Dissipative time evolution of observables in non-equilibrium statistical quantum systems

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Abstract. We discuss differential– versus integral–equation based methods describing out–of thermal equilibrium systems and emphasize the importance of a well defined reduction to statistical observables. Applying the projection operator approach, we investigate on the time evolution of expectation values of linear and quadratic polynomials in position and momentum for a statistical anharmonic oscillator with quartic potential. Based on the exact integro-differential equations of motion, we study the first and naive second order approximation which breaks down at secular time-scales. A method is proposed to improve the expansion by a non–perturbative resummation of all quadratic operator correlators consistent with energy conservation for all times. Motion cannot be described by an effective Hamiltonian local in time reflecting non-unitarity of the dissipative entropy generating evolution. We numerically integrate the consistently improved equations of motion for large times. We relate entropy to the uncertainty product, both being expressible in terms of the observables under consideration.

1 Introduction

Non-equilibrium aspects of quantum field systems are of actual interest. Among other problems, one challenge is the description of time evolution of macroscopic quantities such as the expectation value of the field strength in systems out of thermal equilibrium. The problem, essentially the basic question for macroscopic dynamics of statistical systems, and thus interesting in itself, also plays a prominent role in context with cosmological inflationary phases. Although a plethora of equivalent descriptions of the collisionless limit are available, it is difficult to elaborate methods which allow to go beyond this thermodynamically trivial limit. One purpose of this paper is to promote a strategy based on which time evolution can be described in a consistent and systematic way.

Although the basic concepts of thermodynamic statistical theory are known for a long time, there still appears to be some confusion about terminology and underlying concepts of non-equilibrium systems and their dynamical description. Another task of this work is to introduce, review and discuss some of the basic ideas in a brief but systematic way. Technically, we adopt the projection operator method as one consistent method to describe time evolution of physical quantities in statistical systems.

To keep complexity minimal, we consider the toy model of the quantum Duffing oscillator for practical calculations, which nevertheless is a system of sufficient complexity to exhibit important features of non-equilibrium thermodynamics. For systematic reasons, we discuss some

properties of that system in the statistically trivial, entropy conserving, approximation first. We present criteria for permissible initial data, study static solutions and their stability, construct the first order integrals of motion and the first order effective Hamiltonian and Lagrangian. The system exhibits phenomena of parametric resonance which best may be displayed in the small coupling limit.

Finally, we attack our main task and investigate on proper non-equilibrium features. In a first step, that requires the study of second order effects which, however, turn out to violate energy conservation at long time scales in the strict power–series expansion. The main result of this investigation is to improve the second order result by taking into account the non–unitary effective evolution of observables which renders the approximation scheme self–consistent and solves the problem of non–conservation of constants of motion. In the appendix, we explicitly derive the basic uncertainty–entropy relation for the set of quadratic observables.

2 Definitions and general properties

(i) A mixed state of a quantum system (configuration), both in zero dimensional quantum mechanics as well as in quantum field theory, is described by a density operator, which, in order to allow a probability interpretation, must be a hermitian trace-class operator with positive eigenvalues. It is an intrinsic feature of quantum systems that the density matrix is fictive in the sense that only its diagonal elements correspond to physical probabilities, the other dependencies being phases which enter in expecta-

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tion values via interference effects[1]. Alternatively, one may characterize a configuration by the expectation values of hermitian operators. A generic set of those representing a complete set of observables is given by the mutually orthogonal hermitian projectors constructed from the eigenvectors of the density matrix. A complete set of (not necessarily commuting) observables contains all information about the density matrix such that any observable can be expressed in terms of the complete set.

(ii) The system may be assigned a dynamical structure. Motion is defined as a sequence of possible states having a constant expectation value of the Hamiltonian operator, the energy of the configuration. Quantum mechanical time parameterizes those configurations which are assumed to have time–independent probabilities and phases for autonomous systems. The time evolution generated by the Hamiltonian can be expressed by first order differential operator–equations in time for the density matrix (von Neumann equation) in the Schrödinger representation. Hermitian Hamilton operators generate unitary time evolution which in turn is necessary for compatibility of the probability interpretation with time evolution. Once the problem of time evolution of the mixed state is solved for a given initial configuration, observables can be calculated as expectation values from the evolved density matrix.

(iii) The statistical description of a system is based on a reduction procedure selecting an in general much smaller number of (macroscopic) observed quantities out of the complete set of observables. This subset defines the level of description. The process of reduction from the density operator to the set of the so–called relevant quantities in general involves loss of information. Here, we will concentrate on levels of descriptions that once chosen, will be kept fixed during time evolution. That constraint can be relaxed too if necessary [1].

(iv) The reduction can be dynamically trivial if it commutes with time evolution. In that case of dynamical closure, the Liouvillian maps the operators of the level of description on a linear combination of them. The observables of a level of description at a certain time are sufficient to determine them at any time and evolution induces neither information gain nor information loss at the level of description, the associated entropy being constant. On account of the canonical commutation relation, the most general Hamiltonian admitting a finite dimensional dynamically closed level of observation can contain constant, linear and quadratic expressions in position and momentum operators[2]. The corresponding dynamically closed sets of observables correspond to sums of polynomials of finite order in the canonical operators. If the reduction is non-trivial, one can extend the level of observation to render it trivial. That may involve an infinite number of operators in which case the system is a truly

interacting one, and the only dynamically closed set of operators corresponds to the complete set of observables.

(v) For truly interacting dynamical systems, the complete initial density matrix influences observables at later times. Its definition calls for an additional principle to construct it from the reduced set of initial data. Information theory proposes to apply Shannon's theory of entropy [2] to that physical problem. Jaynes' principle of maximum entropy [3] fixes the generalized canonical density operator as initial condition. It can be shown not to contain more information than the initial set of observables. We want to point out that this choice is the statistically most probable, but the underlying concept of ensemble averages of identical systems evolving from variant initial preparations does not imply the actual preparation of the system in that state.

We confront two strategies to arrive at a description of the motion of observables.

(A) Solve the complete problem of time evolution for the mixed initial state and extract the interesting quantities. The reduction procedure explicitly is postponed after time evolution.

(B) Construct equations of motion for the relevant quantities. They turn out to be integro-differential equation in time necessary to include the effects of the past history on the relevant observables.

Solution (A) appears to be be more attractive for field theorists since methods of field theory can be applied with rather little modification. The problem boils down to solve the initial value problem for mixed states for which the appropriate tool of the closed–time–path method has been developed [4]. We sketch the systematic procedure (A) according to the program outlined in (i)-(v), and discuss associated technical and conceptual problems.

Starting with the equations of motion in differential form, one gets an infinite hierarchy of first order differential equations for the complete set of observables, corresponding to the Schwinger–Dyson hierarchy of equal time correlators, and analogous to the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy of many–particle physics [5]. The hierarchy may be represented in compact form in terms of a classical effective potential generating the equal–time correlators [6] by transforming to the Wigner representation. In principle, the reduction amounts to eliminate the irrelevant quantities resulting in a finite set of infinite order differential equations for the reduced set of observables the integration of which involves an infinite number of initial conditions. At that point the statistical assumption about the initial density matrix enters to determine all derivatives of the observables at the initial time t_0. The essential feature of those effective equations of motion is non–locality in time which becomes apparent when converting them into integral equations. Suppose we only knew the relevant observables at a later time $t_1 > t_0$, then neither retrodictions nor predictions can be made on account of the lacking knowledge on the derivatives at t_1, or the complete history of observables. In that sense, reduction necessarily goes along with current temporal information loss. A complete calculation of the present observables

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[1] That is the fundamental difference to classical phase space averages

[2] Regardless of additional dependencies on other c-number quantities, including time and classical field strength, we call it free (effective) Hamiltonian

can only be done on grounds of the complete past initial density matrix where missing information was induced by the principle of maximum uncertainty. The corresponding reduced entropy at later times is always larger than the entropy of the initial state which introduces thermodynamic irreversibility in a natural way.

