

Comparison between quantum and classical dynamics in the effective action formalism

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A major difficulty in comparing quantum and classical behavior resides in the structural differences between the corresponding mathematical languages. The Heisenberg equations of motion are operator equations only formally identical to the classical equations of motion. By taking the expectation of these equations, the well-known Ehrenfest theorem provides identities which, however, are not a closed system of equations which allows to evaluate the time evolution of the system. The formalism of the effective action seems to offer a possibility of comparing quantum and classical evolutions in a systematic and logically consistent way by naturally providing approximation schemes for the expectations of the coordinates which at the zeroth order coincide with the classical evolution [1].

The effective action formalism leads to equations of motion which differ from the classical equations by the addition of terms nonlocal in the time variable. This means

that for these equations an initial value problem is not meaningful and they have to be interpreted in an appropriate way. Here we analyze situations in which the nonlocal terms can be reasonably approximated by local ones, so that the quantum corrections do not modify the locality of classical equations. In the simplest approximation, the effective Lagrangian differs from the corresponding classical one by a renormalization of both the potential- and the kinetic-energy terms. We shall not discuss the causal formalism used, for example, in refs. [2-4], as in the approximation considered this would lead to the same local equations.

The present contribution describes the beginning of a systematic study of semiclassical evolutions using the effective action formalism. In the first part, after introducing the formalism of the effective action and its expansion in powers of \hbar (loop expansion) in the context of quantum mechanics, we concentrate on the structure of the first-order corrections in \hbar . These corrections are evaluated to the second order in the derivative expansion [5], by two different methods. The first is based on a Euclidean approach [6], the second one on an adiabatic approximation in evaluating functional determinants.

In the second part of the article we put the formalism at work, choosing as our case study a two-dimensional (2D) anharmonic oscillator of the kind considered in molecular physics. The results of the simulations show that by increasing \hbar the effective dynamics tends to regularize the classical motion and becomes qualitatively very similar to the quantum evolution provided the energy is sufficiently small.

The evaluation of the effective dynamics in more general cases will be presented in a forthcoming paper.

PART I

1. – Effective action in quantum mechanics

In this section we define the effective action [7]. For simplicity, consider a one degree of freedom Hamiltonian,

$$(1.1) \quad \hat{H}(\hat{p}, \hat{q}) = \hat{H}_0(\hat{p}, \hat{q}) + \hat{U}(\hat{q}),$$

where

$$(1.2) \quad \hat{H}_0(\hat{p}, \hat{q}) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2$$

and the confining potential $\hat{U}(\hat{q})$ is an even polynomial of \hat{q} . We choose the constant of $\hat{U}(\hat{q})$ so that the lowest eigenvalue of \hat{H} is 0. The generating functional of the Green functions is

$$(1.3) \quad Z[J] = \langle 0 | \mathcal{T} (e^{\frac{i}{\hbar} \int dt J(t) \hat{q}(t)}) | 0 \rangle,$$

where $|0\rangle$ is the ground state of \hat{H} , $\hat{q}(t) = e^{\frac{i}{\hbar} \hat{H} t} \hat{q} e^{-\frac{i}{\hbar} \hat{H} t}$, $J(t)$ is a source vanishing for $|t| \rightarrow \infty$ and \mathcal{T} is the time-ordering operator. In eq. (1.3), as well as in the following,

the integrations with boundaries not explicitly indicated are to be understood between $-\infty$ and $+\infty$. The generating functional of the connected Green functions is defined as $W[J] = -i\hbar \ln Z[J]$ and the Legendre transform of $W[J]$ gives the effective action. By indicating with q the variable conjugated to J , *i.e.*,

$$(1.4) \quad q(t) = \frac{\delta W[J]}{\delta J(t)},$$

we define

$$(1.5) \quad \Gamma[q] = W[J] - \int dt q(t)J(t),$$

where J has to be thought, inverting relation (1.4), as a functional of q . The functional $\Gamma[q]$ represents the analog of the classical action, $S[q] = \int dt (\frac{1}{2}m\dot{q}^2(t) - V(q(t)))$, where $V(q) = \frac{1}{2}m\omega^2 q^2 + U(q)$, and can be written in the form

$$(1.6) \quad \Gamma[q] = S[q] + \tilde{\Gamma}_h[q],$$

with $\tilde{\Gamma}_0[q] = 0$. The Legendre transform can be calculated using the methods of ref. [8].

From the functional derivative of the classical action with respect to the position $q(t)$, one obtains the Euler-Lagrange equation of motion

$$(1.7) \quad \frac{\delta S[q]}{\delta q(t)} = -J(t).$$

In the same way the functional derivative of the effective action $\Gamma[q]$ with respect to the $q(t)$ given by (1.4) yields

$$(1.8) \quad \frac{\delta \Gamma[q]}{\delta q(t)} = -J(t).$$

This equation can be rewritten in the form

$$(1.9) \quad m\ddot{q}(t) + \partial_q V(q(t)) - \frac{\delta \tilde{\Gamma}_h[q]}{\delta q(t)} = J(t).$$

As we shall see in the next section, $\tilde{\Gamma}_h[q]$ admits an expansion in powers of \hbar , whose coefficients have a simple diagrammatic interpretation (loop expansion). In this way we can view the quantum integro-differential equation (1.9) as a perturbation of the classical equation of motion.

In order to interpret the solutions of eq. (1.8), we rewrite $Z[J]$, defined in (1.3), in the equivalent form

$$(1.10) \quad Z[J] = \langle 0|U_S^J(+\infty, -\infty)|0\rangle = \langle 0|\mathcal{T}(e^{-\frac{i}{\hbar} \int dt(\hat{H} - \hat{q}J(t))})|0\rangle,$$

where $U_S^J(t_b, t_a)$ is the evolution operator from t_a to t_b in the Schrödinger representation and in the presence of the external source $J(t)$. Note that in quantum mechanics $J(t)$ is an external force. The variable conjugated to J then is

$$(1.11) \quad q(t) = \frac{\langle \alpha_{[J]} | U_S^J(t, 0)^\dagger \hat{q} U_S^J(t, 0) | \beta_{[J]} \rangle}{\langle \alpha_{[J]} | \beta_{[J]} \rangle},$$

where

$$(1.12) \quad \langle \alpha_{[J]} | = \langle 0 | U_S^J(+\infty, 0),$$

$$(1.13) \quad | \beta_{[J]} \rangle = U_S^J(0, -\infty) | 0 \rangle.$$

Since generally $| \beta_{[J]} \rangle$ differs from $| \alpha_{[J]} \rangle$, $q(t)$ is a nondiagonal matrix element of \hat{q} between two states which evolve in the presence of $J(t)$. The solution of eq. (1.8) therefore can be complex valued. In the harmonic case $U(q)$ constant, $| \alpha_{[J]} \rangle$ and $| \beta_{[J]} \rangle$ are coherent states and coincide, up to a phase, if $\bar{J}(\omega) = 0$, where \bar{J} is the Fourier transform of the external force. In the anharmonic case, more complicated conditions have to be imposed on J so that the two states coincide. If these conditions are satisfied, $q(t)$ is the expectation value of the position operator.

