Current fluctuations in the nonequilibrium Lorentz gas

Andrea Gamba [a] Lamberto Rondoni [b]

[a] *DIMAT, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy*

[b] *DIMAT and INFM, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy*

Abstract

To extend Onsager-Machlup's theory, Bertini, De Sole, Gabrielli, Jona-Lasino and Landim proposed a fluctuation theory for the steady states of stochastic nonequilibrium systems, which preditcs a temporal asymmetry between a fluctuation and its relaxation. Here, this theory is considered in the context of the nonequilibrium Lorentz gas. This system is determinisitc and time reversible, but is chaotic and dissipative, hence its evolution is close to that of irreversible stochastic processes.

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1 Introduction

Large fluctuations around steady states occur rarely but are responsible for many physical processes (phase transitions, nucleation, chemical reactions, DNA mutations, etc.), and shed some light on the emergence of the irreversible behaviour of macroscopic systems from reversible microscopic dynamics [1,2]. A fundamental question concerns the relation between fluctuation and relaxation paths around a steady state (be it equilibrium or not). Temporal asymmetries between these paths have been observed experimentally in stochastically perturbed analog electric devices [2], and should be observable in more general mesoscopic systems, as predicted by the theory recently developed by Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim for nonequilibrium steady states [3]. This theory generalizes Onsager-Machlup's

Email address: `lamberto.rondoni@polito.it` (Lamberto Rondoni).

theory [4] to steady states in Local Thermodynamic Equilibrium (LTE). For stochastic particle systems which admit the hydrodyamic description

$$\partial_t \varrho = \nabla \cdot [D(\varrho) \nabla \varrho] \equiv \mathcal{D}(\varrho) \ , \qquad \varrho = \varrho(u,t) \tag{1}$$

where ϱ is a vector of macroscopic observables, and u a space variable, the theory of Ref.[3] asserts that the spontaneous fluctuations are governed by:

$$\partial_t \varrho = \mathcal{D}^* (\varrho) \tag{2}$$

where $\mathcal{D}^*$ is in general nonlocal, and different from $\mathcal{D}$. Equation (2) is called *adjoint* hydrodynamic equation. The theory rests on the following:

Assumptions: 1) *The "mesoscopic" evolution is a Markov process* X_t;[1]

2) *the macroscopic description is given by the fields* ϱ *(the local thermodynamic variables) whose evolution is described by diffusion type equations like (1)*;

3) *The probability measures describing the evolution of* X_t *and of its time reverse* X_t^**, respectively* P_{st} *and* P_{st}^**, are related by*

$$P_{st}^*(X_t^* = \phi_t, t \in [t_1, t_2]) = P_{st}(X_t^* = \phi_{-t}, t \in [-t_2, -t_1]) \tag{3}$$

Moreover, if L *is the generator of* X_t*, the adjoint dynamics is generated by the adjoint operator* L^**, which admits a hydrodynamic description*;

4) *The stationary measure* P_{st} *admits a large deviation principle stating that the local observable* ϱ_N*, in a volume* V *contanining* N *particles, obeys:*

$$P_{st}(\varrho_N(X_t) \sim \hat{\varrho}(t), t \in [t_1, t_2]) \approx e^{-N[S(\hat{\varrho}(t_1)) + J_{[t_1,t_2]}(\hat{\varrho})]} \ , \tag{4}$$

where $\hat{\varrho}$ *is a given density profile,* J *vanishes if* $\hat{\varrho}$ *is a solution of Eq.1, and* $S(\hat{\varrho}(t_1))$ *is the "entropy" cost to produce the initial profile* $\hat{\varrho}(t_1)$*.*

The generalization given in [3] of Onsager-Machlup's theory follows from these assumptions, and amounts to this:

Fluctuation principle. *In a stationary non equilibrium system, a spontaneous macroscopic fluctuation most likely follows a path which is the time reversal of the relaxation path, according to the adjoint hydrodynamics (Eq.(2)).*

The point is that $\mathcal{D}^* \neq \mathcal{D}$, in general. The question then arises as to whether the consequent asymmetry between a spontaneous fluctuation and its relax-

[1] We call microscopic the deterministic dynamics of many particles constituting a macroscopic system, and mesoscopic the associated reduced stochastic description.

