Equilibration problem for the generalized Langevin equation

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Abstract. - We consider the problem of equilibration of a single oscillator system with dynamics given by the generalized classical Langevin equation. It is well-known that this dynamics can be obtained if one considers a model where the single oscillator is coupled to an infinite bath of harmonic oscillators which are initially in equilibrium. Using this equivalence we first determine the conditions necessary for equilibration for the case when the system potential is harmonic. We then give an example with a particular bath where we show that, even for parameter values where the harmonic case always equilibrates, with any finite amount of nonlinearity the system does not equilibrate for arbitrary initial conditions. We understand this as a consequence of the formation of nonlinear localized excitations similar to the discrete breather modes in nonlinear lattices.

Introduction. – One of the simplest phenomenological ways of modeling the interactions of a system with a heat bath is through the Langevin equation which, for a single particle, of unit mass and moving in a one dimensional potential $V(x)$, is given by

$$\ddot{x} = -dV(x)/dx - \gamma\dot{x} + \eta(t) \ , \tag{1}$$

where $\eta(t)$ is a Gaussian white noise which satisfies the fluctuation-dissipation (FD) relation $\langle\eta(t)\eta(t')\rangle = 2k_BT\gamma\delta(t-t')$. Here T is the temperature of the heat bath. The dynamics in eq. (1) ensures that at long times the system reaches thermal equilibrium. Thus the phase space density $P(x,p,t)$, where $p = \dot{x}$, converges in the limit $t \to \infty$ to the Boltzmann distribution $e^{-\beta H_s}/Z$ where $H_s = p^2/2 + V(x)$ and Z is the corresponding partition function. The proof for this uses the correspondence between the Langevin equation and the Fokker-Planck equation [1].

However the δ-correlated nature of the noise is unphysical and this has led to the study of the generalized Langevin equation [2,3]

$$\ddot{x} = -dV(x)/dx - \int_{-\infty}^{t} dt'\gamma(t-t')\dot{x}(t') + \eta(t) \ , \tag{2}$$

where the noise is correlated and the the dissipative term involves a memory kernel. The noise is again Gaussian and is related to the dissipative term through the generalized FD relation

$$\langle\eta(t)\eta(t')\rangle = k_BT\gamma(t-t') \ . \tag{3}$$

A standard method of microscopically modeling a heat bath is to consider an infinite collection of harmonic oscillators, with a distribution of frequencies, coupled linearly to the system. In that case it can be shown [4, 5] that the effective equation of motion of the system is precisely given by eq. (2) where the dissipation kernel $\gamma(t)$ depends on the bath oscillator frequencies and the coupling constants. Unlike the case with δ-correlated noise there exists no general proof that, for a general potential $V(x)$, the system will reach thermal equilibrium at long times. The reason for this is that in this case the construction of a Fokker-Planck description is difficult and is known in few cases (*e.g.* harmonic oscillator case treated in Ref. [6]). For the special case of a harmonic potential and with certain restrictions on the form of $\gamma(t)$ one can prove equilibration by a direct solution of the equations of motion [7]. In the quantum mechanical case the oscillator bath model has been widely used to model the effects of noise, dissipation and decoherence in quantum systems [8,9]. In this case the approach to equilibrium has been proved only for a special class of potentials for the cases where the system-reservoir coupling is weak [10].

A number of papers [11–13] have attempted to understand various aspects of the generalized Langevin equation such as anomalous diffusion, nonstationarity and ergodic-

