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Physica E 29 (2005) 435–441
PHYSICA E
www.elsevier.com/locate/physe

Quantum ratchets at high temperatures

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Available online 1 July 2005

Abstract

Using the continued-fraction method we solve the *Caldeira–Leggett* master equation in the phase–space (*Wigner*) representation to study quantum ratchets. Broken spatial symmetry, irreversibility and periodic forcing allows for a net current in these systems. We calculate this current as a function of the force under adiabatic forcing. Starting from the classical limit we make the system quantal. In the quantum regime, tunnel events and over-barrier wave reflection phenomena modify the classical result. Finally, using the phase–space formalism we give some insights about the decoherence in these systems.

PACS: 05.40.−a; 03.65.Yz; 05.60.−k

Keywords: Brownian motion; Transport; Open quantum systems; Decoherence; Phase–space methods

1. Introduction

Transport properties in periodical structures with broken spatial symmetry (ratchet systems) have attracted a lot of attention in the past decade [1]. These systems, under out-of-equilibrium conditions, can display net current even when the time and space average of all applied forces is zero. For this reason, these systems are also called *Brownian* motors [2]. Realizations of *Brownian* motors can be found, for example, in biological and condensed matter systems [3].

In the classical limit, the dynamics is governed by classical *Langevin* or equivalently *Fokker–Planck* equations. This limit has been extensively studied in the recent past, establishing the main phenomenologies of the ratchet effect (non-vanishing rectified current, etc.) [1]. The inclusion of quantum fluctuations in the system enriches the ratchet phenomenology [4]. However, the difficulties to deal with quantum dissipative systems, make their study harder and one finds less works on this regime [3–9].

Recently, it has been shown that it is possible to solve quantum master equations using continued fraction methods [10,11]. Such master equations are the "quantum generalization" of the classical

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1386-9477/$ - see front matter
doi:10.1016/j.physe.2005.05.043

Fokker–Planck equations for some ranges of the parameters (weak coupling, high temperature, etc.). Adapting this technique from the classical case [10], the authors of Ref. [11] have studied the ratchet effect as a function of the temperature. In this work we extend the study to the force dependence of the rectified velocities in the high temperature/weak coupling regime.

2. Theoretical framework

The out-of-equilibrium dynamics of classical systems is well established since a century ago with the seminal works of *Einstein* and *Langevin*. The *Langevin* (*Fokker–Planck*) equations describe satisfactorily the stochastic behavior of these systems. However, their quantization represents, in most cases, a difficult task [12]. The most satisfactory approach consists of quantizing the Hamiltonian of the system plus its environment. The minimal bath model is a large collection of harmonic oscillators. This approach, in the classical limit, recovers the *Langevin* description of open systems.

In the quantum realm, a closed evolution equation is not possible in the general case. This is mainly due the non-*Markovian* nature of the quantum correlations. Nevertheless, under some approximations, it is possible to derive a *Markovian* quantum master equation. Thus, it is typically assumed that the relaxation times are much longer that the quantum correlations of the bath,

$$\frac{1}{\gamma} \gg \frac{\hbar}{T}, \tag{1}$$

with γ the damping parameter measuring the strength of the coupling to the bath. Under these conditions (high temperatures and/or weak coupling) the evolution is given by the celebrated *Caldeira–Leggett* master equation [13],

$$\mathrm{i}\hbar\partial_t\varrho = [H_\mathrm{S}, \varrho] + \frac{\gamma}{2\hbar}[x, \{p, \varrho\}] - \frac{\mathrm{i}\gamma M k_\mathrm{B} T}{\hbar}[x, [x, \varrho]]. \tag{2}$$

Here ϱ is the reduced density matrix, obtained after tracing out the environmental degrees of freedom and H_S is the system Hamiltonian, in our case $H_\mathrm{S} = p^2/2m + V(x)$. The first term in (2) gives the unitary evolution, the second yields the dissipation and the last is responsible for the diffusion.

An alternative description of quantum systems is provided by the phase–space (*Wigner*) formalism. The central object is the *Wigner* function, defined in terms of the density matrix as [14]

$$W(x,p) = \frac{1}{2\pi\hbar}\int \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}py/\hbar}\varrho(x + y/2, x - y/2). \tag{3}$$

This representation not only gives a phase–space description for quantum systems, but it allows to extend classical concepts and tools into the quantum domain. Besides, it facilitates the study of quantum analogues to classical phenomena (quantum chaos, phase–space trajectories, etc.) and provides a natural quantum–classical connection.