2. – Loop expansion of the effective action

The effective action cannot be evaluated exactly for anharmonic systems, *i.e.*, $U(q) \neq$ constant. A widely used approximation scheme is the loop expansion (see, for example, [9, 10]), or semiclassical approximation, consisting in an expansion of $\Gamma[q]$ in powers of \hbar . At the lowest order the effective action coincides with the classical action, whereas the one-loop term is expressed by means of a functional determinant.

In order to obtain the loop expansion, we express $Z[J]$ as a path integral. Equation (1.10) can be rewritten, using the Gell-Mann and Low theorem [11], as

$$(2.1) \quad Z[J] = \frac{\langle 0_0 | \mathcal{T} (e^{-\frac{i}{\hbar} \int dt [\hat{U}(\hat{q}_0(t)) - \hat{q}_0(t) J(t)]}) | 0_0 \rangle}{\langle 0_0 | \mathcal{T} (e^{-\frac{i}{\hbar} \int dt \hat{U}(\hat{q}_0(t))}) | 0_0 \rangle},$$

where $\hat{q}_0(t) = e^{\frac{i}{\hbar} \hat{H}_0 t} \hat{q} e^{-\frac{i}{\hbar} \hat{H}_0 t}$ and $| 0_0 \rangle$ is the ground state of \hat{H}_0 . Equation (2.1) is equivalent to

$$(2.2) \quad Z[J] = \frac{e^{-\frac{i}{\hbar} \int dt U\left(\frac{\delta}{\delta J^i(t)}\right)} Z_0[J'] \Big|_{J'=J}}{e^{-\frac{i}{\hbar} \int dt U\left(\frac{\delta}{\delta J^i(t)}\right)} Z_0[J'] \Big|_{J'=0}},$$

where $Z_0[J]$ in terms of Feynman path integrals [12] reads

$$(2.3) \quad Z_0[J] = \lim_{T \rightarrow \infty} \int dx dy \int d[q]_x^y e^{\frac{i}{\hbar} \int_{-T}^T dt [\frac{m}{2} \dot{q}^2(t) - \frac{m}{2} \omega^2 q^2(t) + J(t)q(t)]} \varphi_0(x) \varphi_0(y).$$

Here $\varphi_0(x) = \langle x|0_0 \rangle$ and $d[q]_x^y$ is the functional measure on paths with endpoints $q(-T) = x, q(T) = y$. The purely oscillating integrand in eq. (2.3) can be regularized by changing ω into $\omega_\epsilon \equiv \omega(1 - i\epsilon)$, with $\epsilon \rightarrow 0^+$ [13]. Comparing eqs. (2.2) and (2.3) we obtain

$$(2.4) \quad Z[J] = \lim_{\epsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \frac{\int dx dy \int d[q]_x^y e^{\frac{i}{\hbar} \int_{-T}^T dt [\frac{m}{2} \dot{q}^2(t) - \frac{m}{2} \omega_\epsilon^2 q^2(t) - U(q(t)) + J(t)q(t)]} \varphi_0(x) \varphi_0(y)}{\int dx dy \int d[q]_x^y e^{\frac{i}{\hbar} \int_{-T}^T dt [\frac{m}{2} \dot{q}^2(t) - \frac{m}{2} \omega_\epsilon^2 q^2(t) - U(q(t))]} \varphi_0(x) \varphi_0(y)}.$$

Now we apply the stationary phase approximation to (2.4), expanding the exponent at the numerator around the solution $q_0(t)$ of

$$(2.5) \quad m\ddot{q}_0(t) = -m\omega_\epsilon^2 q_0(t) - \partial_q U(q_0(t)) + J(t),$$

which vanishes for $|t| \rightarrow \infty$. We find

$$(2.6) \quad Z[J] \simeq e^{\frac{i}{\hbar} (S[q_0] + \int dt J(t)q_0(t))} \times \lim_{\epsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \frac{\int d[q]_0^0 e^{\frac{i}{\hbar} \int_{-T}^T dt [\dot{q}^2(t) - \omega_\epsilon^2 q^2(t) - \frac{1}{m} \partial_q^2 U(q_0(t))q^2(t)]}}{\int d[q]_0^0 e^{\frac{i}{\hbar} \int_{-T}^T dt [\dot{q}^2(t) - \omega_\epsilon^2 q^2(t)]}}.$$

Note that the integrations over x and y disappear since $\varphi_0(\cdot)$ is proportional to $\delta(\cdot)$ in the limit $\hbar \rightarrow 0$. The Gaussian integrals in (2.6) can be performed yielding

$$(2.7) \quad Z[J] \simeq e^{\frac{i}{\hbar} (S[q_0] + \int dt J(t)q_0(t))} \times \lim_{\epsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \left(\frac{\det(-\partial_t^2 - \omega_\epsilon^2 - \frac{1}{m} \partial_q^2 U(q_0(t)))}{\det(-\partial_t^2 - \omega_\epsilon^2)} \right)^{-\frac{1}{2}},$$

where the differential operators act on functions $y(t)$ with Dirichlet boundary conditions $y(-T) = y(T) = 0$. From eq. (2.7) we obtain

$$(2.8) \quad W[J] = W_0[J] + \hbar W_1[J] + \mathcal{O}(\hbar^2) \\ = S[q_0] + \int dt J(t)q_0(t) \\ + \lim_{\epsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \frac{i\hbar}{2} \ln \left(\frac{\det(-\partial_t^2 - \omega_\epsilon^2 - \frac{1}{m} \partial_q^2 U(q_0(t)))}{\det(-\partial_t^2 - \omega_\epsilon^2)} \right) + \mathcal{O}(\hbar^2).$$