ity. In this paper we address the question of approach to equilibrium for the generalized Langevin equation. For a particle in a harmonic potential $V(x) = \omega_0^2 x^2/2$ and coupled to a heat bath with a finite band-width (and hence long-time memory) we show that equilibration is not always ensured and depends on the oscillator frequency ω_0. We find the necessary conditions for equilibration which is related to the existence of bound states (localized modes) of the coupled system-plus-bath. We note that Ref. [13] looks at the question of ergodicity which is similar to the question addressed here. One of their results is that the motion of a harmonic oscillator coupled to a general heat bath is ergodic. This is based on the fact that the coefficients in the Fokker-Planck equation asymptotically approach constant values. Our work shows that this condition does *not* ensure ergodicity. Next we consider a particle in a nonlinear potential $V(x) = \omega_0^2 x^2/2 + ux^4/4$ and coupled to a special bath, the so-called Rubin model [5,14]. The usual expectation would be that nonlinearity should help in equilibration. However surprisingly we find the contrary to be true. For values of ω_0 for which the linear system (with $u = 0$) does equilibrate, we show that switching on the nonlinearity can lead to loss of equilibration. We relate this to the formation of nonlinear localized modes which are similar to the discrete breather modes found in nonlinear lattices [15, 16].

Definition of model. – We consider the following Hamiltonian of the usual model of a system coupled to a bath of N oscillators:

$$H = H_s + \sum_{\alpha=1}^{N} \frac{P_\alpha^2}{2} + \frac{\omega_\alpha^2}{2}\left(X_\alpha - \frac{c_\alpha x}{\omega_\alpha^2}\right)^2 , \qquad (4)$$

where $\{X_\alpha,\ P_\alpha\}$ denotes degrees of freedom of the $\alpha^{\rm th}$ bath oscillator ($\alpha = 1, 2, ...N$), ω_α is its frequency, and c_α is the strength of the coupling to the system. For dissipation it is necessary that the frequencies ω_α have a continuous spectrum in the limit $N \to \infty$. We assume that at time $t = t_0$ the system and bath are decoupled ($\{c_\alpha\} = 0$). The bath is in thermal equilibrium and described by the canonical distribution $e^{-\beta H_b}$ where $H_b = \sum_\alpha [\ P_\alpha^2/2 + \omega_\alpha^2 X_\alpha^2/2\ ]$ and the system is in an arbitrary initial state $\{x(t_0),\ p(t_0)\}$. The coupling is switched on at time $t = t_0$. It can then be shown that eliminating the bath degrees of freedom leads to the following equation of motion for the system (for $t > t_0$):

$$\ddot{x} = -\frac{dV(x)}{dx} - \gamma(0)x + \int_{t_0}^{t} dt' \frac{d\gamma(t-t')}{dt'} x(t') + \eta(t) , \quad (5)$$

with the dissipation kernel given by $\gamma(t) = \sum_\alpha (c_\alpha^2/\omega_\alpha^2)\cos(\omega_\alpha t)$. In the limit $t_0 \to -\infty$, using $\gamma(t \to \infty) = 0$, we get eq. (2). The noise correlations satisfy the generalized FD relation in eq. (3) where the noise average $\langle ... \rangle$ is obtained by averaging over the initial conditions of the bath.

Equilibration in a harmonic potential. – We first consider the case with $V(x) = \omega_0^2 x^2/2$. For this case eq. (5) is a linear inhomogeneous equation whose solution is:

$$\begin{aligned} x(t) &= H(t-t_0)x(t_0) + G(t-t_0)p(t_0) \\ &\quad + \int_{t_0}^{t} dt' G(t-t')\eta(t') , \end{aligned} \qquad (6)$$

where $H(t)$ and $G(t)$ are the solutions of the homogeneous part of eq. (5) (with $t_0 = 0$) for initial conditions $H(0) = 1,\ \dot{H}(0) = 0$ and $G(0) = 0,\ \dot{G}(0) = 1$ respectively. For equilibration we require that, in the long time limit, the solution in eq. (6) should not depend on initial conditions. Thus a necessary condition is that $G(t \to \infty) \to 0$. At large times it can be shown that $H(t) \to \dot{G}(t)$ and hence $H(t \to \infty) \to 0$ also. Let us define the Green's function $G^+(t) = G(t)\theta(t)$. It is easy to see that G^+ satisfies the equation of motion:

$$\ddot{G^+} + \omega_0^2 G^+ + \int_{-\infty}^{\infty} dt' \gamma^+(t-t')\dot{G^+}(t') = \delta(t) ,$$

where $\gamma^+(t) = \gamma(t)\theta(t)$. Defining the Fourier transforms $G^+(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} G^+(t)$ and $\gamma^+(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}\gamma^+(t)$ we find that $G^+(\omega)$ is given by

$$G^+(\omega) = \frac{1}{-(\omega^2 - \omega_0^2) - i\omega\gamma^+(\omega)} \qquad (7)$$

with $\gamma^+(\omega) = \gamma_R^+(\omega) + i\gamma_I^+(\omega)$ where the real and imaginary parts are given by: $\gamma_R^+(\omega) = \sum_\alpha (\pi c_\alpha^2/2\omega_\alpha^2)[\delta(\omega + \omega_\alpha) + \delta(\omega - \omega_\alpha)]$, $\gamma_I^+(\omega) = \sum_\alpha c_\alpha^2 \omega/[\omega_\alpha^2(\omega^2 - \omega_\alpha^2)]$. Now from eq. (7) it follows that $G^+(t \to \infty) = \lim_{t\to\infty}(1/2\pi)\int d\omega e^{-i\omega t} G^+(\omega)$ will vanish (this follows from the Riemann-Lebesgue lemma [17]) *unless* $G^+(\omega)$ blows up at some real value of ω. Thus the condition under which $G^+(t \to \infty)$ does not vanish is that the equation

$$-(\omega^2 - \omega_0^2) - i\omega\gamma^+(\omega) = 0 \qquad (8)$$

has a real ω solution, which we will denote by Ω_b. It follows from eq. (8) that $\gamma_R(\Omega_b) = 0$ which means that Ω_b necessarily lies outside the bath band-width. This solution corresponds to a bound state. To see this we now solve the equations of motion of the coupled system-plus-bath by a resolution into its normal modes. Let us denote the normal mode frequencies by Ω_Q and the corresponding eigenfunction by $\mathbf{U}_Q = \{U_{0,Q}, U_{\alpha=1,Q}, ...U_{\alpha=N,Q}\}$ where U_{0Q} corresponds to the system variable x. They satisfy the equations:

$$\begin{aligned} -\Omega_Q^2 U_{0Q} &= -\omega_0^2 U_{0Q} + \sum_\alpha c_\alpha \left(U_{\alpha Q} - \frac{c_\alpha U_{0Q}}{\omega_\alpha^2}\right) \\ -\Omega_Q^2 U_{\alpha Q} &= -\omega_\alpha^2 \left(U_{\alpha Q} - \frac{c_\alpha U_{0Q}}{\omega_\alpha^2}\right) \quad \alpha = 1...N \end{aligned} \qquad (9)$$

A bound state [18] occurs if there is a mode such that its frequency Ω_b lies outside the bandwidth of the isolated bath. The corresponding eigenfunction $\mathbf{U}_b$ will have a finite weight at the system point (*i.e.* $U_{0b} = O(1)$). Solving, for $U_{\alpha b}$, the second equation in eq. (9) and substituting into the first equation, we find that the condition for a bound state is given precisely by the solution (if it exists) of eq. (8). The corresponding eigenfunction is given by: $U_{\alpha b} = c_\alpha U_{0b}/(-\Omega_b^2 + \omega_\alpha^2)$, $\alpha = 1...N$ and $U_{0b} = [1 + \sum_\alpha c_\alpha^2/(-\Omega_b^2 + \omega_\alpha^2)^2]^{-1/2}$. The general solution of the full equations of motion in terms of normal modes is

$$Y = U \cos\Omega(t-t_0) U^{-1} Y(t_0) + U \frac{\sin\Omega(t-t_0)}{\Omega} U^{-1} \dot{Y}(t_0) \ ,$$