In the *Wigner* representation the master equation (2), can be written as

$$\partial_t W = \left[-p\partial_x + V'\partial_p + \gamma_T\,\partial_p\,(p + \partial_p) + \sum_{s=1}^{\infty} \kappa^{(s)}\, V^{(2s+1)}(x)\,\partial_p^{(2s+1)} \right] W. \tag{4}$$

The first two terms correspond to the *Poisson* bracket (*Liouville* equation). This *Poisson* bracket plus the third term yields the classical *Fokker–Planck* equation, evidencing the classical character of the noise and relaxation. The last term is purely quantal and comes from the unitary evolution of the closed system (*Wigner–Moyal* bracket).

Eq. (4) is written in dimensionless form [11]. The variables have been scaled with help from a reference length x_0, mass M and frequency Ω_0. For example, action variables are scaled by the characteristic action $S_0 = M\Omega_0 x_0^2$, energy by $E_0 = M\Omega_0^2 x_0^2$, etc. Then the coefficient in the quantum sum is given in terms of the *de Broglie* wavelength by,

$$\kappa^{(s)} = (-1)^s \lambda_{\mathrm{dB}}^{2s}/(2s+1)!. \tag{5}$$

Besides, $\gamma_T \propto \gamma\sqrt{T}$ and $\hbar$ is introduced in terms of S_0 via the quantum parameter K:

$$\hbar/S_0 = 2\pi/K \quad \text{and} \quad \lambda_{\mathrm{dB}} \propto 1/K. \tag{6}$$

Note that the classical limit is naturally recovered letting $K \to \infty$.

To conclude, the calculation of observables in the *Wigner* formalism is an example of extension of classical methods to the quantum domain. The quantum mechanical expectation value is obtained via $W(x,p)$ as a classical "average"

$$\langle A \rangle \equiv \mathrm{Tr}(\hat{\varrho}\,\hat{A}) = \int \mathrm{d}x\,\mathrm{d}p\, W(x,p) A(x,p), \tag{7}$$

with $A(x,p)$ the classical observable corresponding to the operator $\hat{A}$ (via Weyl's rule).

3. Continued-fraction approach

A suitable non-perturbative technique to solve classical *Fokker–Planck* equations of systems with a few variables is the continued-fraction method [15]. This is a special case of the expansion into complete sets (Grad's) method to solve kinetic equations in statistical mechanics. The technique had already been adapted to quantum dissipative systems in studies of spins and quantum non-linear optics. Recently, this method has been extended to quantum Brownian motion problems described by *Caldeira–Leggett* type equations exploiting the *Fokker–Planck*-like structure of the quantum master equation in the *Wigner* representation [10,11].

The idea of the method consists of expanding the desired solution W of the dynamical equation ($\partial_t W = \mathscr{L} W$) into an appropriate basis of functions. The equations for the expansion coefficients (C_i) have then the form of a system of coupled differential equations, say

$$\dot{C}_j = \sum_{i=-I}^{I} Q_{j,j+i} C_{j+i}. \tag{8}$$

The goal is to find a basis in which the range of index coupling I of the coefficients C_i is as short as possible. Indeed, for finite coupling range ($I < \infty$) the differential recurrence relation (8) can be solved by iterating a simple algorithm, the structure of which is like that of a continued fraction,

$$C = \cfrac{p_1}{q_1 + \cfrac{p_2}{q_2 + \cfrac{p_3}{q_3 + \cdots}}}. \tag{9}$$

In the case of the *Caldeira–Leggett* equation the expansion is on an x and p basis:

$$W(x,p) \propto \sum_{n,\alpha} C_n^{\alpha} u_{\alpha}(x) \psi_n(p). \tag{10}$$

Then, the recurrence (8) is replaced by a two index one, $\dot{C}_n^{\alpha} = \sum_{m,\beta} Q_{\alpha\beta}^{nm} C_m^{\beta}$, which can be transformed into a one index recurrence introducing appropriate vectors and matrices:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{C}_{\alpha} = \sum_{i=-I}^{i=I} \mathbb{Q}_{\alpha,\alpha+i} \mathbf{C}_{\alpha+i}. \tag{11}$$