We want argue that, strictly speaking, the cut hierarchy is not a permissible dynamical approximation. There, one keeps only those equations which involve the time derivatives of the variables of interest. In order to arrive at a closed set of equations, the irrelevant quantities generally still being present in the system have to be expressed somehow in terms of the relevant ones. There is no systematics of how to do that. In some particular cases, as the large N–expansion of $O(N)$ symmetric scalar theories, the hierarchy by chance closes without further assumptions [7]. In the classical theory of gases Boltzmann introduced the famous Stoßzahlansatz for two particle correlators at that point. Generally dynamics then is represented by a finite closed set of effective (macroscopic) equations of motion. Of course no statistical assumptions about the complete initial state has to be inferred.

We want to point out that the truncation of the differential hierarchy explicitly alters the dynamics of the system in an uncontrolled way. Any finite order hierarchy of equations of motion exhibits features of a closed dynamic system discussed in (iv) and is thus a priori inequivalent to the reduced truly interacting evolution. It is always local in time which presumes memory loss at microscopic scales and automatically reduces to a Markovian description, even in cases where the complete system behaves differently. Some truncations are compatible with the existence of a macroscopic effective Hamiltonian (Lagrangian) being a function of a finite set of effective variables. The very existence of that Hamiltonian description, however, automatically conserves the relevant reduced von Neumann entropy such that the system can neither exhibit equilibration nor thermodynamic irreversibility in the strict sense[3]. Also, due to the Liouville–theorem the volume of cells in the phase space remains constant under effective Hamiltonian evolution. The volume, on the other hand, corresponds to the classical particle number density, which enters in the entropy functional of Boltzmann.

The argument may best be illustrated for the class of effectively Gaussian approximations which can be obtained by time dependent Hartree–Fock variational methods [9], the method of equal–time Green functions [8, 10], optimized expansions [11] or the truncation of the Schwinger–Dyson hierarchy to the one and two particle Green function. All those methods are physically equivalent in the Gaussian limit where the Hamiltonian is assumed to have free form, or, equivalently the density matrix is approximated by a generalized Gaussian wave package. One considers time dependent spatially bilocal functions — essentially equal–time two point correlators —

as coefficients in the quadratic expressions which are determined by the corresponding variational and expansion methods. But those bilocal coefficients enter in the generalized uncertainty which is a constant of time in the Gaussian approximation. On account of the uncertainty–entropy relation, also entropy remains constant contradicting information loss inherent in the incomplete description. Under certain conditions, the effective Gaussian theory can even be shown to have a representation in terms of a free theory after requantisation [12]. Although this approximation may supply a fairly good description at short terms or close to equilibrium, they are thermodynamically trivial approximations and cannot account for full long term evolution since they effectively correspond to the collisionless[4] limit of the physical system. We will show that in fact an effective Gaussian density matrix, whatever its time dependence be, does not evolve to the Gaussian approximation of the interacting density matrix at large times. The 'equilibration' observed in those approximations [8,13] can thus not be identified with physical entropy generating processes, but converges to static values by dephasing effects.

In general, the dynamics of a cut hierarchy effectively corresponds to current preparation of the system to have the canonical density matrix of the level of observation. Thus, dynamical closure is attained at the price of effectively time dependent probabilities being typical for non–autonomous systems. The procedure presumes that the density matrix decoheres for macroscopic observables including the existence of a classical limit for the variables of the level of observation. Such an effective theory may exist, depending on the particular system under consideration, but it remains to show that it represents motion also at macroscopically large time scales.

The problems with the differential representations can be avoided if we adopt solution (B) which intrinsically accounts for non–locality in time. The practical method we apply is the projection operator method in Schrödinger representation which yields the Robertson equation [14] being equivalent to the generalized Langevin–equation [1, 15] in the Heisenberg representation. Although those equations of motion are closed in the variables of the level of observation only, expectation values of arbitrary operators can be expressed by non–local time dependence. The exact reduced equations of motion turn out to have a rather complicated structure and suitable approximation schemes have to be developed within that framework. Splitting off a dynamically closed part from the Hamiltonian, the entropy generating contributions involve quadratic and higher powers in the remaining truly interacting Hamiltonian. There, a non-unitary operator enters, responsible for time evolution in the projected subspace. Approximating that operator by a unitary one again amounts to introduce a Gaussian approximation which differs formally only at third order from the exact solution but nevertheless involves unphysical consequences. It conflicts with entropy generated at second order and, more

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[3] Effective irreversibility, sometimes misleadingly related to ergodicity [5], may occur in infinite–dimensional systems [8], but has to be justified a posteriori and cannot be concluded on grounds of an approximation scheme

[4] Strictly speaking, the term collisionless is not precise since the limit does account for effective elastic scattering

severely, results in non-conservation of the energy at secular scales.

3 Basic setup

We briefly sketch the result of the projection operator approach [1,15]. For convenience, we define a level of observation by the finite set of hermitian operators $\mathcal{E} = \{\mathcal{F}_\nu\}$ including $\mathcal{F}_0 = \mathbb{1}$. For the corresponding operator expectation values $g_\nu(t) = \text{tr}\,(\mathcal{F}_\nu \rho(t))$, the closed exact equation of motion is found to read

$$
\frac{d}{dt}\text{tr}\,(\mathcal{F}_\nu \mathcal{R}(t)) = -i\,\text{tr}\,(\mathcal{F}_\nu L \circ \mathcal{R}(t))
$$
$$
- \int_0^t dt'\,\text{tr}\,(\mathcal{F}_\nu L \circ T(t,t') \circ Q(t') \circ L \circ \mathcal{R}(t')). \quad (1)
$$

The accompanying canonical density operator $\mathcal{R}(t) = \exp(-\mu_\nu(t)\mathcal{F}_\nu)$ which minimizes the entropy in $\mathcal{E}$ contains time dependent Lagrange multipliers $\mu(t)$ which are functions of $g_\nu(t)$ such that $g_\nu(t) = \text{tr}\,(\mathcal{F}_\nu \mathcal{R}(t))$. We emphasize that $\mathcal{R}(t)$ does not evolve with L and must not be confused with the density-operator $\rho(t)$ of the system. All trace expressions at the r.h.s. of (1) can at least in principle be expressed in terms of the g_ν, and the system is a closed integro-differential equation in the c-number expectation values. The projector $Q(t)$ is defined by

$$
\text{tr}(\mathcal{O}_1 Q(t) \circ \mathcal{O}_2) = \text{tr}(\mathcal{O}_1 \mathcal{O}_2) - \frac{\partial \text{tr}(\mathcal{O}_1 \mathcal{R}(t))}{\partial g_\nu(t)}\text{tr}(\mathcal{F}_\nu \mathcal{O}_2), \quad (2)
$$

and the non-unitary evolution operator $T(t,t')$ is a solution of

$$
\frac{\partial}{\partial t}T(t,t') = -iQ(t) \circ L \circ T(t,t') \quad (3)
$$

and

$$
\frac{\partial}{\partial t'}T(t,t') = iT(t,t') \circ Q(t') \circ L \quad (4)
$$

with initial condition $T(t,t) = 1$.

Here, we will complete $\mathcal{E}$ such that the action of the Hamiltonian $[H,\mathcal{X}] = L \circ \mathcal{X}$ can be split into $L = L_0 + L_1$, and the free part be dynamically closed with respect to the level of observation, $L_0 \circ \mathcal{F}_\nu = [H_0, \mathcal{F}_\nu] = \Omega_{\nu\mu}\mathcal{F}_\mu$. In that case, in the integral (1), the complete Liouvillian can be replaced by L_1.

Expectation values of operators which are not in the linear hull of $\mathcal{E}$ get additional contributions to their $\mathcal{R}$-averages,

$$
\text{tr}(\mathcal{O}\rho(t)) = \text{tr}\,(\mathcal{O}\mathcal{R}(t))
$$
$$
- i\int_0^t dt'\text{tr}\,(\mathcal{O}T(t,t') \circ Q(t') \circ L \circ \mathcal{R}(t')) \quad (5)
$$

where again the dynamically closed part in L does not contribute to the integral. The integral vanishes for $\mathcal{O} \in \mathcal{E}$.