where $Y = \{x, X_1, ...X_\alpha ...X_N\}^T$. From this one can identify the part of $x(t)$ involving $p(t_0)$. Comparing with eq. (6) we get $G(t) = \sum_Q U_{0Q}^2 \sin(\Omega_Q t)/\Omega_Q$. If there are no bound states then the frequencies Ω_Q form a continuous spectrum, the sum can be converted into an integral, and in the limit $t \to \infty$ the infinite oscillations lead to the integral vanishing. In the presence of a bound state we get a non-vanishing contribution given by

$$G(t \to \infty) = U_{0b}^2 \frac{\sin(\Omega_b t)}{\Omega_b} \ . \tag{10}$$

Thus we again arrive at the conclusion that in the presence of bound states, thermal equilibration is not achieved and the steady state properties depend on the initial conditions of the system. The long time form in eq. (10) can also be obtained directly from eq. (7) by integrating around the singularity given by eq. (8). In the absence of bound states, eq. 6 gives the unique steady state solution $x(t) = \int_{-\infty}^{\infty} dt' G^+(t-t')\eta(t')$, and one can verify that:

$$\begin{aligned} \langle \frac{\omega_0^2 x^2}{2} \rangle = \frac{\omega_0^2 k_B T}{2\pi} \int_{-\infty}^{\infty} d\omega |G^+(\omega)|^2 Re[\gamma^+(\omega)] &= \frac{k_B T}{2} \\ \langle \frac{p^2}{2} \rangle = \frac{k_B T}{2\pi} \int_{-\infty}^{\infty} d\omega \ \omega^2 |G^+(\omega)|^2 Re[\gamma^+(\omega)] &= \frac{k_B T}{2} \ , \end{aligned}$$

where the integrals are easy to evaluate if one chooses appropriate contours [7]. The inset in fig. (1) gives a numerical demonstration of the nonequilibration problem (see following section for details of numerics).

Equilibration in a nonlinear potential. – Usually one expects that introducing nonlinearity should help in equilibration and we will now test this expectation. We will consider a particular model of a heat bath for which it will be possible to analyze things in detail. This is the Rubin model in which the bath is a one-dimensional chain of coupled oscillators. Thus the full Hamiltonian is: $H = H_s + \sum_{i=1}^N [p_i^2/2 + (x_{i+1} - x_i)^2/2] + (x_1 - x)^2/2$, with $x_{N+1} = 0$ and where $x = x_0$ refers to the system. Transforming to normal mode coordinates of the bath we recover the form eq. (4) with $\omega_\alpha = 4\sin^2(q_\alpha/2)$ and $c_\alpha = [2/(N+1)]^{1/2} \sin(q_\alpha)$ with $q_\alpha = \alpha\pi/(N+1)$ and $\alpha = 1, 2...N$. From this we can find the explicit form of $\gamma^+(\omega)$ which is:

$$\begin{aligned} i\omega\gamma^+(\omega) &= -(1 - e^{iq}) \quad \text{for } |\omega| = 2|\sin(q/2)| \ < \ 2 \\ &= -(1 + e^{-\sigma}) \quad \text{for } |\omega| = 2\cosh(\sigma/2) \ > \ 2. \end{aligned} \tag{11}$$

For a harmonic potential $V(x) = \omega_0^2 x^2/2$ we see from eq. (8) that the condition for getting bound states is $\omega_0^2 > 2$. The bound-state mode is given by $x_i^b = A(-1)^i e^{-\sigma i} \cos(\Omega_b t)$. where $\Omega_b = \omega_0^2/\sqrt{\omega_0^2 - 1}$ is the bound state frequency, $\sigma = \ln(\omega_0^2 - 1)$ and A is an arbitrary constant which can be fixed by normalization.