This recurrence relation can be solved with *matrix* continued-fraction methods. In [11] the explicit form of matrices $\mathbb{Q}$ was derived. In particular, for periodic potentials $[V(x) = V(x+L)]$ explicit recurrence relations were constructed using *Hermite* functions for the momentum basis and *plane waves* ($u_{\alpha} \propto \mathrm{e}^{\mathrm{i}\alpha x}$) for the position basis. This choice provides a finite coupling range I, making possible its solution by the above-sketched method.

Solving the quantum master equation in this way, the *Wigner* function is obtained (i.e., the density matrix), so any observable can be calculated.

4. Results for quantum ratchets

In the context of *Brownian* motion, the simplest model that allows for broken spatial symmetry is the two harmonic potential,

$$V(x) = -V_0[\sin x + (r/2)\sin(2x)], \tag{12}$$

(other ratchet systems can be modelized using tight binding Hamiltonians, rotational spin systems, optical lattices, etc.). The potential (12) has a steeper side to the left, which we will call the "hard" direction, while we will refer to the other direction as the "easy" one (to the right).

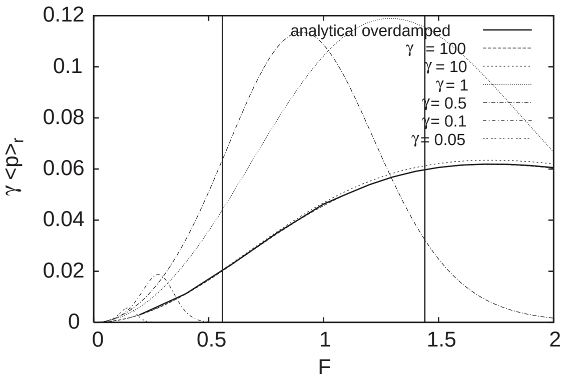

Fig. 1. Rectified velocity vs. force for a classical particle in a ratchet potential (a square wave $\pm F$ is used). Results are shown for various values of the damping γ, as well as the analytical overdamped result. The vertical lines mark the two critical forces in the deterministic case $F_{\mathrm{c}}^{\pm}$ [Eq. (14)].

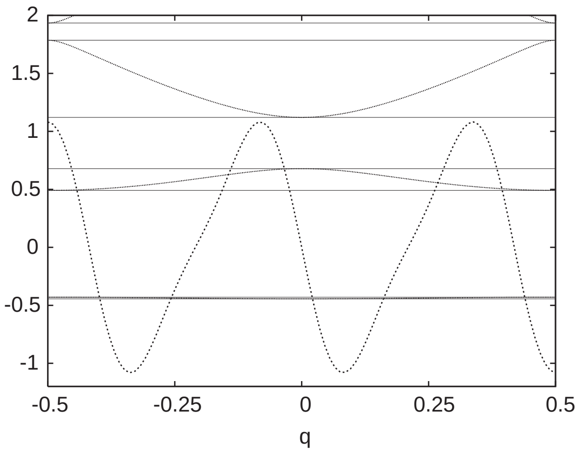

Fig. 2. Energy bands for $K=5$. The potential profile $V(x) = -V_0[\sin x + (r/2)\sin(2x)]$ is plotted (dashes) to show the number of bands below the barrier. In the calculations, we use $r = 0.44$ which smoothens the potential profile.

Using the continued-fraction technique, we can solve the *Caldeira– Leggett* equation. In particular, for the case of the two harmonic potential (12) the coupling range I is 2 (i.e., equal to the number of harmonics of the potential).

Our purpose is to study the transport properties in this system. We limit ourselves to the case of a square-wave force switching alternatively between $\pm F$ with a period $2\pi/\omega$. Then the rectified velocity is defined as,

$$\gamma\langle p\rangle_{\mathrm{r}} = \gamma\langle p\rangle_{+F} + \gamma\langle p\rangle_{-F}. \tag{13}$$

As we consider adiabatic conditions ($\omega \to 0$), the $\langle p\rangle_{\pm F}$ are the corresponding stationary velocities; they can be calculated immediately with the general result (7).