4 Zero-dimensional system

We will investigate on the time evolution of an anharmonic oscillator defined by the Hamiltonian

$$
H = H_0 + H_1, \quad H_0 = \frac{1}{2}(p^2 + sx^2), \quad H_1 = \frac{\lambda}{2}x^4 \quad (6)
$$

with canonical commutator $[x,p] = i$. The parameter $s = \pm 1$ allows to switch to the broken symmetry case. We define the level of description by a dynamically closed set of observables for H_0 given by $\mathcal{E} = \{\mathbb{1}\,, x, p, x^2, p^2, xp + px\}$. That set plays a preferred role since, due to its bilinear nature, the accompanying density operator $\mathcal{R}(t)$ is quasi-Gaussian which allows to apply a modified Wick theorem in the evaluation of expectation values. Inclusion of the quadratic variables also ensures the existence of the accompanying canonical operator, and allows for direct comparison with approximations of Gaussian type. The equations of motion are found to read

$$
\frac{d}{dt}\bar{x} = \bar{p} \quad (7)
$$
$$
\frac{d}{dt}\bar{p} = -s\bar{x} + 4\lambda\bar{x}^3 - 6\lambda\bar{x}x_2 + \Sigma_p(t) \quad (8)
$$
$$
\frac{d}{dt}x_2 = w \quad (9)
$$
$$
\frac{d}{dt}p_2 = 8\lambda\bar{p}\bar{x}^3 - sw - 6\lambda w x_2 + \Sigma_{p^2}(t) \quad (10)
$$
$$
\frac{d}{dt}w = 2p_2 + 8\lambda\bar{x}^4 - 2sx_2 - 12\lambda x_2^2 + \Sigma_w(t) \quad (11)
$$

with $\bar{x} = \langle x \rangle, \bar{p} = \langle p \rangle, x_2 = \langle x^2 \rangle, p_2 = \langle p^2 \rangle, w = \langle xp + px \rangle$ and

$$
\Sigma_\nu(t) = -\int_0^t dt'\text{tr}(\mathcal{F}_\nu L_1 \circ T(t,t') \circ Q(t') \circ L_1 \circ \mathcal{R}(t')) \quad (12)
$$

accounting for entropy increase. Note that $\dot{\bar{x}}$ and $\dot{x}_2$ do not get further corrections since the potential is a function of position only. The energy is of the form

$$
\text{tr}\,(H\rho(t)) = \frac{1}{2}(p_2 + sx_2) + \frac{\lambda}{2}(3x_2^2 - 2x^4) + \epsilon(t),
$$
$$
\epsilon(t) = -i\int_0^t dt'\text{tr}(H_1 T(t,t') \circ Q(t') \circ L_1 \circ \mathcal{R}(t')),
$$
$$
(13)
$$

and is conserved in time. The key challenge is to find a sensible approximation for the operator $T(t,t')$. However it is worthwhile to study the first order system without integrals first.

5 First order approximation

5.1 Permissible initial conditions

The first order system may be integrated numerically with initial conditions for $\bar{x}, \ldots, w$. Those as well as their time

evolved counterparts are subject to the positivity conditions, $x_2 \geq 0, p_2 \geq 0, \delta^2 x = x_2 - \bar{x}^2 \geq 0, \delta^2 p = p_2 - \bar{p}^2 \geq 0$, and the uncertainty relation ($\delta^2 w = w - 2\bar{x}\bar{p}$)

$$\mathcal{A}^2 := (\delta^2 x)(\delta^2 p) - \frac{1}{4}(\delta^2 w)^2 \geq \frac{1}{4}. \qquad (14)$$

which follows immediately from Schwarz' inequality relation[5] $\langle A^2 \rangle \langle B^2 \rangle \geq |\langle AB \rangle|^2$. Coefficients that do not fulfill that relations cannot appear as expectation values averaged with a physical accompanying density operator $\mathcal{R}$.

5.2 Static solutions and their stability

Static solutions of (7–11) include the trivial configuration $\bar{x} = \bar{p} = w = 0$. More interestingly, the set of equations permits also non-trivial positional expectation values

$$\bar{x} = \pm\sqrt{\frac{s + 6\lambda x_2}{4\lambda}}, \quad p_2 = -\frac{1}{4\lambda}(s + 2\lambda x_2)(s + 6\lambda x_2),$$
$$w = \bar{p} = 0. \qquad (15)$$

In the unbroken case $s = 1$, for any choice of x_2, the value p_2 is always negative excluding a static configuration with non-trivial positional expectation value.

In the broken case $s = -1$, however, the positivity requirement for p_2 permits static solutions in the range $1/(6\lambda) \leq x_2 \leq 1/(2\lambda)$. They may have expectation values for position with $|\bar{x}| \leq 1/\sqrt{2\lambda}$, where the bounds correspond to the classical local minima of the potential. Classically, one would not expect static solutions for values of $\bar{x}$ other than the minimum $1/\sqrt{2\lambda}$. An additional restriction is given by the uncertainty relation,

$$(1 - 2\lambda x_2)^2(-1 + 6\lambda x_2) \geq 4\lambda^2. \qquad (16)$$

For $\lambda \ll 1$, this condition narrows the region of static solutions $1/(6\lambda) + 3\lambda/2 + \mathcal{O}(\lambda^2) \leq x_2 \leq 1/(2\lambda) - 1/\sqrt{2} + \mathcal{O}(\lambda)$ by a small amount. For increasing λ, the window gets smaller and finally completely vanishes at $\lambda = \frac{2}{9}\sqrt{\frac{2}{3}} \approx 0.18$, corresponding to $x_2 = \frac{5}{4}\sqrt{\frac{3}{2}} \approx 1.53$ and $\bar{x} = (27/2)^{1/4}/2 \approx 0.96$. For larger couplings, no static solutions exist. In that case, the minimal quantum uncertainty suffices to overcome the potential barrier and the motion can escape the initial half.

To study the stability of the static points in the broken phase, we consider a set of initial conditions with $\bar{p} = w = 0$ and x_2, p_2 satisfying the staticity requirement. We chose $\bar{x}(0) = \bar{x}^{\text{static}} + \delta$, where $\delta/\bar{x} \ll 1$ to model perturbed initial conditions. For $\delta > 0$ a numerical integration shows that the position observable periodically increases to a maximum, at which the width $\delta^2 x$ develops a local minimum. The motion of $\bar{x}$ remains in the initial

half, but the amplitude is large with respect to the initial coordinate.

For $\delta < 0$, the qualitative picture is completely different. There the average position performs an oscillation to the negative initial value, while the width oscillates only slightly. It is surprising that motion is just opposite to the classically expected roll–down in the potential. Again quantum effects largely dominate over the classical picture.

In both cases, the motion of the position coordinate does not remain near the initial preparation. In that sense, static solutions are not attractive, and cannot be regarded as stable.

An explanation for the different quantitative behavior depending on the sign of δ can be given on grounds of the phase space trajectories. As we will show below, the system (7–11) is equivalent to the Eqns. (19–20). Reading the second time derivatives as curvature vector in the $(\bar{x}, x_2)$ phase space, the expansion around $\bar{x}^{\text{static}}$ shows that the direction of curvature is determined by the sign of the small parameter δ at the static point. That indicates a bifurcation point and quantitatively explains the dynamic instability near the staticity conditions.

5.3 First order integrals of motion

Rewriting the system (7–11) it in terms of the quantum widths $X = \sqrt{\delta^2 x}$, $P = \sqrt{\delta^2 p}$, $W^2 = \delta^2 w$,

$$\frac{d}{dt}W^2 = 2P^2 - 2(s + 6\lambda x_2)X^2,$$
$$\frac{d}{dt}P^2 = -(s + 6\lambda x_2)W^2,$$
$$\frac{d}{dt}X^2 = W^2, \qquad (17)$$

one verifies the time independence of $\mathcal{A}$. It is remarkable that the uncertainty appears as constant of motion which moreover in independent of the coupling. Physically, on account of the uncertainty–entropy relation (see Appendix), constant uncertainty means that quantum effects do not increase entropy. To first order, the value of the set of observables $\mathcal{E}$ at a given time is sufficient to determine their time evolution locally in time, and to express all observables of the system.