We now introduce the nonlinear term $ux^4/4$ and study its effect numerically. Let us choose $\omega_0^2 = 1$, in which case, in the absence of the nonlinear term, there are no bound states and we expect equilibration. In our simulation we consider a heat bath with $N = 1000$ particles whose initial positions and momenta are chosen from the Boltzmann distribution $e^{-H_b/T}$ with $T = 1$. The system has the initial state $\{p(0) = 0, x(0)\}$. We solve the equations of motion numerically with this initial state with the system-bath coupling turned on at time $t = 0$. We compute the expectation values $K_e(t) = \langle p^2 \rangle$ and $P_e(t) = \langle x \ \partial H/\partial x \rangle$ where $\langle .... \rangle$ denotes an average over the bath initial conditions. In our simulations we averaged over 10^4 initial conditions. We have checked that results do not change on increasing the bath size or number of aveages. For equilibration we expect the steady state values $K_e = P_e = T$. In fig. 1 we see that for the initial condition $x(0) = 7.0$ the linear problem equilibrates as expected. On the other hand for a small value of the nonlinearity parameter $u = 0.1$ the system *fails to equilibrate*. For a different initial condition $x(0) = 5.0$ the system equilibrates. The loss of equilibration infact occurs whenever $x(0)$ is greater than a critical value $x_c \approx 5.6$.

The dependence of equilibration on initial conditions can be traced to the formation of localized states that can be generated once we have nonlinearity. These *nonlinear localized modes* [15,16] are stable time-dependent solutions of the equations of motion that are localized and largely monochromatic and have the same form as the impurity bound states namely $x_i^b(t) = A(-1)^i e^{-\sigma i} \cos(\Omega_b t)$. If we plug this into the equations of motion and neglect terms containing higher harmonics ($\sim 3\Omega_b$) we then get the following conditions relating Ω_b, σ and A (for the parameter choice $\omega_0 = 1$):

$$A^2 = \frac{4e^\sigma}{3u}, \quad \Omega_b^2 = 2 + e^\sigma + e^{-\sigma} \ . \tag{12}$$

Note that, of the three parameters needed to describe a bound state namely Ω_b, σ, A only two get fixed and we thus have a continuum set of possible bound states which can be described by a single parameter. It is clear that for any non-zero u we can always choose $\sigma > 0$ and determine A, Ω_b from eq. (12). Hence bound states exist for *any* value of u. A clean way to numerically observe these localized modes is by initially preparing the bath at $T = 0$

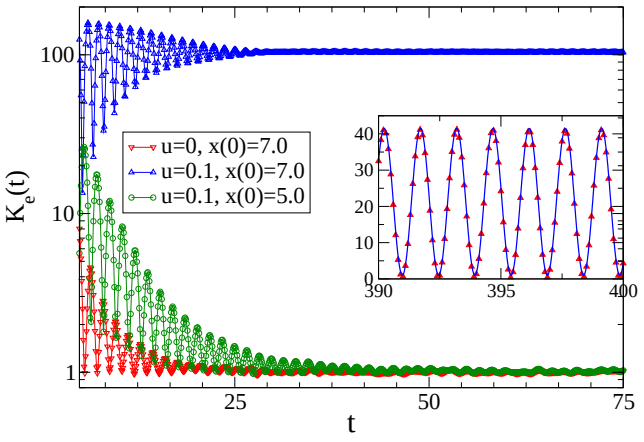

Fig. 1: Plot of average kinetic energy $K_e(t)$ as a function of time for different initial conditions. The purely linear case always equilibrates (for $\omega_o = 1$) while in the nonlinear case, equilibration depends on initial conditions. The behaviour of $P_e(t)$ is similar. The inset shows the nonequilibration problem in the linear case. The parameter value $\omega_0^2 = 3.0$ gives a bound state with $\Omega_b = 3/2^{1/2}$ and we plot $K_e(t)$ at large times for $x(0) = 5.0$ and $T = 1$. The solid line gives the analytic prediction $K_e(t) = \ddot{G}(t)^2 x(0)^2 + T$ with $G(t)$ given by eq. (10).