ation can be obtained from deterministic, reversible microscopic dynamics. In fact, one generally assumes that the thermodynamic behaviour of, e.g., classical fluids is due to the chaotic reversible dynamics of their particles, which appear stochastic at a mesoscopic, or coarse grained, level. [2]

Unfortunately, it is hard to construct models of steady states of particle systems on which these ideas can be directly tested. For instance, one needs two reservoirs at different temperatures, in order to produce a steady heat flow in a system coupled to them. The corresponding thermodynamic limits pose formidable mathematical problems, while the present computer technology cannot simulate sufficiently large reservoirs. Therefore, the question whether, and how, some deterministic reversible dynamics may account for the behaviour predicted by Ref.[3] is open.

Nevertheless, quite realistic molecular dynamics models have been produced [7], which turn succesful in self-consistent calculations of transport coefficients. Hence, simplified versions of these models, like the nonequilibirum Lorentz gas (NLG) [8], have been considered for theoretical purposes.

Although the NLG seems suitable to assess the theory of [3] in the context of microscopic, deterministic, reversible dynamics (cf. Section 3), our results show no clear asymmetry between relaxation and fluctuation paths. Different regions of the NLG parameters space might yield different results. But it is more likely that more realisitc models will be needed for the asymmetries of [3] to be observed.

2 Structure of the adjoint hydrodynamics

Let ϱ be a n-dimensional vector, and consider the deterministic dynamics

$$\dot{\varrho} = \mathcal{D}(\varrho) \ , \tag{5}$$

where $\mathcal{D}$ is a vector field with an attracting fixed point $\hat{\varrho}$. The components of ϱ may be viewed as the values taken by a given observable on the n different sites of a spatially discrete system, $\hat{\varrho}$ as a steady state, and (5) as the corresponding hydrodynamic law. Perturbing Eq.(5) with a Gaussian noise ξ, with mean $\langle \xi(t) \rangle = 0$ and $\langle \xi_i\,(t)\,\xi_j\,(t') \rangle = K_{ij}\delta\,(t-t')$, where K is symmetric and

[2] The analogy between physical systems and chaotic dynamcal systems must be taken with a grain of salt. The coarse graining of dynamical systems concerns their phase space, while the physical mesoscopic level refers to real space. Furthermore, chaotic dynamics have fast decays of correlations, and don't need the thermodynamic limit, but then they only yield *fictitious* thermodynamic behaviours [5,6].

positive definite, Eq.(5) results from the maximization of the probability of the paths $\varrho(t)$ connecting the states $\varrho_i = \varrho(t_i)$ and $\varrho_f = \varrho(t_f)$, i.e. from the minimization of

$$J_{[t_i,t_f]}(\varrho) = \frac{1}{2}\int_{t_i}^{t_f} (\dot{\varrho} - \mathcal{D})^T K^{-1} (\dot{\varrho} - \mathcal{D})\, \mathrm{d}t \equiv \frac{1}{2}\int_{t_i}^{t_f} \langle \dot{\varrho} - \mathcal{D}\, ,\, \dot{\varrho} - \mathcal{D}\rangle\, \mathrm{d}t \qquad (6)$$

where $\langle x, y\rangle = x^T K^{-1} y$, and the superscript T indicates matrix transposition. In fact, consider the discretized version of the perturbed equation $\dot{\varrho} = \mathcal{D}(\varrho) + \xi$:

$$\frac{\varrho_{k+1} - \varrho_k}{\Delta t} = \mathcal{D}(\varrho_k) + \xi_k \ , \quad \text{with } \langle \xi_k\rangle = 0 \ , \quad \langle \xi_{l,i}\xi_{k,i}\rangle = \frac{1}{\Delta t}\delta_{l,k} \qquad (7)$$

where k labels the time instants, and the noise vectors $\xi_k = \{\xi_{k,i}\}_{i=1}^n$ are normally distributed. The time evolution is then described by the conditional probability P that ϱ_{k+1} equals r_{k+1}, given that ϱ_k equals r_k, i.e. by:

$$P(\varrho_{k+1} = r_{k+1} | \varrho_k = r_k) = \int d\xi_k\ p(\xi_k)\ \delta\left(\frac{r_{k+1} - r_k}{\Delta t} - \mathcal{D}(r_k) - \xi_k\right) \ . \qquad (8)$$