A second constant of motion is given by

$$h = \frac{1}{2}p_2 + \frac{1}{2}sx_2 + \frac{\lambda}{2}(3x_2^2 - 2\bar{x}^4) \qquad (18)$$

which equals the expectation value of the Hamiltonian averaged with $\mathcal{R}$. That statement is not so trivial as seems at first sight. It is a consequence of the fact of dynamical closure of H_0 which makes the corrections in the integral in (13) of second order.

Let us further make a comparison with the standard perturbative approximation. There, one expands H around the classical expectation value of momentum and position, i.e. $x = \bar{x} + \delta x$, where δx is supposed to be

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[5] This condition generally gives stronger constraints than the usual procedure to minimize the positive–definite expression $\langle (A - \lambda B)^2 \rangle \geq 0$

small. Applying that approximation to the Hamiltonian and keeping only quadratic terms in δx, one finds for the λ–dependent contribution to the energy $\lambda(6\bar{x}^2 x_2 - 5\bar{x}^4)/2$, which differs from h if δx is not small, to wit, if quantum or statistical corrections become important which is in fact the case. Note also that in the case of symmetric configurations $\bar{x} = 0$, the quartic potential part does not contribute to energy in that approximation at all. Thus the standard perturbative first order effective potential does not coincide with the consistent Gaussian dynamical potential, in agreement with [8].

5.4 First order effective Hamiltonian and effective Lagrangian

The energy integral can be used to eliminate $\bar{p}, p_2, w$ from the system (7–11),

$$\ddot{\bar{x}} = -s\bar{x} + 4\lambda\bar{x}^3 - 6\lambda\bar{x}x_2, \qquad (19)$$

$$\ddot{x}_2 = 4h - 4sx_2 - 18\lambda x_2^2 + 12\lambda\bar{x}^4. \qquad (20)$$

This system is not a Hamiltonian system in the kinetic momenta $\dot{\bar{x}}, \dot{x}_2$. A necessary condition of the existence of a Hamiltonian $\dot{\bar{x}}^2 + \dot{x}_2^2 + J(\bar{x}, x_2)$ would require J to be a solution of

$$\frac{\partial J}{\partial \bar{x}} = -\ddot{\bar{x}}(\bar{x}, x_2), \quad \frac{\partial J}{\partial x_2} = -\ddot{x}_2(\bar{x}, x_2). \qquad (21)$$

However, the integrability condition $\partial^2 J/(\partial\bar{x}\partial x_2) = \partial^2 J/(\partial x_2\partial\bar{x})$ is not fulfilled by the corresponding expressions of (19,20).

Nevertheless, an effective Hamiltonian which reproduces the equations motion of (7-11) together with the constant of uncertainty $\mathcal{A}^2$ can be constructed. We introduce the canonical pairs $(\bar{x}, \pi)$ and (x_2, π_2) and cast the conserved energy (18) in canonical variables. Then, p_2 becomes a function of $(\bar{x}, x_2, \pi, \pi_2)$ and has to be consistent with the Hamiltonian equations of motions,

$$\bar{p} = \dot{\bar{x}} = \frac{\partial H}{\partial \pi} = \frac{1}{2}\frac{\partial p_2}{\partial \pi}, \qquad w = \dot{x}_2 = \frac{\partial H}{\partial \pi_2} = \frac{1}{2}\frac{\partial p_2}{\partial \pi_2}. \quad (22)$$

On the other hand, the constant uncertainty requires p_2 to be a solution of the partial differential equation

$$\frac{1}{16}\left(\frac{\partial p_2}{\partial \pi_2}\right)^2 - \frac{\bar{x}}{4}\frac{\partial p_2}{\partial \pi_2}\frac{\partial p_2}{\partial \pi} + \frac{x_2}{4}\left(\frac{\partial p_2}{\partial \pi}\right)^2 = p_2 X^2 - \mathcal{A}^2. \quad (23)$$

Splitting off a summand $\mathcal{A}^2/X^2$ the remaining function has to be a homogeneous expression in π, π_2 of order two. We find

$$p_2 = \frac{\mathcal{A}^2}{X^2} + (4x_2\pi_2^2 + 4\bar{x}\pi_2\pi + \pi^2), \quad \bar{p} = (2\bar{x}\pi_2 + \pi), \quad (24)$$

which relates observables to the canonical variables. The corresponding Hamiltonian function has the form

$$H(\bar{x}, \pi; x_2, \pi_2) = 2x_2\pi_2^2 + 2\bar{x}\pi_2\pi + \frac{1}{2}\pi^2 + V(\bar{x}, x_2),$$

$$2V(\bar{x}, x_2) = \frac{\mathcal{A}^2}{X^2} + sx_2 + \lambda(3x_2^2 - 2\bar{x}^4). \qquad (25)$$

It can be checked that the remaining Hamiltonian equations of motion $\partial H/\partial\bar{x} = -\dot{\pi}$, $\partial H/\partial x_2 = -\dot{\pi}_2$ are in fact compatible with the original set of equations of motion. The corresponding effective Lagrangian is related to H by a Legendre transformation, $L = \pi_2\dot{x}_2 + \pi\dot{\bar{x}} - H$. Equation (22) supplies the necessary relations of canonical and kinematical momenta, and we finally get

$$L = \frac{1}{2}\dot{X}^2 + \frac{1}{2}\dot{\bar{x}}^2 - V(\bar{x}, x_2). \qquad (26)$$

In terms of the coordinates $\bar{x}, X$, the Lagrangian is composed of a kinematical kinetic contribution, a potential $(sX^2 + s\bar{x}^2 + \lambda(3X^4 + 6X^2\bar{x}^2 + \bar{x}^4))/2$ and an additional term $\mathcal{A}^2/(2X^2)$ having the form of the energy of circular motion with angular momentum $\mathcal{A}$.

5.5 The small coupling limit and parametric resonance

In the strict limit $\lambda = 0$ the equations of motion (19,20) decouple trivially. However, that limit does not provide a sensible starting point for a perturbative expansion since the perturbation series turns out to be non-analytic around zero coupling. We thus concentrate on the limit $\lambda \to 0^+$ in which the equation of motion for $\bar{x}$ has the structure

$$\ddot{\bar{x}} + \bar{x}\omega^2(t) = 0 \qquad (27)$$

of a linear oscillator with a time dependent frequency-factor. It can be seen by completely eliminating x_2 from the system (19,20) that for finite $\bar{x}$ the quantities x_2, p_2 and w consistently have to be taken of order $1/\lambda$. Consequently, also the energy being a function of those quadratic expectation values grows with the inverse coupling and will be rescaled into the finite quantity $\tilde{h} = 18\lambda h + 1$. The time dependent mass-term $\omega^2 = (s + 2z\sqrt{\tilde{h}})/3$ can be rewritten in terms of the function $z = (9\lambda x_2 + s)/\sqrt{\tilde{h}}$ which is a solution of $z'' + z^2 - 1 = 0$, where the prime denotes differentiation with respect to the rescaled time $\tau = t(2\sqrt{\tilde{h}})^{1/2}$. Note that in this limit, there is no back-reaction on the frequency-factor by the motion of the position coordinate. A first integral is given by

$$\frac{1}{2}(z')^2 = A + z - \frac{z^3}{3} \qquad (28)$$

where A encodes the initial conditions of x_2. Solutions for $z(\tau)$ are periodic if $|A| < 2/3$ with minima in the strip $|z| < 1$ and maxima for $1 < z < 2$.