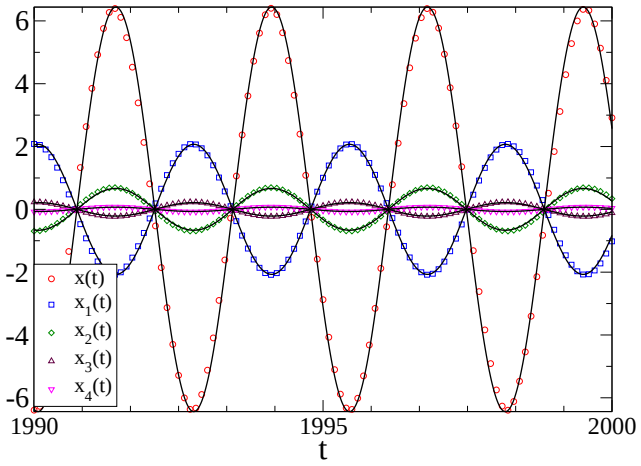

Fig. 2: Plots of the positions of various particles $x(t)$ and $x_i(t)$ for $i = 1, 2, 3, 4$ as functions of time plotted after the system has reached a steady state. Initial condition was $x(0) = 7.0$ and all other positions and momenta set to zero. The solid lines correspond to the analytical prediction for the breather mode with $A = 6.44$, $\sigma = 1.135$ and $\Omega_b = 2.331$.

and the system with initial conditions $\{p(0) = 0, x(0)\}$. Then at very long times we find that this initial condition relaxes to a localized mode if $x(0)$ is sufficiently large. In fig. 2 we plot the coordinates $\{x(t), x_i(t)\}$ for $i = 1, 2, 3, 4$ as functions of time (for parameter values $\omega_0 = 1$ and $u = 0.1$) . For the initial condition $x(0) = 7.0$ it is clear that the long time solution is quite accurately described by the localized mode solution. In the fits with the localized mode we fix A from the numerically obtained amplitude of $x(t)$ and obtain σ and Ω_b from eq. (12). For the initial condition $x(0) = 5.0$ we find that the initial energy quickly dissipates into the bath and at long times is distributed uniformly. A more accurate form for the localized mode can be obtained by including higher harmonics. At the next order, the solution is given by $x_i^b = A^{(1)}(-1)^i e^{-\sigma^{(1)} i} \cos \Omega_b t + A^{(2)}(-1)^i e^{-\sigma^{(2)} i} \cos 3\Omega_b t$, where again there is only one unknown constant. In our example we find that $A^{(2)} << A^{(1)}$ (For all values of u we get $A^{(2)}/A^{(1)} < 1/21$).

Thus we have shown that the finite-temperature non-equilibration problem is related to the formation of nonlinear localized modes which, unlike in the harmonic case, depends on initial conditions.

Discussion. – In summary we have examined the conditions necessary for thermal equilibration of a particle in a potential well and evolving through a generalized Langevin equation. For the case of a harmonic potential we show that for finite band-width baths the system will not always equilibrate. Using the microscopic model of a bath as a collection of oscillators we show that non-equilibration arises because of the formation of bound states in the coupled system-plus-bath. Surprisingly we find that making the system nonlinear does not restore equilibration. On the contrary nonlinearity assists in the formation of localized modes and hence causes loss of equilibration for arbitrary initial conditions. These nonlinear localized modes are usually studied in the context of periodic nonlinear lattices, while here they arise in a situation where only one spring is nonlinear. In this paper we have considered a special one-dimensional bath. However localized modes also occur in higher dimensional nonlinear lattices with finite band-widhts [16] and hence we expect that the problem of equilibration is quite general.

In Ref. [19] electronic systems described by the tight binding noninteracting Hamiltonian were discussed and it was shown that the formation of bound states with finite band width reservoirs leads to a similar problem of equilibration. One example which was studied was that of a single site attached to a one-dimensional free electron reservoir. An interesting question that the present study raises is whether the introduction of an onsite interaction, say of the Hubbard type, would lead to similar effects as the nonlinear term in the case of the oscillator.

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