In Ref. [11] we considered the temperature dependence of the ratchet current. In this article, we study the force dependence of $\gamma\langle p\rangle_{\mathrm{r}}$ at fixed temperature. A high enough temperature is chosen to circumvent validity problems of the master equation (see Eq. (1) and discussion below).

4.1. Classical limit

First, it is convenient to understand the classical phenomenology. We plot in Fig. 1 the effect of finite inertia on the curves $\gamma\langle p\rangle_{\mathrm{r}}$ vs. F at a fixed temperature $k_{\mathrm{B}}T/E_0 = 1$.

The results obtained can be summarized as follows: (i) the rectified velocity is positive, i.e., the net drift is to the "easy" side; (ii) at high γ the results converge to the known overdamped analytical result; (iii) finite inertia (γ) shifts the curves to lower forces and narrows them; (iv) at low enough damping the net current drops to zero.

There are two main points to be understood here: the dependence on γ of the efficiency of the rectification and the window of forces where it occurs. Recall that in the zero noise limit ($T=0$), there exist two critical forces (for $r > 1/4$),

$$F_{\mathrm{c}}^{-}/V_0 = 1 + r, \quad F_{\mathrm{c}}^{+}/V_0 = 1 - r, \tag{14}$$

where $F_{\mathrm{c}}^{\pm}/V_0$ are the critical forces for barrier disappearance to the right and left sides. In our case, $r = 0.44$, then $F_{\mathrm{c}}^{-}/V_0 > F_{\mathrm{c}}^{+}/V_0$. Thus, in the $T=0$ limit we expect a current to the right (i.e., positive).

Borromeo et al. studied the classical inertial, deterministic ($T=0$) case [16]. They found that the net current starts at F_{c}^{+}/V_0. Then rectification grows quickly with F, up to F_{c}^{-}/V_0. From this force the rectification starts to decrease with F, tending to zero at large forces. They also observed that inertia narrows the curves, and fits them to the window $(F_{\mathrm{c}}^{+}/V_0, F_{\mathrm{c}}^{-}/V_0)$. In addition, for intermediate damping the ratchet efficiency grows inversely proportional to the damping. Finally, at very low damping the rectified velocity drops to zero. Thus, our findings agree with the efficiency and narrowing characteristics of Ref. [16] for the noiseless limit. Nevertheless the temperature smoothens the curves in our case, allowing for rectified velocity below F_c^+.

This range below F_c^+ is indeed quite rich already in the $T \to 0$ limit. There are two more characteristic forces $F_1(\gamma)$ and $F_2(\gamma)$ ($F_1 < F_2 < F_c$). Below F_1 the locked solution ($\langle p \rangle \simeq 0$) is the attractor globally stable. Above F_2 the stable attractor is the running solution ($\langle p \rangle \simeq F/\gamma$). Between F_1 and F_2 there exist bistability between these solutions. However, both for locked and running solutions there is little asymmetry in the response [as then $\langle p \rangle$ is nearly independent of $V(x)$]. Therefore, the asymmetry in the response concentrates in the range $F_1 < F < F_2$. Then, since both F_1 and F_2 decrease with γ [15, p. 330], the window with the maximum rectification is shifted to lower F as γ is decreased, in accordance with our results.

4.2. Quantum corrections

After the exploration of the classical limit, we proceed to make the system quantal, by decreasing K (see Section 2), and see how this affects the ratchet effect. The physical meaning of K can be seen calculating the bands of the closed system, which depend only on K [11]. The number of bands grows with K (as a rule of thumb the number of bands below the potential is approximately $K/2$) while the bandwidth increases with decreasing K. We plot in Fig. 2 the bands for the case $K = 5$.

We show results for the rectified current $\gamma\langle p \rangle_r$ in Fig. 3. We present curves at $k_BT/E_0 = 1$ and $\gamma = 0.05$ for different values of K. It is observed that the deviation from the classical case is systematic in K. First, we find a reduction of the ratchet effect at low forces. The reduction continues at intermediate forces, while at high forces an enhancement is observed, with respect to the classical case. Finally, a slight shift of the peaks of the curves to higher forces is found as K is decreased.