For physical solutions of the system (27–28) we have to keep in mind that only positive values of x_2 can be generated by hermitian density matrices[6]. Consequently, $z\sqrt{\tilde{h}} - s$ has to remain positive in the course of time evolution. In the case of the unbroken potential $s = 1$, this further restricts motion of z to the strip $2 < 2z\sqrt{\tilde{h}} < (-1 + \sqrt{6 + 3\tilde{h}})$ where the bounds correspond to the local extrema of a periodic motion during which ω^2 remains positive.

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[6] $\delta^2 x > 0$ is trivially valid since λx_2 is of the same order as $\bar{x}$
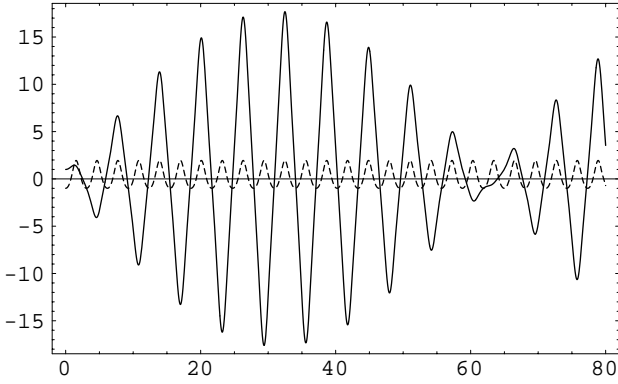
Fig. 1. Time evolution of the effective mass $\omega^2(t)$ (dashed line) and $\bar{x}(t)$ with parameters $\tilde{h} = 3.1$, $z_0 = -0.56$, $\bar{x}_0 = 1$, $\bar{x}'_0 = z'_0 = 0$

Fig. 2. The same as in Fig. 1, but with $\tilde{h} = 1.84$

The more interesting case is the broken phase $s = -1$. There, the solutions which fulfill the positivity requirement for x_2 can now be found in the domain $-2 < 2z\sqrt{\tilde{h}} < (1 + \sqrt{6 + 3\tilde{h}})$ and correspond all to oscillatory z. However, if the initial conditions are varied, the behavior of ω^2 becomes quantitatively different. In particular, in the range $1 < 2z\sqrt{\tilde{h}} < (1 + \sqrt{6 + 3\tilde{h}})$, the factor ω^2 is positive but becomes negative for $-2 < 2z\sqrt{\tilde{h}} < 1$. In the first region, the motion of $\bar{x}$ is quasi-harmonic with variable frequency, but turns into exponential behavior if the lower strip of z is reached by time evolution. Physically, oscillatory and tunneling phases alternate. Negative square of frequency flips the sign of the curvature of $\bar{x}$ and bends trajectories in a direction opposite to the oscillations. However, since there is no back reaction on the motion of $\bar{x}$ from the frequency-factor, the tunneling phases are short, and exponential growth stops before the numerical value of $\bar{x}$ can become large. The period of $\bar{x}$ is roughly determined by ω^2 averaged over one period of z. Depending on the quotient of those two periods, a variety of resonance phenomena can appear. Figure 1 displays the case of a frequency coefficient close to $1:2$. The periodic kick of the motion of $\bar{x}$ results in large resonant amplitudes. Figure 2 shows a frequency quotient of $3:8$. The dents in the motion of $\bar{x}$ correspond to tunneling phases.

6 Second order motion

Realistic thermodynamic behavior includes entropy generating processes which necessitates the inclusion of the non-local integral contributions in (1). The evaluation of that term, however, requires an approximation for the evolution operator $T(t, t')$. A strict expansion in powers of the coupling constant to second order amounts to the replacement $L \rightarrow L_0$ in the definition of $T(t, t')$ which has been applied recently in the context of field theory [17]. On account of the dynamical closure, $T(t, t')$ even exponentiates to the product of the free unitary time evolution operator with Q. That approximation, however, suffers from
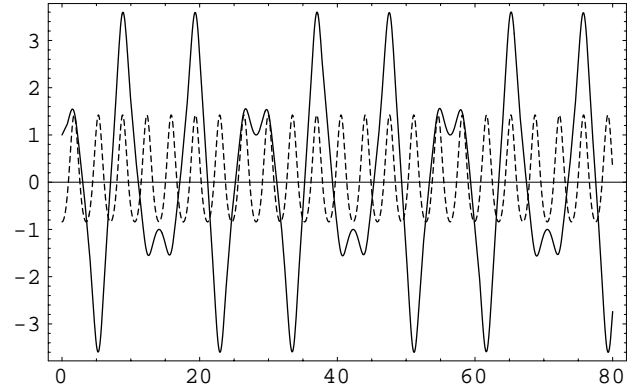
non-conservation of the energy (13) at secular scales. A numerical integration shows that the runaway of energy sets in even at times before the interesting transition from regular motion to the stochastic entropy generating phase appears. Moreover, since energy turns out to increase even exponentially, the expectation values also grow in an unphysical manner. A first attempt to cure the situation is to replace the free Hamiltonian in $T(t, t')$ by a resummed quadratic one. At first sight this concept appears promising, since it still benefits from a dynamic closure relation. We discuss this approach first before we turn to a further essential modification.

6.1 Resummed Hamiltonian approach

The resummed first order Hamiltonian is defined to be of at most quadratic in position and momenta but with explicit time dependence through coefficients $(a, \ldots, e)$, and has to reproduce the equations of motion (7–11). We make the Ansatz $H^r(t) = H_0 + \lambda H_1^r(t)$ with

$$H_1^r(t) = ap + bx + c(xp + px) + dx^2 + ep^2. \tag{29}$$

Plugging this expression into (1) and keeping terms to first order in the coupling, the equations of motion turn into

$$\begin{aligned}
\dot{x} &= \bar{p}(1 + 2\lambda e) + 2\lambda c\bar{x} + \lambda a, \\
\dot{p} &= -\bar{x}(s + 2\lambda d) - 2\lambda c\bar{p} - \lambda b, \\
\dot{x}_2 &= w(1 + 2\lambda e) + 2\lambda a\bar{x} + 4\lambda cx_2, \\
\dot{p}_2 &= -w(s + 2\lambda d) - 4\lambda cp_2 - 2\lambda b\bar{p}, \\
\dot{w} &= 2p_2(1 + 2\lambda e) - 2x_2(s + 2\lambda d) - 2\lambda b\bar{x} + 2\lambda a\bar{p},
\end{aligned} \tag{30}$$

which when compared with the original first order set of equations defines

$$a = \xi(2\bar{p}x_2 - w\bar{x}), \quad b = -4\bar{x}^3 + \xi(2p_2\bar{x} - \bar{p}w),$$
$$c = \frac{1}{2}\xi W^2, \quad d = 3x_2 - \xi P^2, \quad e = -\xi X^2. \tag{31}$$

The one-parameter solution parameterized by ξ is a consequence of time independent uncertainty which still is an

integral of motion of (30). The remaining freedom has to be fixed by the condition that H^r is a constant of time which is equivalent to the fact that the expectation value of H^r equals the expectation value of H,

$$\xi = \frac{3(2\bar{x}^4 - x_2^2)}{w^2 - 4x_2 p_2 + 6(x_2\bar{p}^2 + \bar{x}^2 p_2 - w\bar{x}\bar{p})}. \qquad (32)$$

Resummation is achieved by absorbing the effective Hamiltonian into the new free one, and compensating by an interaction counter term,

$$H = H^r + H_2, \quad H_2 = H_1 - \lambda H_1^r(t). \qquad (33)$$

In the integrals of the dissipative contributions in (12), we have to replace L_1 by L_2. However, the set of observables $\mathcal{E}$ is still dynamically closed with respect to H^r such that only H_1 of H_2 contributes. Finally, the resummation enters in the expansion of the evolution operator $T(t,t')$ where we replace $L \to L^r(t)$ in (4). We have to consider the particular combination $T(t,t') \circ Q(t')$ appearing in the entropy generating contribution which can be integrated formally directly from its definition,

$$T^r(t,t') \circ Q(t') = \mathcal{T} \exp\left(-i\int_{t'}^{t} d\tau Q(\tau) \circ L^r(\tau) \circ \right) Q(t'). \qquad (34)$$

At that point, dynamical closure guarantees the important relation $Q(t'') \circ L^r(t) \circ Q(t') = L^r(t) \circ Q(t')$ valid even in the case where the time arguments of the projectors differ. All Q but the one at the most r.h.s in the summands of the formal exponential can be dropped, and we arrive at the desired relation

$$T^r(t,t') \circ Q(t') = \mathcal{U}(t,t') \circ Q(t'),$$

$$\mathcal{U}(t,t') = \mathcal{T} \exp\left(-i\int_{t'}^{t} d\tau L^r(\tau) \circ \right). \qquad (35)$$

We want to point out that this relation does not automatically imply the equality of $T^r(t,t')$ and $\mathcal{U}(t,t')$. The replacement is non-trivial also in the sense that acting on the projector, the action of a non-unitary operator is replaced a unitary one.