For the probability of a path $\gamma = \{\varrho_i = r_0, \varrho_1 = r_1, ..., \varrho_f = r_{m+1}\}$, this yields:

$$P(\gamma) = \left(\frac{\Delta t}{(2\pi)^n |K|}\right)^{\frac{1}{2}} e^{\frac{\Delta t}{2}\sum_{k=0}^{m}\left\langle \frac{r_{k+1}-r_k}{\Delta t} - \mathcal{D}(r_k), \frac{r_{k+1}-r_k}{\Delta t} - \mathcal{D}(r_k)\right\rangle} \ . \qquad (9)$$

For small Δt, the argument of the exponential approximates $J_{[t_i,t_f]}$. Its extremum with $t_i = -\infty$, taken over all paths $\varrho(t)$ connecting ϱ_i to ϱ_f, $S(\varrho_f) = \inf_{\varrho(-\infty)=\varrho_i} J_{[-\infty,t_f]}(\varrho)$, called "entropy functional", identifies the most likely path. Let ∇_ϱ indicate differentiation with respect to the components of ϱ, and suppose that $\mathcal{D}$ be decomposed as a sum of two parts:

$$\mathcal{D}(\varrho) = -\frac{1}{2}K\nabla_\varrho V(\varrho) + \mathcal{A}(\varrho) \, , \qquad \text{with } \ \langle K\nabla_\varrho V\, ,\, \mathcal{A}\rangle = 0 \qquad (10)$$

where $\hat{\varrho}$ minimizes V. This decomposition is used in the context of finite dimensional Langevin equations [11]. In Ref. [3] it is observed that a similar decomposition arises in the hydrodynamic limit of stochastic multiparticle systems, in which case K is the matrix of the transport coefficients which link the thermodynamic forces to the corresponding fluxes $\dot{\varrho}$. The entropy functional can then be written as

$$J_{[t_i,t_f]}(\varrho) = \frac{1}{2}\int_{t_i}^{t_f} \left\langle \dot{\varrho} + \frac{1}{2}K\nabla_\varrho V - \mathcal{A}\,,\, \dot{\varrho} + \frac{1}{2}K\nabla_\varrho V - \mathcal{A} \right\rangle \mathrm{d}t = \tag{11}$$

$$\frac{1}{2}\int_{t_i}^{t_f} \left\langle \dot{\varrho} - \frac{1}{2}K\nabla_\varrho V - \mathcal{A}\,,\, \dot{\varrho} - \frac{1}{2}K\nabla_\varrho V - \mathcal{A} \right\rangle \mathrm{d}t + [V(\varrho_f) - V(\varrho_i)]\,. \tag{12}$$

The minimization of (11) leads to Eq.(5), for relaxation paths, while the minimization of (12) leads to to the fluctuation paths governed by:

$$-\dot{\varrho} = \mathcal{D}^*(\varrho) = -\frac{1}{2}K\nabla_\varrho V - \mathcal{A}(\varrho)\ . \tag{13}$$

This implies an asymmetry between fluctuation and relaxation (not present in Onsager-Machlup's theory) due to the fact that $K\nabla_\varrho V$ and $\mathcal{A}$ have opposite time reversal transformation properties. Onsager-Machlup's theory is recovered in the linear regime (K independent of ϱ) with $\mathcal{A} = 0$, but symmetric fluctuation-relaxation paths are obtained also in the nonlinear case, if $\mathcal{A} = 0$.

This theory can be extended to infinite dimensional ϱ's, as in Ref.[3], where the hydrodynamic limit of certain classes of lattice gases is considered. This yields evolution equations like (1), where $\mathcal{D}$ is an elliptic differential operator. The analogy with the Langevin case is due to the fact that the probabilities of the fluctuation paths are given by large deviation expressions like $\exp(-J)$. So, most relations used in the finite dimensional Langevin case hold in the infinite dimensional setting, provided that K is a positive definite elliptic operator, and that ∇_ϱ is replaced by the functional derivative $\delta/\delta\varrho$. The "quasi potential" V can now be identified with the "entropy" cost $S(\varrho_f) = \inf \mathrm{J}_{[-\infty,t_f]}(\varrho)$ for the fluctuation ϱ_f to be created at time t_f.