Setting $q = q_0 + \hbar q'$ and remembering that $\left. \frac{\delta S[q]}{\delta q(t)} \right|_{q_0} = -J(t)$, the effective action to one-loop order is

$$\begin{aligned}
 (2.9) \quad \Gamma[q] &= \Gamma_0[q] + \hbar \Gamma_1[q] + \mathcal{O}(\hbar^2) \\
 &= W_0[J] + \hbar W_1[J] - \int dt q(t) J(t) + \mathcal{O}(\hbar^2) \\
 &= S[q - \hbar q'] + \hbar W_1[J] - \hbar \int dt q'(t) J(t) + \mathcal{O}(\hbar^2) \\
 &= S[q] + \frac{i\hbar}{2} \lim_{\epsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \ln \left(\frac{\det(-\partial_t^2 - \omega_\epsilon^2 - \frac{1}{m} \partial_q^2 U(q(t)))}{\det(-\partial_t^2 - \omega_\epsilon^2)} \right) \Bigg|_{\text{Dirichlet}(\pm T)} + \mathcal{O}(\hbar^2).
 \end{aligned}$$

3. – Derivative expansion of the effective action

The classical action $S[q]$ is the time integral of a density (the Lagrangian) which is an ordinary function of $q(t)$ and $\dot{q}(t)$. As a consequence, the classical equation of motion (1.7) is a differential equation. On the other hand, the effective action $\Gamma[q]$ is nonlocal in time and, therefore, the variational equation (1.8) is also nonlocal. If $q(t)$ varies slowly, however, it is possible to expand $\Gamma[q]$ around a constant value of q (derivative expansion [6, 14]). In this expansion one finds that also $\Gamma[q]$ can be written as the time integral of a density, which is a series of terms involving time derivatives of $q(t)$ of increasing order:

$$(3.1) \quad \Gamma[q] = \int dt \left(-V_e(q(t)) + \frac{Z(q(t))}{2} \dot{q}^2(t) + A(q(t)) \dot{q}^4(t) + B(q(t)) \ddot{q}^2(t) + \dots \right).$$

As we shall see, the derivative expansion (3.1) does not generally converge and has only an asymptotic validity for $q(t) \rightarrow \text{constant}$. The absence in (3.1) of odd powers of $\dot{q}(t)$ is a consequence of the time reversal symmetry of the Hamiltonian.

Except for V_e and Z , all the terms in the derivative expansion (3.1) are at least of order \hbar :

$$(3.2) \quad V_e(q) = \frac{1}{2} m q^2 \omega^2 + U(q) + \hbar V_{e1}(q) + \mathcal{O}(\hbar^2),$$

$$(3.3) \quad Z(q) = m + \hbar Z_1(q) + \mathcal{O}(\hbar^2),$$

$$(3.4) \quad A(q) = \hbar A_1(q) + \mathcal{O}(\hbar^2),$$

$$(3.5) \quad B(q) = \hbar B_1(q) + \mathcal{O}(\hbar^2).$$

The effective potential $V_e(q)$, well known in quantum field theory in the study of spontaneous symmetry breaking [5], is everywhere convex [15]. It may happen that the effective

potential evaluated at a finite \hbar order loses somewhere its convexity if the classical potential is not everywhere convex [16]. In this paper we restrict ourselves to a phase-space region where the evaluated effective potential is convex.

If the derivative expansion (3.1) is truncated at a finite order $2N$, the corresponding variational equation is a differential equation of order $2N$. We thus have a Cauchy problem with $2N$ initial conditions. It is clear that these conditions do not determine completely the initial wave function of the system. They are constraints which must be imposed in the choice of the initial wave function for a comparison between true and effective quantum evolutions. We confine ourselves to the second order in the derivative expansion (DE2), that is

$$(3.6) \quad \Gamma[q] \simeq \int dt \left(-V_e(q(t)) + \frac{Z(q(t))}{2} \dot{q}^2(t) \right).$$

This is the simplest approximation to the effective action which preserves the structure of the classical equations of motion.

In the following we work out and compare two methods to obtain the derivative expansion of the effective action. The first is an adaptation to quantum mechanics of a method [6] used in quantum field theory and based on the Euclidean functional formalism. In the second method, we relate the derivative expansion to the adiabatic approximation of a differential equation with slowly varying coefficients. In this way we are able to give an estimate of the validity of the derivative expansion.

3.1. Derivative expansion: Euclidean approach. – The derivative expansion of the effective action can be obtained starting from the Euclidean generating functional

$$(3.7) \quad Z_E[J] = \frac{\int d[q]_x^y e^{-\frac{1}{\hbar}(S_E[q] - \int dt J(t)q(t))} \varphi_0(x)\varphi_0(y) dx dy}{\int d[q]_x^y e^{-\frac{1}{\hbar}S_E[q]} \varphi_0(x)\varphi_0(y) dx dy},$$

where the Euclidean action $S_E[q]$ is defined by

$$(3.8) \quad S_E[q] = \int dt \left(\frac{1}{2}m\dot{q}^2(t) + \frac{1}{2}m\omega^2 q^2(t) + U(q(t)) \right).$$

Setting $W_E[J] = \hbar \ln Z_E[J]$ and $q(t) = \frac{\delta W_E[J]}{\delta J(t)}$, we introduce the Euclidean effective action

$$(3.9) \quad \Gamma_E[q] = W_E[J] - \int dt J(t)q(t).$$

In analogy with the results of sect. 2, to one-loop order we have

$$(3.10) \quad \Gamma_E[q] = -S_E[q] - \frac{\hbar}{2} \ln \frac{\det \left[\frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)} \right]}{\det \left[\frac{\delta^2 S_E[0]}{\delta q(t)\delta q(s)} \right]} + \mathcal{O}(\hbar^2),$$

where the differential operator $\frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)}$ can be rewritten as

$$(3.11) \quad \frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)} = [-m\partial_t^2 + m\omega^2 + \partial_q^2 U(q(t))] \delta(t-s).$$

The second order in the derivative expansion of the Euclidean effective action is

$$(3.12) \quad \Gamma_E[q] = - \int dt \left[V_e(q(t)) + \frac{1}{2} Z(q(t)) \dot{q}^2(t) \right],$$

where $V_e(q)$ and $Z(q)$ are the same functions that appear in (3.1).