It turns out to be useful to let $\mathcal{U}$ act on the operators to its left, $\text{tr}\left((\mathcal{U}^\dagger(t,t') \circ \mathcal{O}_1) \circ \mathcal{O}_2\right) = \text{tr}(\mathcal{O}_1 \mathcal{U}(t,t') \circ \mathcal{O}_2)$. On account of the two properties of L^r being a derivation and anti-hermitian, the adjoint action simply amounts to exchange time arguments, $\mathcal{U}^\dagger(t,t') = \mathcal{U}(t',t)$. We introduce the evolved operator $\mathcal{O}(t,t') = \mathcal{U}^\dagger(t,t') \circ \mathcal{O}$ which solves

$$\partial_{t'} \mathcal{O}(t,t') = -iL^r(t') \circ \mathcal{O}(t,t') \qquad (36)$$

and is related to the Dirac representation induced from L^r by $\mathcal{O}_D(t,t') = \mathcal{U}(t,t') \circ \mathcal{O} = \mathcal{O}(t',t)$. Since the Liouvillian is a derivation, it suffices to investigate on the evolution of $x, p, \mathbb{1}$ representing an operator basis. Dynamical closure guarantees the success of the Ansatz

$$x(t,t') = x\alpha_x(t,t') + p\beta_x(t,t') + \gamma_x(t,t'),$$
$$p(t,t') = x\alpha_p(t,t') + p\beta_p(t,t') + \gamma_p(t,t') \qquad (37)$$

with $\alpha_x(t,t'), \ldots, \gamma_p(t,t')$ to be determined by coefficient comparison. That gives rise to the system

$$\partial_{t'}\alpha_x(t,t') = -2\lambda c(t')\alpha_x(t,t') + (s + 2\lambda d(t'))\beta_x(t,t'),$$
$$\partial_{t'}\beta_x(t,t') = -(1 + 2\lambda e(t'))\alpha_x(t,t') + 2\lambda c(t')\beta_x(t,t'),$$
$$\partial_{t'}\gamma_x(t,t') = -\lambda a(t')\alpha_x(t,t') + \lambda b(t')\beta_x(t,t'). \qquad (38)$$

Integrals are found to read

$$\alpha_x(t,t')\bar{x}(t') + \beta_x(t,t')\bar{p}(t') + \gamma_x(t,t') = \bar{x}(t), \qquad (39)$$

which corresponds to the quantity $\text{tr}(x(t,t')\mathcal{R}(t'))$ independent of t', and

$$\alpha_x^2(t,t')X^2(t') + \beta_x^2(t,t')P^2(t') + \\ \alpha_x(t,t')\beta_x(t,t')W^2(t') = X^2(t), \qquad (40)$$

expressing the t' independence of $\text{tr}(x(t,t')x(t,t')\mathcal{R}(t'))$. We remark that these constants imply unitary evolution of the accompanying operator, $\mathcal{U}(t,t')\mathcal{R}(t') = \mathcal{R}(t)$, and are compatible with a time independent uncertainty product. The complete solution of (38) can be parameterized by the angle variable

$$\Psi(t,t') = \int_{t'}^{t} d\tau \mathcal{A}\left(X^{-2}(\tau) - 2\lambda\xi(\tau)\right). \qquad (41)$$

We find

$$\alpha_x(t,t') = \mathcal{A}^{-1}X(t)P(t')\cos(\Psi(t,t') + \eta(t')),$$
$$\beta_x(t,t') = \mathcal{A}^{-1}X(t)X(t')\sin(\Psi(t,t')) \qquad (42)$$

with

$$\cos\eta(t) = \mathcal{A}X^{-1}(t)P^{-1}(t),$$
$$\sin\eta(t) = W^2(t)X^{-1}(t)P^{-1}(t)/2, \qquad (43)$$

which satisfies the initial conditions $\alpha_x(t,t) = 1$, $\beta_x(t,t) = 0$. The coefficients for $p(t,t')$ are also solutions of the differential equations (38), but with integration constants $\bar{p}(t)$ and $P^2(t)$ at the r.h.s. of (39,40). The corresponding angle variable gets shifted to $\Psi(t,t') - \eta(t) + \pi/2$ and we get

$$\alpha_p(t,t') = -\mathcal{A}^{-1}P(t)P(t')\sin(\Psi(t,t') - \eta(t) + \eta(t')),$$
$$\beta_p(t,t') = \mathcal{A}^{-1}P(t)X(t')\cos(\Psi(t,t') - \eta(t)). \qquad (44)$$

Now all necessary tools are at hand to evaluate the integrals in (12) and (13) necessary solve the integro-differential equation of motion in a resummed Hamiltonian approximation. We have integrated the system numerically and still find non-conservation of energy at typical time scales of order $2\pi/(4\lambda)$ for $\lambda \ll 1$. The factor 2π corresponds to the natural period of the oscillator with unit circular frequency, and $1/4$ can be identified to coming from the fourth powers of the harmonic functions in α, β due to the quartic interaction Hamiltonian. At a technical level, the problem is that quadratic Hamiltonians, even with time dependent coefficients, automatically conserve the uncertainty $\mathcal{A}^2$, and motion stays within this equivalence class fixed by the initial conditions. Plugging that

approximation into the entropy generating integrals of the equations of motion, the dissipative corrections, although formally of second order, do not remain small at large time scales. The effective unitary evolution operator generated by an effective quadratic Hamiltonian cannot be used as a sensible approximation in the entropy generating corrections. The inconsistency becomes apparent when one compares the uncertainty $\mathcal{A}$ determined by the initial conditions with the actual uncertainty expressed by the evolved value of the observables.

7 Consistent effective approximation

Although the effective Hamiltonian constructed in the previous section turns out to be inconsistent with time–variant uncertainty and time evolution at large time scales, it still approximates time evolution locally in time at short time scales. It can be seen from numerical integration that the quadratic Hamiltonian adjusted to a set of given quantities $x(t), \ldots, w(t)$ considered as initial conditions evolves them quite accurately. Local in time, motion appears to be generated by a quadratic Hamiltonian which can be used to approximate only the enveloping curves of the true trajectories, but the locally best approximating effective Hamiltonian does not evolve to the enveloping Hamiltonian being the best approximation at a later time. One may argue that a non-quadratic extension may solve the problem of energy conservation. However, on account of the basis of observables chosen, the accompanying density operator still remains quadratic, and the exact Wick theorem valid, such that the non-quadratic extension effectively boils down to the quadratic effective theory.

We thus abandon the query for an effective Hamiltonian completely in favor of the construction of an effective time evolution operator. Physically, we have to admit effective equations of motions for the observables which are not generated by a Hamiltonian function. This step is also necessary to account for irreversibility.

The complete effective time evolution operator $\mathcal{V}(t, t')$ be subject to the following assumptions.
(a) Transitivity, $\mathcal{V}(t, t') \circ \mathcal{V}(t', t'') = \mathcal{V}(t, t'')$
(b) Initial value, $\mathcal{V}(t, t) = \mathbb{1}$.
(c) Its adjoint acts like an exponentiated derivative operator on products, i.e. $\mathcal{V}(t, t')^\dagger \circ (\mathcal{O}_1 \mathcal{O}_2) = (\mathcal{V}^\dagger(t, t') \circ \mathcal{O}_1)(\mathcal{V}^\dagger(t, t') \circ \mathcal{O}_2)$. Time evolution commutes with forming operator products.