Writing the generator of the stochastic dynamics on the lattice gas as a sum of hermitian and anti-hermitian parts: $L = \frac{1}{2}(L^+ + L^-) + \frac{1}{2}(L^+ - L^-)$, the term $\mathcal{A}$ in Eq.(10) arises as the scaling limit of $L^+ - L^-$. Since the adjoint generator can be written as $L = \frac{1}{2}(L^+ + L^-) - \frac{1}{2}(L^+ - L^-)$, the adjoint hydrodynamics must then have the form (13). If L is self-adjoint, one obtains $\mathcal{D}(\varrho) = \mathcal{D}^*(\varrho)$.

3 The nonequilibrium Lorentz gas

The NLG is arguably the simplest particle model which affords a nonequilibrium steady state, with a net current. It consists of a two dimensional lattice of hard scatterers (Fig.1), and of noninteracting particles subject to a constant external force $\mathbf{F} = (\varepsilon, 0)$ and to an isokinetic "thermostat" [8–10]. In

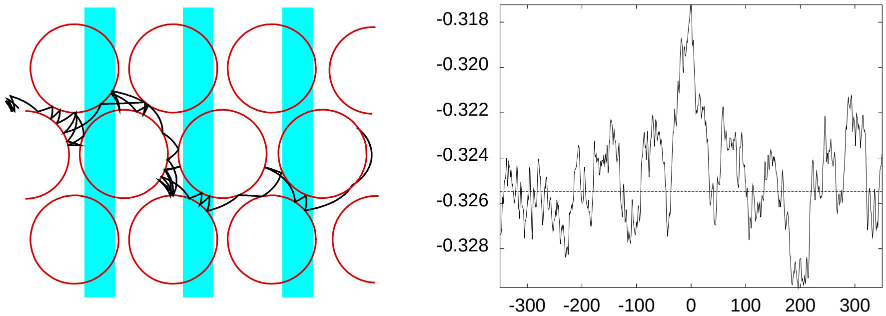


Fig. 1. Trajectory of a Lorentz particle, and (shaded) integration region Ω for the local fluctuations (left panel). Typical fluctuation-relaxation path (right panel). The irregular curve is the instantaneous current inside Ω, and the straight line is the average current. The paths of the global current are analogous.

Lorentz's original model, the moving particles are in LTE with the scatterers, [3] and are randomly placed in the plane. Let $m = 1$ be the mass of the particle, $K = 1/2$ its initial kinetic energy, $\mathbf{x} = (x, y)$ its position, and $\mathbf{p} = (p_x, p_y)$ its momentum. The equations of motion between two collisions read:

$$\dot{\mathbf{x}} = \mathbf{p} \ ; \quad \dot{\mathbf{p}} = \mathbf{F} - \alpha \mathbf{p} \quad \text{with “thermostat”} \quad \alpha = \varepsilon p_x \ . \tag{14}$$

The dynamics is dissipative (phase space volumes contract on average), reversible and, for sufficiently small ε, hyperbolic with one ergodic measure for the forward time statistics [9]. Moreover, there is a Kawasaki formula for the nonlinear response, which reduces to a kind of Ohm's law at small ε. [4] This is due to the fact that the ergodic measure assigns different weights to phase space trajectories corresponding to opposite currents, thus breaking the temporal symmetry on the statistical (average, or “macroscopic”) level, despite the reversibility of the dynamics. Moreover, the deterministic evolution may be reduced to a stochastic process, by means of a kind of coarse graining in phase space, which can be viewed as a less detailed description of the dynamics. For the equilibrium Lorentz gas, this description is based on the Markov partitions constructed by Sinai and Bunimovich, later refined also by Chernov (cf. Ref.[12]). The refined method has been adapted to the NLG in Ref.[9].