The effective potential can be found by combining (3.10) and (3.12) for $q(t)$ constant

$$(3.13) \quad \int dt V_{e1}(q) = \frac{1}{2} \ln \det \left[\frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)} \right] - \frac{1}{2} \ln \det \left[\frac{\delta^2 S_E[0]}{\delta q(t)\delta q(s)} \right].$$

Employing the functional analogue of the identity $\ln \det \mathbb{A} = \text{tr} \ln \mathbb{A}$, valid for any Hermitian matrix \mathbb{A} , we get

$$(3.14) \quad \ln \det \left[\frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)} \right] = \text{tr} \ln \left[\frac{\delta^2 S_E[q]}{\delta q(t)\delta q(s)} \right].$$

We use the Dirac notation to write

$$(3.15) \quad \left(-\partial_t^2 + \omega^2 + \frac{1}{m} \partial_q^2 U(q) \right) \delta(t-s) = \langle t | \left(\hat{P}^2 + \omega^2 + \frac{1}{m} \partial_q^2 U(q) \right) | s \rangle,$$

where the \hat{P} operator is defined in the $\{|t\rangle\}$ basis by $\langle t | \hat{P} | s \rangle = -i \frac{\partial}{\partial t} \delta(t-s)$. Equation (3.13) becomes

$$(3.16) \quad \int dt V_{e1}(q) = \frac{1}{2} \int dt \left\{ \langle t | \ln \left(\hat{P}^2 + \omega^2 + \frac{1}{m} \partial_q^2 U(q) \right) | t \rangle - \langle t | \ln \left(\hat{P}^2 + \omega^2 \right) | t \rangle \right\}.$$

With the help of the identity $\int dp |p\rangle \langle p| = 1$, where $\hat{P}|p\rangle = p|p\rangle$, we can write

$$(3.17) \quad \langle t | \ln \left(\hat{P}^2 + \omega^2 + \frac{1}{m} \partial_q^2 U(q) \right) | t \rangle = \frac{1}{2\pi} \int dp \ln \left(p^2 + \omega^2 + \frac{1}{m} \partial_q^2 U(q) \right).$$

The integral in the above expression can be evaluated exactly and from (3.16) we finally get

$$(3.18) \quad V_{e1}(q) = \frac{1}{2} \left(\sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q)} - \omega \right).$$

The determination of $Z_1(q)$ is more involved. From eq. (3.12) we see that $Z(q)$ is the coefficient of the term containing $\dot{q}(t)^2$ in the effective action. We can thus write

$$(3.19) \quad \int dt Z_1(q(t)) \dot{q}^2(t) = \ln \det \left[\frac{\delta^2 S_E[q]}{\delta q(t) \delta q(s)} \right] - \left(\ln \det \left[\frac{\delta^2 S_E[q_c]}{\delta q(t) \delta q(s)} \right] \right)_{q_c \rightarrow q(t)},$$

with the assumption that we consider in the r.h.s. only those terms with at most two time derivatives of $q(t)$. The first term in the r.h.s. of (3.19) is essentially the one-loop Euclidean effective action, while the second one comes from the effective potential. The second functional determinant in (3.19) has to be evaluated with a constant q_c which, at the end, must be replaced with $q(t)$. The terms due to the normalization of $Z_E[J]$, being common to both the effective action and the effective potential, cancel each other. Again we change the logarithm of the determinant into the trace of the logarithm and write the differential operators in Dirac notation. It is useful to introduce two operators, \hat{P} and \hat{T} , satisfying the commutation relation $[\hat{T}, \hat{P}] = i$, and with elements $\langle t | \hat{P} | s \rangle = -i \frac{\partial}{\partial t} \delta(t-s)$, $\langle p | \hat{T} | q \rangle = i \frac{\partial}{\partial p} \delta(p-q)$, where $|t\rangle, |s\rangle$ and $|p\rangle, |q\rangle$ are eigenstates of \hat{T} and \hat{P} , respectively. In addition, we write the difference of two logarithms of positive-definite operators in the parametric form

$$(3.20) \quad \ln \hat{A} - \ln \hat{B} = \int_0^\infty \frac{ds}{s} \left(e^{-\hat{B}s} - e^{-\hat{A}s} \right).$$

We then arrive at the following expression:

$$(3.21) \quad \int dt Z_1(q(t)) \dot{q}^2(t) = \int dt \langle t | \int_0^\infty \frac{ds}{s} e^{-[m\hat{P}^2 + m\omega^2 + \partial_q^2 U(q(t))]s} - e^{-[m\hat{P}^2 + m\omega^2 + \partial_q^2 U(q(\hat{T}))]s} | t \rangle.$$

Since we keep only terms at most quadratic in $\dot{q}(t)$, we can expand $\partial_q^2 U(q(\hat{T}))$ as follows:

$$(3.22) \quad \partial_q^2 U(q(\hat{T})) = \partial_q^2 U(q(t)) + \hat{Q}a(t) + \frac{1}{2} \hat{Q}^2 b(t),$$

where $\hat{Q} = \hat{T} - t$, $a(t) = \partial_t \partial_q^2 U(q(t))$ and $b(t) = \partial_t^2 \partial_q^2 U(q(t))$. All the terms proportional to \hat{Q}^n , with $n \geq 3$, are neglected since they do not contribute to the determination of $Z_1(q)$. The expressions for $\langle t | e^{-m\hat{P}^2 s} | t \rangle$ and for $\langle t | e^{-[m\hat{P}^2 + Qa(t) + \frac{1}{2} \hat{Q}^2 b(t)]s} | t \rangle$ are known [17] and can be inserted in (3.21). Finally we can expand the integrand in eq. (3.21) maintaining only the terms linear in $b(t)$ and at most quadratic in $a(t)$. Performing the integration over the variable s , we obtain

$$(3.23) \quad Z_1(q) = \frac{1}{32m^2} \frac{(\partial_q^3 U(q))^2}{\left(\omega^2 + \frac{1}{m} \partial_q^2 U(q)\right)^{\frac{5}{2}}}.$$