We will further specify to the 'collisionless' approximation of $\mathcal{V}(t, t')$ by the additional assumptions that
(i) — the operator linearly maps the basis $x, p, \mathbb{1}$ onto itself. That replaces the notion of 'free motion', and generalizes dynamical closure to non-Hamiltonian evolution.
(ii) — $\mathcal{V}(t, t')$ is compatible with time evolution of the accompanying density operator, i.e. $\mathcal{V}(t, t') \circ \mathcal{R}(t') = \mathcal{R}(t)$. That condition actually defines $\mathcal{V}$ consistently with the equations of motion, and the evolution of $\mathcal{R}$, which is just contrary to the strategy of the previous chapter, where the evolution operator generated by the effective Hamiltonian was responsible for time evolution of $\mathcal{R}$.

At a technical level, time dependent uncertainty $\mathcal{A}(t)$ is introduced into the coefficients α, β which are no longer subject to the set of differential equations (38). If we define the evolved operators by $\mathcal{O}(t, t') = \mathcal{V}^\dagger(t, t') \circ \mathcal{O}$, the basis still can be expanded as in (37). The requirements (ii,c) automatically lead to the relations

$$\operatorname{tr}(x(t, t')\mathcal{R}(t')) = \bar{x}(t), \ \operatorname{tr}(x(t, t')x(t, t')\mathcal{R}(t')) = x_2(t),$$
$$\operatorname{tr}(p(t, t')\mathcal{R}(t')) = \bar{p}(t), \ \operatorname{tr}(p(t, t')p(t, t')\mathcal{R}(t')) = p_2(t),$$
$$(45)$$

which we identified as constants of motion of the resummed evolution equations. In addition to these, we find

$$\operatorname{tr}((x(t, t')p(t, t') + p(t, t')x(t, t'))\mathcal{R}(t')) = w(t) \quad (46)$$

the r.h.s. of which was fixed by initial conditions in resummed Hamiltonian dynamics. These equations are sufficient to express the evolution coefficients of x and p in a manner analogously to (42,44) together with (43), but with $\mathcal{A}$ replaced by the actual uncertainty $\mathcal{A}(t')$ in (42,44) and $\mathcal{A}(t)$ in (43). The angle variable $\Psi(t, t')$, however, remains undetermined for the moment.

In the evaluation of $T(t, t') \circ Q(t')$, we consistently have to replace the resummed unitary operator $\mathcal{U}(t, t')$ by $\mathcal{V}(t, t')$. The dissipative contributions $\Sigma_\nu(t)$ and $\epsilon(t)$ are now found to read ($\Psi \equiv \Psi(t, t')$, $\bar{x} \equiv \bar{x}(t)$, $\bar{x}' \equiv \bar{x}(t'), \ldots$)

$$\Sigma_\nu(t) = \lambda^2 \int_0^t dt' \sigma_\nu(t, t'), \qquad \epsilon(t) = \lambda^2 \int_0^t dt' \epsilon(t, t'),$$
$$(47)$$

with

$$\sigma_p(t, t') = 6\mathcal{A}'^{-3} X^3 X'^3 \sin\Psi \left(12\mathcal{A}'^2 \cos^2\Psi - \sin^2\Psi\right) \bar{x}',$$
$$\sigma_{p_2}(t, t') = 12\mathcal{A}'^{-3} X'^3 X^2 P \times$$
$$\left(XX' \left(4\mathcal{A}'^2(2\cos(2\Psi - \eta) - \cos\eta)\cos^2\Psi - \right.\right.$$
$$\left.(2\cos(2\Psi - \eta) + \cos\eta)\sin^2\Psi\right)$$
$$+ \bar{x}\bar{x}' \left(6\mathcal{A}'^2(3\cos(2\Psi - \eta) - \cos\eta)\cos\Psi - \right.$$
$$\left.\left.3\cos(\Psi - \eta)\sin^2\Psi\right)\right)$$
$$+ 2\bar{p}\sigma_p(t, t'),$$
$$\sigma_w(t, t') = 48\mathcal{A}'^{-3} X^3 X'^3 \sin\Psi \times$$
$$\left(XX' \left(4\mathcal{A}'^2 \cos^2\Psi - \sin^2\Psi\right)\cos\Psi + \right.$$
$$\left.\bar{x}\bar{x}' \left(12\mathcal{A}'^2 \cos^2\Psi - \sin^2\Psi\right)\right),$$
$$\epsilon(t, t') = -\sigma_w(t, t')/8.$$
$$(48)$$

The last equality is due to the particular form of the operator $xp + px$ which, when commuted with a homogeneous operator, evaluates to twice the degree of homogeneity in x.

A complete solution involves also to determine the unknown angle variable $\Psi(t, t')$. Analogously to the construction of the effective Hamiltonian, we exploit the remaining freedom to require the energy to be a conserved quantity within our approximation scheme. Differentiating the corresponding expressions (13) with respect to time, on finds that the term $d\epsilon(t)/dt$ has to be compensated by the integrand of the term $\Sigma_{p^2}(t)/2$. That gives rise to a differential
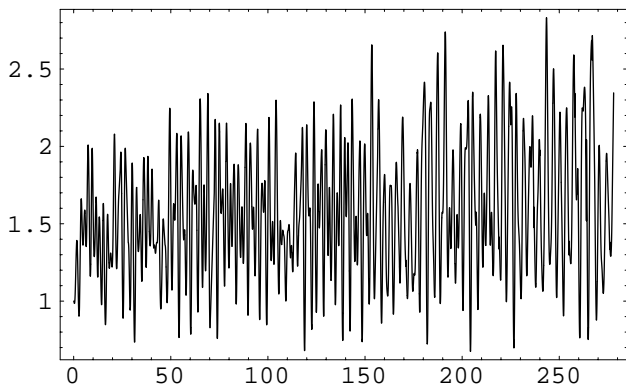
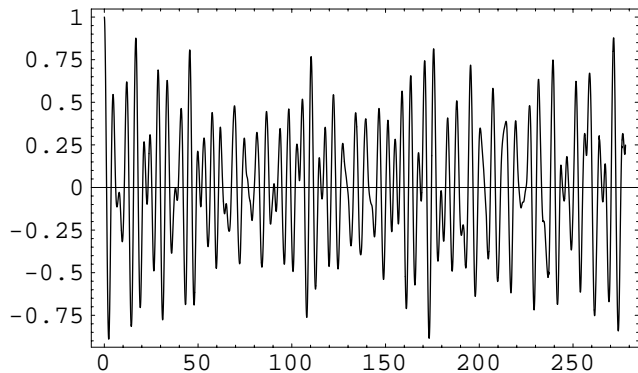**Fig. 3.** Time evolution of the uncertainty of the position operator $X(t)$

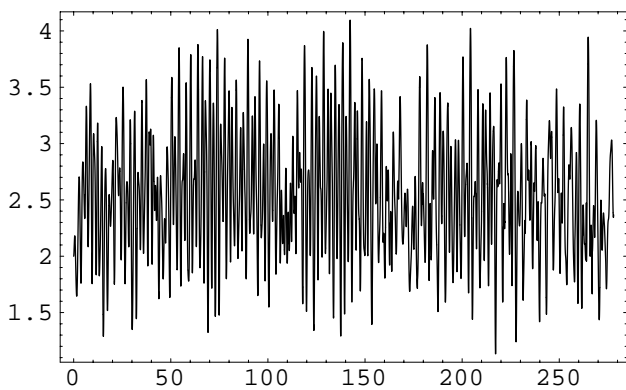**Fig. 5.** Time evolution of the position average $\bar{x}(t)$