The reduction/enhancement of the rectified velocity with respect to the classical limit was already investigated in [11]. These deviations can be understood in terms of quasiclassical corrections to classical transport, which is modified by tunnel events and over-barrier wave reflection (reflection of particles with energy above the barrier; those energies are attained by thermal activation). Modeling with an asymmetric *saw tooth* potential one finds that tunnel events are more frequent in the hard direction than in the easy one for moderate to weak amplitude forces (leading to reduction of the ratchet effect) [1,11]. On the contrary, the phenomenon of the wave reflection is less intense in the easy direction [11].

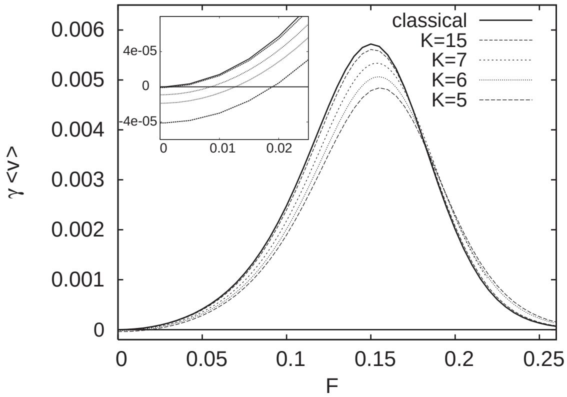

Fig. 3. Rectified velocity vs. force for a quantum particle in a ratchet potential (excited with $\pm F$). Results are shown for various values of the quantumness parameter K (see main text). The damping and temperature are fixed at $\gamma = 0.05$ and $k_BT/E_0 = 1$. We show for reference the classical case (solid). Inset: Amplification of the very low force range. A small negative rectified current is observed at $F = 0$ for the quantum curves.

In particular, at $F \simeq \gamma$ we obtained in Ref. [11] that, depending on the inertia and temperature, the reduction/enhancement is a consequence of the "competition" of tunnel events and wave reflection. Increasing the force both the contributions of wave reflection and tunnel transmission grow [11, Appendix F]. However, wave reflection grows like $\sim F$, while tunnel transmission goes exponentially with F. Thus, when $F > \gamma$, but not too high, tunnel contributions are favored more than wave reflection. As a consequence, one finds a reduction of the rectified velocity in the range of inertia where an enhancement at $F \lesssim \gamma$ takes place. Finally, at high enough forces the barrier is sufficiently lowered. Then, there are many particles with energies above the barrier (experiencing wave reflection). In addition, at high forces tunnel events also favor the enhancement [1].

As for the shift to higher forces, Shushin and Pollak showed [17] that quantum corrections produce a suppression of the diffusion in the underdamped regime. This effect yields an effective increased barrier, which manifest itself in a shift to higher forces in the quantum curves.

In Fig. 3 (see the inset) we also observe a small current at $F=0$. We believe that this "little" violation of the second law (transformation of thermal fluctuations in net current in absence of forcing) is a consequence of the approximations done in the derivation of the *Caldeira–Leggett* equation [8] (since the starting formalism is thermodynamically consistent).

5. Phase space representation

We plot a (stationary) *Wigner* distribution in Fig. 4. In order to see quantum effects clearly we choose the lowest K case considered (recall $K \propto S_0/\hbar$).

The white islands in the graph represent zones with negative values of the *Wigner* function. Apart from this negative zones, the *Wigner* distribution lies mainly on its classical counterpart.

Negative zones are a consequence of quantum interference. Thus, one would expect that decoherence yields positive *Wigner* functions. In fact, in the harmonic dissipative case, it was shown that after a finite time the *Wigner* function becomes positive [18]. However, our plots show that more general (non linear) potentials allow for non-positive *Wigner* distributions at long times.

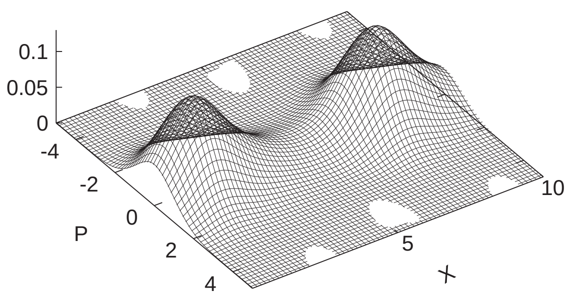

Fig. 4. *Wigner* function for a particle in a ratchet potential. The quantumness parameter is $K=5$, the damping is $\gamma=0.05$ and $F=0$. White "islands" correspond to zones of negative W ($\sim -10^{-5}$). These negative zones are of size comparable to those of Hamiltonian case [11]. Note the spatial asymmetry induced by the ratchet potential.