3'2. Derivative expansion as a WKB-like approximation. – The functional determinant in the one-loop term of the effective action (2.9) can be expressed by means of the Gelfand-Yaglom formula [18-20] as

$$(3.24) \quad \Gamma[q] = S[q] + \frac{i\hbar}{2} \lim_{\varepsilon \rightarrow 0^+} \lim_{T \rightarrow \infty} \ln \left(\frac{\omega_\varepsilon F_\varepsilon(T)}{\sin(2\omega_\varepsilon T)} \right) + \mathcal{O}(\hbar^2),$$

where $F_\varepsilon(t)$ is the solution of

$$(3.25) \quad \begin{cases} \ddot{F}_\varepsilon(t) + (\omega_\varepsilon^2 + \frac{1}{m} \partial_q^2 U(q(t))) F_\varepsilon(t) = 0, \\ F_\varepsilon(-T) = 0, \\ \dot{F}_\varepsilon(-T) = 1. \end{cases}$$

Note that the time variable appearing in the above equations is the real time. At first sight it might seem that, on account of the factor i in (3.24), the one-loop contribution to $\Gamma[q]$ is imaginary if $q(t)$ is real. Actually, the effect of the regularization $\omega \rightarrow \omega_\varepsilon$ is such that $\Gamma_1[q]$ has generally both a real and an imaginary part. As we shall see, the latter disappears if $q(t)$ varies slowly with time. Without the regularization the expression for $\Gamma_1[q]$ would be ill-defined, both numerator and denominator oscillating with T .

We obtain the derivative expansion of the effective action at order \hbar starting from eq. (3.24). For the moment we neglect the frequency regularization which we will reintroduce later. In order to deal with convergent integrals, we suppose that $q(t) = 0$ for $|t| > s$. At the end of the calculation, *i.e.*, after the limits $T \rightarrow \infty$ and $\varepsilon \rightarrow 0^+$ have been taken, we will let $s \rightarrow \infty$.

If we set $q(t) = Q(\rho t)$, $q(t)$ varies slowly if ρ is small. The expansion of $\Gamma[q]$ around $q(t)$ constant is therefore related to the asymptotic expansion of $F(t)$ for $\rho \rightarrow 0$. Introducing the variable $\tau = \rho t$ and setting $\Phi(\tau) \equiv F(\tau/\rho)$ and $k^2(\tau) \equiv \omega^2 + (1/m) \partial_q^2 U(Q(\tau))$, eq. (3.25) becomes

$$(3.26) \quad \begin{cases} \frac{d^2}{d\tau^2} \Phi(\tau) + \frac{1}{\rho^2} k^2(\tau) \Phi(\tau) = 0, \\ \Phi(-\rho T) = 0, \\ \frac{d}{d\tau} \Phi(-\rho T) = \frac{1}{\rho}. \end{cases}$$

An approximate solution of (3.26) for $\rho \rightarrow 0$ can be found by means of the WKB method [21] with the parameter ρ playing the role of \hbar . The N -th order solution is

$$(3.27) \quad \Phi_{2N}(\tau) = \frac{1}{\sqrt{W_{2N}(\tau)}} \left[c_+ e^{\frac{i}{\rho} \int^\tau W_{2N}(\tau') d\tau'} + c_- e^{-\frac{i}{\rho} \int^\tau W_{2N}(\tau') d\tau'} \right],$$

where $W_{2N}(\tau)$ is obtained, neglecting all the terms of order higher than ρ^{2N} , from the

recursive relation

$$(3.28) \quad W_{2N}(\tau) = \left[k^2(\tau) + \rho^2 \sqrt{W_{2(N-1)}(\tau)} \frac{d^2}{d\tau^2} \left(\frac{1}{\sqrt{W_{2(N-1)}(\tau)}} \right) \right]^{\frac{1}{2}},$$

with

$$(3.29) \quad W_0(\tau) = k(\tau).$$

Imposing the initial conditions and going back to the variable t , we find that at the lowest order the solution of (3.25) is

$$(3.30) \quad F_0(t) = \frac{e^{i \int_{-T}^t dt' \sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q(t'))}} - e^{-i \int_{-T}^t dt' \sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q(t'))}}}{2i \sqrt{\omega \sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q(t))}}}.$$

When the regularization $\omega \rightarrow \omega_\epsilon$ is reintroduced and $F_0(t)$ is evaluated at the time T , the second exponential, proportional to $e^{-2i\omega_\epsilon(T-s)}$, vanishes for large T and can be neglected, since the limit $T \rightarrow \infty$ has to be performed before the limit $\epsilon \rightarrow 0^+$. We obtain therefore

$$(3.31) \quad \Gamma[q] \simeq S[q] - \frac{\hbar}{2} \int_{-s}^s dt \left(\sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q(t))} - \omega \right).$$

Recalling (3.2), the first quantum correction to the classical potential is

$$(3.32) \quad V_{e1}(q) = \frac{1}{2} \left(\sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q)} - \omega \right).$$

The next order of the WKB approximation gives

$$(3.33) \quad \Gamma[q] \simeq S[q] - \frac{\hbar}{2} \int_{-s}^s dt \left(\sqrt{\omega^2 + \frac{1}{m} \partial_q^2 U(q(t))} - \omega \right) + \frac{\hbar}{2} \int_{-s}^s dt \frac{1}{32m^2} \frac{(\partial_q^3 U(q(t)))^2}{(\omega^2 + \frac{1}{m} \partial_q^2 U(q(t)))^{\frac{5}{2}}} \dot{q}^2(t),$$

which implies

$$(3.34) \quad Z_1(q) = \frac{1}{32m^2} \frac{(\partial_q^3 U(q))^2}{(\omega^2 + \frac{1}{m} \partial_q^2 U(q))^{\frac{5}{2}}}.$$

Equations (3.32) and (3.34) agree with the results found in subsect. 3'1.

If the classical potential $V(q)$ is not everywhere convex, in the regions where $\omega^2 + \frac{1}{m}\partial_q^2 U(q)$ is negative the effective potential $V_{e1}(q)$ and $Z_1(q)$ become imaginary. Moreover, $Z_1(q)$ has a divergence at the points where $\omega^2 + \frac{1}{m}\partial_q^2 U(q) = 0$ and this corresponds to the fact that the WKB approximation loses its validity near the turning points $k^2(\tau) = 0$.