Unfortunately, no rigorous results seem to be available on the symmetry properties of the generator of the corresponding Markov chain. Furthermore, this process concerns phase space, not real space, and explicit knowledge of its generator may not suffice to our purpose. Therefore, numerical simulations appear to be the only presently available option to investigate the symmetry

[3] Note, LTE requires finite mass scatterers and an infinite time limit. The infinite mass limit, if desired, must be taken after the time limit. Exchanging the order of these limits corresponds to physical situations without LTE, like in our NLG.

[4] Because of lack of LTE, this is only a *formal* Ohm's law, and the dissipation is not the irreversible entropy production of Irreversible Thermodynamics [6].

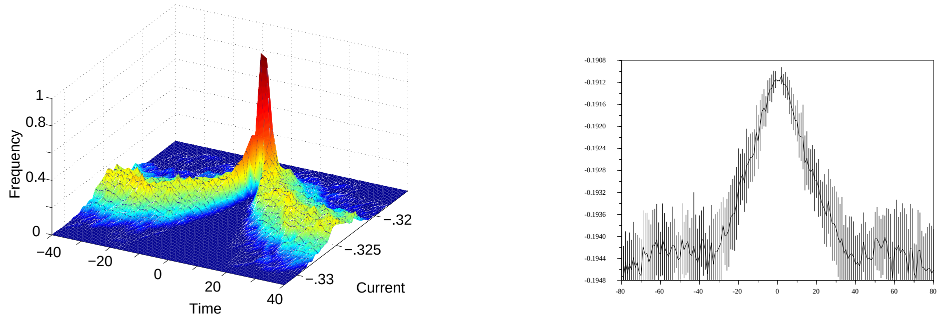


Fig. 2. Histogram of large (local) current fluctuations in the Lorentz gas with $\varepsilon = 1.5$ (left panel). The histogram is symmetric with respect to the origin of times (threshold times). The global current behaves analogously, as the plot of the crest of its histogram, in the right panel, shows. Error bars are drawn for completeness.

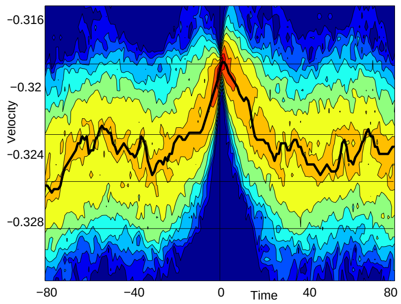
properties of the stochastic process and of the fluctuation-relaxation paths of the NLG. In fact, a numerical study [13] of the symbolic dynamics of the NLG suggests that the real space projection of the NLG phase space stochastic process does have asymmetric transition probabilities (as expected), and that the asymmetry grows with ε [13]. This makes the NLG an ideal candidate to test the theory of Ref.[3] in the context of deterministic reversible dynamics.

The only relevant observable here seems to be the instantaneous current due to N particles. We take $N \sim 10^6$ and follow the particles for the time needed to undergo $\sim 10^4$ collisions. Then, the x component of the current averaged over the ensemble of particles is integrated either over the shaded domain Ω of Fig.1, to give the local current in Ω, or over the whole space, to give the global current. The resulting signal (Fig.1) is analyzed and fluctuations exceeding a given threshold (2.5 standard deviations from the mean) are collected. Then, a time interval centered on the instant of time in which the current reaches the threshold is discretized, together with the range of observed currents, in order to obtain a grid of rectangular bins in the current-time plane. This grid is used to construct the histogram of the current paths before and after the threshold, thus identifying the most frequent fluctuation-relaxation path (Fig.2). Our results for the local and global currents of the NLG appear symmetric under time reversal, which raises some questions on the kind of observables and of reversible deterministic dynamics compatible with the theory of Ref.[3]. These questions are listed below, and will be investigated in the future.

1. We collected large current fluctuations exceeding 2.5 standard deviations from the mean, for two forces ε. Would other observables, other thresholds and other forces give different results?

2. The NLG is periodic in space, and homogeneously driven, instead of boundary driven. Is this the source of the observed fluctuation-relaxation symmetry?