By decoherence we mean that an initial reduced density matrix, $\varrho(t_0)$ evolves with time to a diagonal one (in a preferred basis), when the system is coupled to the environment [19]. The basis $\{|n\rangle\}$ in which ϱ becomes diagonal, $\varrho = \sum |c_n|^2 |n\rangle\langle n|$, it is the so-called *pointer* basis [19]. The preferred basis depends on the *Hamiltonian* of the system (H_S) and the interaction between the system and the bath. For example, in linear quantum *Brownian* motion (free particle and harmonic oscillator), the pointer states are localized in phase–space, the so-called coherent states (familiar from quantum optics). Mixtures of these states yield positive W.

The fact that our stationary W retains the negative islands (after decoherence), implies that such coherent states cannot be the pointer basis in our case. Actually, in the limit of weak damping and high temperature, one expects that the stationary solution of (2) corresponds to the canonical density matrix,

$$\varrho = \frac{1}{\mathscr{Z}} \mathrm{e}^{-\beta H_S} = \frac{1}{\mathscr{Z}} \sum \mathrm{e}^{-\beta E_k} |k\rangle\langle k|. \tag{15}$$

Accordingly, the pointer states would correspond to *eigenstates* of the system Hamiltonian.

This can be additionally supported by the following. Consider the approximate Bloch functions that can be analytically obtained in the extreme quantum case ($K \lesssim 1$) [11]. Weighting the corresponding $|k\rangle\langle k|$ by the thermal factor $\mathrm{e}^{-\beta E_k}$ and integrating over k's in the lowest bands, one obtains Wigner functions displaying a structure similar to the stationary solutions obtained here by solving the Caldeira–Leggett equation for small γ/T.

6. Conclusions

The continued-fraction method is an established technique to solve classical *Fokker–Planck* equations. Admittedly, compared with direct simulations, the method has several shortcomings (it is quite specific for the concrete problem; the stability and convergence fails in some ranges of parameters, etc.). However, it also has valuable advantages (it is free from statistical errors, its non-perturbative character, high efficiency, etc.) [15].

When transferred to the quantum case the method inherits these shortcomings plus the problem of the critical election of the basis and recurrence index [11]. However, no quantum *Langevin* simulations are available, while numerical solutions of master equations are computationally expensive. Notable exceptions are the different versions of the quantum stochastic calculus [20], which can be viewed as a sort of quantum counterpart of the classical *Langevin* simulations.

Let us emphasize that the continued-fraction technique gives the exact solution of the quantum master equation (*Wigner* distribution), allowing the calculation of any observable [see Eq. (7)]. This method has also "spectral advantages" since it does not require the calculation of the eigenvalues, circumventing the demanding problem of continuum spectrum. Moreover, a quantum–classical connection is attained in a natural way (tuned by K). Finally, the method enjoys the advantages of working in phase–space.

In this work, we have studied the ratchet effect in the quantum case for high temperature/weak damping conditions as a function of the amplitude of the forcing. Starting from the classical case, we have proceeded to make the system quantal. The deviations from the classical limit have been understood in terms of tunnel events and thermally activated over-barrier wave reflection.

The representation of the *Wigner* functions has shown that, contrary the harmonic case, ratchet (cosine) potentials do not exhibit positive *Wigner* functions at long times. We have argued that in the weak damping and high temperature regime the pointer basis are the *eigenstates* of the system *Hamiltonian*, yielding in our case a non-positive W.

We finally, mention that the limitations of the master equation considered do not allow us to study the low temperature regime, where quantum corrections will be more important. These problems are brought to the fore with an unphysical violation of the second law of thermodynamics. This situation constitutes a motivation to develop corrections to the *Caldeira– Leggett* equation, which could hopefully be solved with the continued fraction method.

Acknowledgements

This work was supported by DGES, project BFM2002-00113, and DGA, Grant no. B059/ 2003. We acknowledge to P.J. Martínez his support during this work.

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