It is clear that the N -th order WKB approximation for $\Phi(\tau)$ corresponds to the derivative expansion of $\Gamma_1[q]$ at order $2N$. One can also check that no terms with an odd number of derivatives appear. The connection to the WKB approximation also shows, as previously stated, that the derivative expansion has only an asymptotic validity for $\dot{q} \rightarrow 0$.

From eq. (3.24) it is clear that if $q(t)$ is real, $\Gamma[q]$ up to one-loop order is not necessarily real. However, from eq. (3.28) we see that, if the classical potential is everywhere convex, all the terms of the derivative expansion of the effective action are real if $q(t)$ is real. The contradiction is only apparent. It can be seen that the imaginary part of $\Gamma[q]$ is due to singularities in the Green functions which do not contribute to the derivative expansion.

In conclusion, in the case of vanishing external source $J(t) = 0$ the DE2 approximation at order \hbar of eq. (1.8) reads

$$(3.35) \quad (m + \hbar Z_1(q(t))) \ddot{q}(t) + \frac{\hbar}{2} \partial_q Z_1(q(t)) \dot{q}^2(t) = -\partial_q (V(q(t)) + \hbar V_{e1}(q(t))) .$$

We discuss the validity of this equation in the case $V(q) = \frac{1}{2}m\omega^2 q^2 + \frac{g}{4!}q^4$. Equation (3.35) is approximate both because the DE2 approximation is adopted and because the terms of order higher than \hbar are neglected. For a solution $q(t)$ of amplitude A these two approximations are valid if

$$(3.36) \quad \frac{\frac{g}{4!}A^4}{\frac{1}{2}m\omega^2 A^2} \ll 1$$

and

$$(3.37) \quad \frac{\hbar g}{m^2 \omega^3} \ll 1 ,$$

respectively. Under these conditions the solutions of eqs. (3.35) and (1.8) remain close for a time t satisfying

$$(3.38) \quad \omega t \frac{\hbar g}{m^2 \omega^3} \frac{\frac{g}{4!}A^4}{\frac{1}{2}m\omega^2 A^2} \ll 1 .$$

PART II

4. - 2D anharmonic oscillator: classical

Classical systems with more than one degree of freedom present a richer variety of phenomena and in particular they may exhibit chaotic behavior for $J = 0$. The formalism

described in Part I can be generalized without difficulties to many degrees of freedom. Here we study the system whose Lagrangian is [22]

$$(4.1) \quad L(\dot{q}_1, \dot{q}_2, q_1, q_2) = \frac{1}{2}m(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{2}m\omega^2(q_1^2 + q_2^2) - gq_1^2q_2^2.$$

Apparently, the system has four free parameters: m , ω , g and the energy E . However, the rescaling $t \rightarrow t/\omega$, $q_i \rightarrow q_i\sqrt{m\omega^2/g}$, $\dot{q}_i \rightarrow \dot{q}_i\sqrt{m\omega^4/g}$, for $i = 1, 2$, yields

$$(4.2) \quad L \rightarrow \frac{m^2\omega^4}{g} \left[\frac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{2}(q_1^2 + q_2^2) - q_1^2q_2^2 \right],$$

where, now, \dot{q}_i , q_i and t are dimensionless. The energy of the system (4.1) is then $E = (m^2\omega^4/g)\varepsilon$, where ε is the dimensionless energy of the rescaled Lagrangian $L = \frac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{2}(q_1^2 + q_2^2) - q_1^2q_2^2$. We conclude that ε is the unique free parameter of the system under consideration.

The rescaled equations of motion

$$(4.3) \quad \ddot{q}_1 = -q_1(1 + 2q_2^2),$$

$$(4.4) \quad \ddot{q}_2 = -q_2(1 + 2q_1^2),$$

have been numerically integrated using a standard fourth-order Runge-Kutta method [23]. A qualitative description of the corresponding solutions has been achieved by constructing the surfaces of section (Poincaré sections) [24] and evaluating the largest Lyapunov exponent [25]. The degree of chaoticity of the system can be summarized by the fraction of regular orbits on the energy shell as a function of the dimensionless energy ε . This fraction is close to unity for $\varepsilon \lesssim 0.75$ and vanishes exponentially for $\varepsilon \gtrsim 0.75$. The border value $\varepsilon = 0.75$ agrees with that obtained from the Toda criterion [26]. In our system, the sign of the curvature of the energy surface where the motion takes place is given by $\text{sign}(\det \text{He}(V))$, where $\text{He}(V)$ is the Hessian of $V = (q_1^2 + q_2^2)/2 + q_1^2q_2^2$, i.e., $\text{He}(V)_{ij} = \frac{\partial^2 V}{\partial q_i \partial q_j}$. This sign changes from positive to negative at $\varepsilon = 3/4$. It is worth noting that the Toda criterion does not detect the first occurrence of chaos in the Poincaré sections [27, 28]. Nevertheless, when $\varepsilon > 3/4$ we find that chaotic orbits are spread all over the sections. For $\varepsilon < 3/4$, the irregular orbits are located in a small region of the Poincaré sections, namely near a perturbed separatrix where chaos initially appears as a consequence of the mechanism of the heteroclinic intersection [29].

5. – 2D anharmonic oscillator: quantum

In the semiclassical and local approximations, the quantum system corresponding to the 2D anharmonic oscillator introduced in the previous section is described by an effective Lagrangian (effective action density)

$$(5.1) \quad L_e(\dot{\mathbf{q}}, \mathbf{q}) = \frac{1}{2}Z_{ij}(\mathbf{q})\dot{q}_i\dot{q}_j - V_e(\mathbf{q}),$$

where $\mathbf{q} = (q_1, q_2)$ and $\dot{\mathbf{q}} = (\dot{q}_1, \dot{q}_2)$. In the rescaled variables used in the classical case, we have

$$(5.2) \quad V_e = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2^2 + \frac{\gamma}{2} \left(\sqrt{\Lambda_+} + \sqrt{\Lambda_-} - 2 \right),$$

$$(5.3) \quad Z_{11} = 1 + \gamma \left\{ \frac{q_1^2}{8} \left[\frac{(1+\eta)^2}{\Lambda_+^{5/2}} + \frac{(1-\eta)^2}{\Lambda_-^{5/2}} \right] + 8q_2^2 \zeta \right\},$$