Fig. 4. Time evolution of the uncertainty of the momentum operator $P(t)$
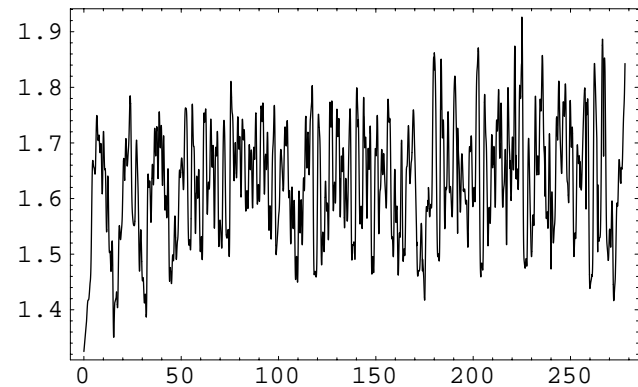

Fig. 6. Time evolution of the relevant entropy $S(t)$

equation for Ψ with solution

$$\Psi(t, t') = \int_{t'}^{t} d\tau \mathcal{A}(\tau) X^{-2}(\tau). \tag{49}$$

It is a non-trivial result that the angle parameter can be expressed in terms of an integral involving the history of $\mathcal{A}$ and X. That nevertheless includes all contributions which can be resummed in an effective evolution operator satisfying conditions (i) and (ii) in a self consistent way. Note also that the first order correction of (41) can be absorbed into the time dependent uncertainty completely. Moreover, since uncertainty is directly related to entropy (see Appendix), the approximation consistently accounts for entropy variations but by construction keeps the energy constant in time.

The complete set of integro-differential equations can now be evaluated numerically. A typical time evolution is displayed in Figs. 3–6 for the initial conditions $\bar{x}(0) = 1$, $x_2(0) = p_2(0) = 2$, $\bar{p}(0) = w(0) = 0$ with $\lambda = 0.1$ and symmetric potential $s = 1$.

It can be proven in the general setting that motion is such that the entropy is always larger or equal than its initial value. We find that our approximation respects that property, but fluctuations at intermediate times are possible. There is no sign that the system approaches a

static point at large time scales which is not to be expected in general.

The numerical strategy to solve the consistency problem for the integro–differential equation was the following. Suppose we knew the exact set of variables in the time range $(0, t)$. Then we benefited from the enveloping Gaussian dynamics and predicted the evolution by integrating the first order system with the initial data at t for a time interval $(t, t + \delta t)$, where δt is typically of the order of a period of $\bar{x}$.

That prediction can be improved iteratively for $(t, t + \delta t)$ by plugging it into the integral at the r.h.s. which represents an inhomogeneity for the differential equation. Note that the integral expands over the complete history of the observables which poses a problem in numerical integration over large time scales. Luckily, the integrand can be split into a sum of products of functions depending solely on t or t', such that the integrals can be reused in the extension procedure of time range. For times including a large number of quasi–periods of the variables, the contribution of the integral, although evaluated exactly, increasingly exhibits stochastic behavior. The method proposed thus supplies a tool to exactly calculate quasi–stochastic dissipative behavior which can be used to test a priori assumptions about stochastic forces.

To complete our considerations let us make some remarks concerning the analysis of time scales involved. The

projection method suggests to introduce the time scale of memory effects τ_{mem} determined by the scale where the effects from the remote past encoded in the kernel of the memory term become negligible. On the other hand, a macroscopic time scale may best be defined to be of order of the variation $g(t)/\dot{g}(t)$, which is not necessarily the same for all observables. In our case, τ_{mem} can be estimated by the time range where trajectories evolving with the enveloping temporally local Hamiltonian significantly start to deviate from the solution of the dissipative system. This time scale is directly related to the variation of the uncertainty $\mathcal{A}$, and thus to the entropy plotted in Fig. 6. Comparison of that with the behavior of the observables shows that the macroscopic time scale of the positional coordinate is of about the same order as τ_{mem}, but the quadratic observables $X(t)$ and $P(t)$ have significantly larger scales. Physically, this can be attributed to the zero-dimensionality of the quantum system under consideration where no fast fade–out of memory effects happens, but rather averaging effects over oscillations dominate. It is very likely that the qualitative picture changes in higher (infinite-) dimensional systems where spatial energy flux may also play an important role.

8 Conclusion and outlook

We proposed a method to calculate the time evolution of observables beyond the effective Hamiltonian approximation in a self–consistent systematic way thus accounting for real dissipative processes. An application of this approximation scheme to field theories is planned. In particular, we are interested in the influence of real collisional processes on long term evolution, and expect to be able to decide whether dephasing or proper entropy generating processes dominate in infinite–dimensional systems. A generalization to gauge and fermion systems is planned, and we intend to develop a systematic expansion to higher orders. Applications may also include dynamical problems in cosmology such as inflationary phases.

Appendix A Entropy, uncertainty and effective Lagrange multipliers

We relate the Lagrange multipliers μ_ν and the relevant entropy $S = \mu_\nu g_\nu$ to the set of observables $\bar{x}, \bar{p}, x_2, p_2, w$. One considers

$$[\mathcal{F}_\mu, \mathcal{R}] = -\mu_\sigma \int_0^1 dx \mathcal{R}^x [\mathcal{F}_\mu, \mathcal{F}_\sigma] \mathcal{R}^{1-x}, \qquad (50)$$

which has vanishing trace. That gives rise to the set of equations $\mu_\sigma g_\rho \Gamma_\rho^{\mu\sigma} = 0$, $[\mathcal{F}_\mu, \mathcal{F}_\sigma] = \Gamma_\rho^{\mu\sigma} \mathcal{F}_\rho$ which are not independent, but lead to

$$\mu_x = \eta(\bar{x}P^2 - \frac{1}{2}\bar{p}W^2), \quad \mu_p = \eta(\bar{p}X^2 - \frac{1}{2}\bar{x}W^2),$$
$$\mu_{x^2} = -\eta P^2/2, \quad \mu_{p^2} = -\eta X^2/2, \qquad (51)$$

where $\eta = 4\mu_w/W^2$. Thus, one more relation is called for to determine the remaining unknown. To that end, we consider the eigenvectors $\mathcal{G}_\pm$ of $\log \mathcal{R}$ being linear combinations of the operators $\mathcal{F}_\nu$. The eigenvalue equation $[\mathcal{G}_\pm, \log \mathcal{R}] = \xi_\pm \mathcal{G}_\pm$ implies $\text{tr}(\mathcal{G}_\mp \mathcal{G}_\pm \mathcal{R}) = e^{\xi_\pm} \text{tr}(\mathcal{G}_\pm \mathcal{G}_\mp \mathcal{R})$, with the conjugate pairs of eigenvectors one of which is found to have the eigenvalues $\xi_\pm = \pm 2\sqrt{\mu_{x^2}\mu_{p^2} - \mu_w^2} = \pm \eta \mathcal{A}$. On the other hand, the traces can be evaluated using Wick's theorem, and one finds

$$\log\left(\frac{2\mathcal{A} - 1}{2\mathcal{A} + 1}\right) = \eta \mathcal{A}, \qquad (52)$$

which expresses the remaining unknown η in terms of the observables. From the constant normalization $\text{tr}\dot{\mathcal{R}}(t) = 0$ we get $\dot{\mu}_0 + \dot{\mu}_i g_i = 0$, and thus $\dot{S} = \mu_i \dot{g}_i$. The summands can be combined in terms of $\mathcal{A}(t)$ and we finally get

$$S(t) = (\mathcal{A}(t) + \frac{1}{2})\log(\mathcal{A}(t) + \frac{1}{2}) - (\mathcal{A}(t) - \frac{1}{2})\log(\mathcal{A}(t) - \frac{1}{2}) \qquad (53)$$

where a possible integration constant was chosen such that entropy vanishes at the minimal possible uncertainty corresponding to $\mathcal{A} = \frac{1}{2}$. $S(t)$ is a monotonically increasing function of $\mathcal{A}(t)$. This relation was found in a different context earlier [16].

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