{K(t-t')}{2\sigma c}\}\left[\dot{x}(t') - \frac{\partial u^h(0,t')}{\partial t'}\right].\qquad(5.50)$$

Putting this in (5.47) we get the Langevin equation (2.1) with

$$\mu(t) = K \exp\{-\frac{Kt}{2\sigma c}\}\,\theta(t)\,,\qquad \tilde{\mu}(\omega) = \frac{2\sigma c}{1 - 2i\sigma c\omega/K}\,.\qquad(5.51)$$

In the limit $K \to \infty$ this becomes the classical Langevin equation (2.9) with friction constant

$$\zeta = 2\sigma c = 2\sqrt{\sigma\tau}\qquad(5.52)$$

This is the Lamb model. It is clear that the quantum generalization is straightforward; one need only quantize the string field.

VI Concluding remarks

Heat bath problems occur in such diverse areas of physics as statistical mechanics, condensed matter, quantum optics, and even atomic physics. The quantum Langevin equation affords a powerful and physically appealing approach to such problems. Our point of view in this work has been that this equation corresponds to a *macroscopic* description of a quantum particle interacting with a heat bath. Our main motive has been to show that this description can be formulated with accuracy and precision, using such general physical principles as causality and the second law of thermodynamics, and such mathematical notions as the theory of positive real functions. We have stressed that this formulation is model-independent.

The fact that the description is macroscopic does not mean to say that the "particle" is necessarily macroscopic; the description applies to a single atom,[15] or to a Josephson junction.[24] Rather, as we have stressed, the bath must be macroscopic, with an infinite number of degrees of freedom. This requirement is not superficially obvious from the general description we give in Section II and derive from the IO model in Section IV. Indeed, the derivation given in Section IV formally applies for a bath consisting of a single particle! Rather, it appears in more subtle ways, e.g., in the requirement that there be a unique equilibrium state.

The IO model has played a prominent role in our discussion. We stress that this is only for reasons of convenience. It is a simple general model that can easily be solved exactly and is therefore very handy for calculations. But the macroscopic description is model-independent.

An additional advantage of the IO model is that it incorporates many other models that have appeared in the literature. This allowed us in Section V to discuss in a unified way such diverse models as the velocity coupling model, the blackbody radiation heat bath, and the FKM model. There, too, we discussed the linear coupling models and pointed out that, since they must be repaired to make them physical and the repair is not unique, they are dangerous to use and have led to errors in the

literature. Moreover, any repaired liner coupling model is an IO model, so one might as well have started with the latter. Based on similar reasoning, we showed that there is no computational advantage in using the rotating wave approximation which, on the contrary, is only a variant of the flawed linear coupling model. And when the flaw is repaired one gets again an IO model!

Acknowledgment

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