$$(5.4) \quad Z_{12} = Z_{21} = \gamma \left\{ \frac{q_1 q_2}{8} \left[\frac{(1+\eta)(1+\xi)}{\Lambda_+^{5/2}} + \frac{(1-\eta)(1-\xi)}{\Lambda_-^{5/2}} \right] + 8q_1 q_2 \zeta \right\},$$

$$(5.5) \quad Z_{22} = 1 + \gamma \left\{ \frac{q_2^2}{8} \left[\frac{(1+\xi)^2}{\Lambda_+^{5/2}} + \frac{(1-\xi)^2}{\Lambda_-^{5/2}} \right] + 8q_1^2 \zeta \right\},$$

where

$$(5.6) \quad \Lambda_{\pm} = 1 + q_1^2 + q_2^2 \pm \Sigma,$$

$$(5.7) \quad \Sigma = \sqrt{q_1^4 + q_2^4 + 14q_1^2 q_2^2},$$

$$(5.8) \quad \eta = (q_1^2 + 7q_2^2)/\Sigma,$$

$$(5.9) \quad \xi = (q_2^2 + 7q_1^2)/\Sigma$$

and

$$(5.10) \quad \zeta = \frac{[(q_1^2 + q_2^2)/\Sigma]^2}{[\sqrt{\Lambda_+ \Lambda_-} (\sqrt{\Lambda_+} + \sqrt{\Lambda_-})^3]}.$$

With respect to the classical system, we have an additional parameter $\gamma = \hbar g/m^2 \omega^3$ which arises from rescaling \hbar . It can be seen that, when \mathbf{q} varies, the effective potential and the symmetric kinetic matrix Z_{ij} can be singular or complex-valued, unless \mathbf{q} is constrained inside a certain region. If we limit ourselves to the region where the effective potential, in the considered approximation, is convex, then L_e is well defined.

The rescaled equations of motion corresponding to the Lagrangian (5.1)

$$(5.11) \quad Z_{11}\ddot{q}_1 + Z_{12}\ddot{q}_2 = -\frac{1}{2} \frac{\partial Z_{11}}{\partial q_1} \dot{q}_1 \dot{q}_1 - \frac{\partial Z_{11}}{\partial q_2} \dot{q}_1 \dot{q}_2 + \left(\frac{1}{2} \frac{\partial Z_{22}}{\partial q_1} - \frac{\partial Z_{12}}{\partial q_2} \right) \dot{q}_2 \dot{q}_2 - \frac{\partial V_e}{\partial q_1},$$

$$(5.12) \quad Z_{12}\ddot{q}_1 + Z_{22}\ddot{q}_2 = -\frac{1}{2} \frac{\partial Z_{22}}{\partial q_2} \dot{q}_2 \dot{q}_2 - \frac{\partial Z_{22}}{\partial q_1} \dot{q}_1 \dot{q}_2 + \left(\frac{1}{2} \frac{\partial Z_{11}}{\partial q_2} - \frac{\partial Z_{12}}{\partial q_1} \right) \dot{q}_1 \dot{q}_1 - \frac{\partial V_e}{\partial q_2},$$

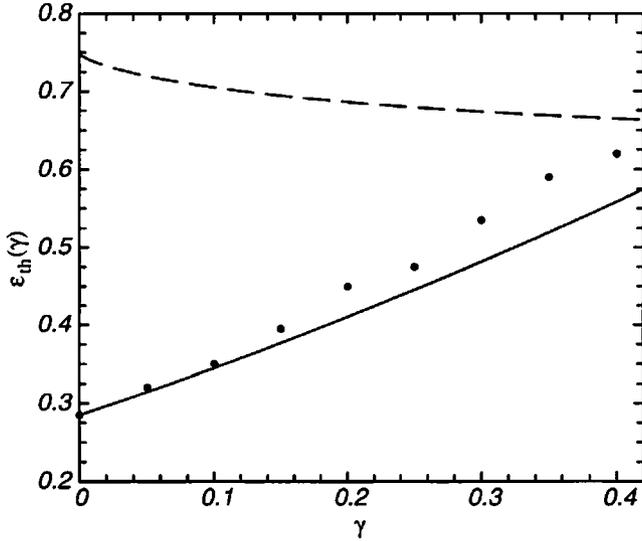


Fig. 1. - Threshold energy ε_{th} at which chaotic behavior shows up in the Poincaré sections of the effective system *vs.* $\gamma = \hbar g/m^2\omega^3$. The solid line is the theoretical estimate $\varepsilon_{\text{th}}(\gamma) = \varepsilon_{\text{th}}(0)(1 + \gamma)^2$. The dashed line represents the maximal energy ε_m below which the effective potential is everywhere convex.

have been numerically solved as in the classical case. These equations are nonlinear and may lead to a chaotic evolution. However, due to the fact that no chaotic behavior is allowed at quantum level, we expect a reduction of chaoticity in the effective system with respect to the classical one. This reduction should depend on the value of the parameter γ , the value $\gamma = 0$ corresponding to the classical system. In fig. 1 we illustrate, for different values of γ , the smallest energy (threshold energy) ε_{th} at which chaos shows up in the Poincaré sections of the effective system [30]. We see that ε_{th} increases with increasing γ . This behavior can be explained as follows. Let us consider the Taylor expansion of the effective Lagrangian around $\mathbf{q} = \mathbf{0}$ and $\dot{\mathbf{q}} = \mathbf{0}$. Up to quadratic terms, we obtain $L_e(\dot{\mathbf{q}}, \mathbf{q}) = \frac{1}{2}(\dot{q}_1^2 + \dot{q}_2^2) - \frac{1}{2}(1 + \gamma)(q_1^2 + q_2^2) + \dots$. In terms of unrescaled variables this corresponds to a shift of the classical frequency $\omega \rightarrow \omega\sqrt{1 + \gamma}$. The rescaled energy $\varepsilon = E/(m^2\omega^4/g)$ picks up a factor $(1 + \gamma)^2$. This means that if $\varepsilon_{\text{th}}(0)$ denotes the threshold energy at $\gamma = 0$, we should have approximately $\varepsilon_{\text{th}}(\gamma) = \varepsilon_{\text{th}}(0)(1 + \gamma)^2$. This prediction is well confirmed in fig. 1. It is easy to see that the increase of the threshold for chaos holds under the general condition that V_{e1} is convex, which, in turn, amounts to

$$(5.13) \quad \text{He} \left(\text{tr} (\text{He}(V))^{\frac{1}{2}} \right) > 0,$$

where V is the classical potential. These results parallel those obtained in [31] for the N -component ϕ^4 oscillators where the mean field plays the role of classical system.

The range of γ values explored in fig. 1 includes situations encountered in molecular

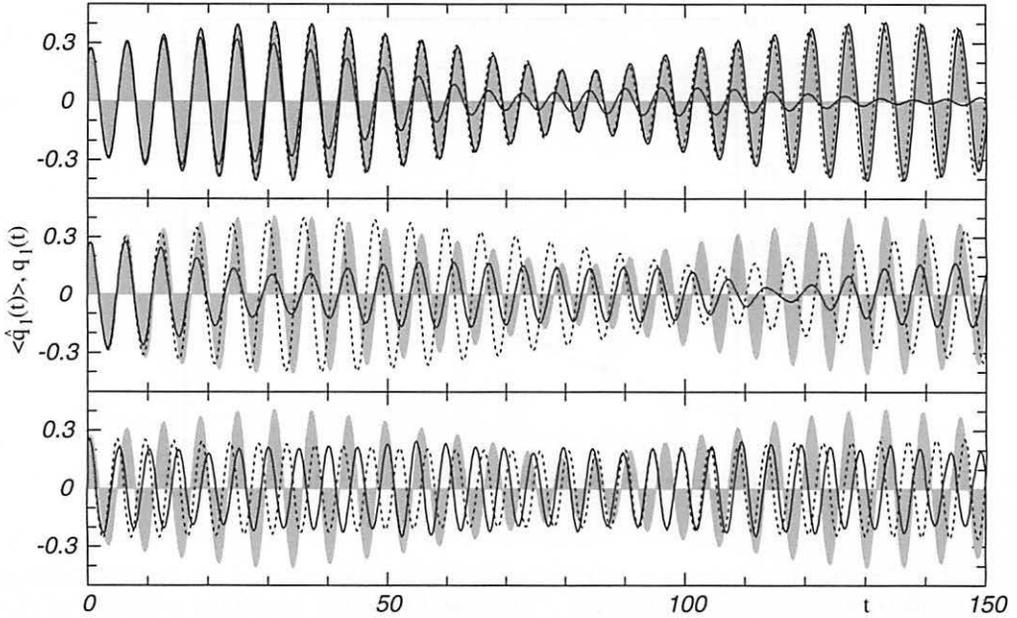


Fig. 2. – Time evolution of the expectation value of the position operator $\langle \hat{q}_1(t) \rangle$ (solid line) compared with the classical (shaded area) and the effective (dots) solutions $q_1(t)$. The three panels correspond, from top to bottom, to $\gamma = 0.01$, 0.1 , and 1 , respectively. In all cases we have a classical rescaled energy $\varepsilon = 0.1$.

physics. In fact, the vibrational Hamiltonian of diatomic molecules is often assumed as a quartic oscillator and using the numerical values of ref. [32] obtained from spectroscopic data, we find that $10^{-4} \lesssim \gamma \lesssim 10^{-1}$.

In the following we compare the solutions of the local effective equations with the classical solutions and with the exact quantum evolutions of coherent states centered at the initial conditions of the local equations. We have already remarked that the initial conditions for the classical and the effective dynamics do not determine completely the initial wave function but provide only a constraint. Therefore the choice of the initial wave function is not unique. A natural choice is represented by a harmonic coherent state which is parametrized by the expectation value of position and momentum. In fact, by performing simulations with initial wave functions which satisfy the proper constraints but are of arbitrary shape, we find that the agreement between the effective and quantum dynamics is very poor when the shape of the initial wave function differs substantially from that of a coherent state.

In rescaled units, the exact quantum dynamics is defined by the Schrödinger equation

$$(5.14) \quad i\gamma \frac{\partial}{\partial t} \psi(q_1, q_2, t) = \hat{H} \psi(q_1, q_2, t),$$

with

$$(5.15) \quad \hat{H} = \frac{1}{2}(\hat{p}_1^2 + \hat{p}_2^2) + \frac{1}{2}(\hat{q}_1^2 + \hat{q}_2^2) + \hat{q}_1^2 \hat{q}_2^2,$$

where $\hat{p}_j = -i\gamma \frac{\partial}{\partial q_j}$ and $\hat{q}_j = q_j$, for $j = 1, 2$, are the rescaled momentum and position operators. In order to solve (5.14), we represent the rescaled Hamiltonian operator (5.15) in the basis of the eigenstates of the associated 2D harmonic oscillator $\hat{H}_0 = \frac{1}{2}(\hat{p}_1^2 + \hat{p}_2^2) + \frac{1}{2}(\hat{q}_1^2 + \hat{q}_2^2)$. The corresponding infinite matrix is truncated and then diagonalized with standard techniques [23]. As initial state we choose the coherent state

$$(5.16) \quad |p'_1 q'_1 p'_2 q'_2\rangle = e^{-\frac{i}{\gamma} q'_1 \hat{p}_1} e^{\frac{i}{\gamma} p'_1 \hat{q}_1} e^{-\frac{i}{\gamma} q'_2 \hat{p}_2} e^{\frac{i}{\gamma} p'_2 \hat{q}_2} |0_0\rangle,$$

where $|0_0\rangle$ is the ground state of \hat{H}_0 . The parameters $p'_1 q'_1 p'_2 q'_2$ are taken equal to the initial conditions used in the integration of the classical and effective Lagrangians.

In fig. 2 we show the evolution of $\langle \hat{q}_1(t) \rangle$ in comparison with the corresponding classical and effective solutions. The three panels correspond, from top to bottom, to increasing values of γ at constant dimensionless classical energies ε . Note that the initial coherent state depends on γ .

Figure 2 shows that by increasing γ there is a crossover in the behavior of the solution of the effective dynamics. At small γ the effective solution stays close to the classical one, while for larger γ it reproduces qualitatively the shape of the quantum evolution. We notice that in the large- γ region the quantum and the effective dynamics do not show, on the time scale considered, a transfer of energy among the degrees of freedom as the classical solution. This seems to indicate that the quantum corrections in the effective dynamics have an anti-mixing influence that regularizes the motion. Of course, over longer times a transfer of energy takes place also in the quantum and effective evolutions. The theoretical interpretation of these results will be discussed elsewhere.

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