3. Is the observed symmetry a mere consequence of the reversibility of the NLG? This does not seem to be the case. In the first place, the microscopic reversibility of the NLG is compatible with its macroscopic irreversibility,



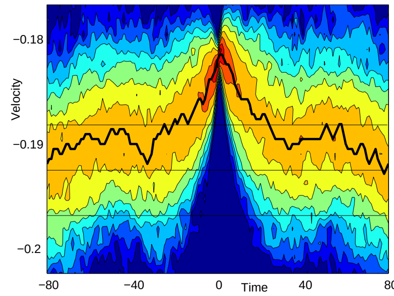


Fig. 3. Contour plots of the probabilities of the local current fluctuations for $\varepsilon = 1.5$ (left panel), and $\varepsilon = 0.75$ (right panel). The histograms appear symmetric (the slight asymmetry for $\varepsilon = 1.5$ seems to be due to the particular size of the bins.

and probably also with its mesoscopic irreversibility, as argued in Section 3. Furthermore, if reversibility was a sufficient condition for the fluctuation-relaxation paths to be symmetric, no known microscopic description of a nonequilibirum steady state would have asymmetric paths. In fact, the most realistic currently available models of such states are hamiltonian, and consist of a many particle system coupled to much larger particle reservoirs at different thermodynamic states (see Fig.4 for one example). Such models are reversible and have only finitely many degrees of freedom. The limit of infinitely many degrees of freedom, which is usually considered and makes the models effectively irreversible, is taken only for mathematical convenience. Indeed, the microscopic time scales are separated from the macroscopic ones, and one has a nonequilibirum steady state on the observation time scales, when the reservoirs are sufficiently large, but still finite.

Were symmetric fluctuation-relaxation paths implied by reversibility, the statistical mechanical approach, based on reversible microscopic dynamics, would unexpectedly fail to describe the asymmetric paths which have been observed in some experimental setup, and are expected in other mesoscopic systems as well. A possible scenario is that the current molecular dynamics models resolve the microscopic and the macroscopic features of physical systems, but not their mesoscopic features. It seems more likely that some microscopic dynamics are not suitable to represent thermodynamic systems. For instance, the NLG is affected by an unphysical dissipation due to the force $\alpha\mathbf{p}$, called Gaussian thermostat, and does not enjoy LTE [6]. We conclude that the NLG, apparently an ideal model to test the theory of Ref.[3], in reality is not sufficiently close to a thermodynamic system, and that more realisitc (but still reversible) models of nonequilibrium systems have to be considered.

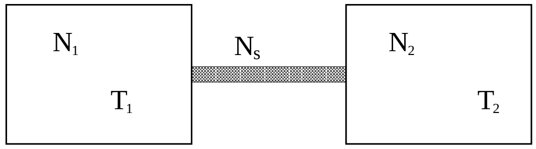


Fig. 4. Model of a nonequilibrium "steady state". The shaded central region is the "system", which is made of $N_s \gg 1$ particles and is coupled to two heat baths. The bath on the left is made of $N_1 \gg N_s$ particles at temperature T_1, while the bath on the right is made of $N_2 \gg N_s$ particles at temperature $T_2 \neq T_1$. The union of the baths and of the system is hamiltonian and has finitely many degrees of freedom.

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References

[1] G. Gallavotti and E.G.D. Cohen, J. Stat. Phys. **80**(5/6), 931 (1995)

[2] D.G. Luchinsky and P.V.E. McClintock, Nature, **389** 463–466, (1997)

[3] L. Bertini et al., Phys. Rev. Lett. 040601–4 (2001); J. Stat. Phys. **107**(3/4), 635 (2002)

[4] L. Onsager and S. Machlup, Phys. Rev. **91**, 1505–1512, (1953)

[5] E.G.D. Cohen and L. Rondoni, Chaos, **8**(2), 357 (1998)

[6] L. Rondoni and E.G.D. Cohen, Physica D, **168-169**, 341 (2002)

[7] D.J. Evans and G.P. Morriss, **Statistical mechanics of nonequilibrium liquids**, Academic Press, London (1990)

[8] B.M. Moran and W.G. Hoover, J. Stat. Phys. **48**(3/4), 709 (1987)

[9] N.I. Chernov et al., Comm. Math. Phys. **154**, 569 (1993)

[10] J. Lloyd et al., Chaos **5**(3), 536 (1995)

[11] M.I. Friedlin and A.D. Wentzell, **Random perturbations of dynamical systems**, Springer, Berlin (1984)

[12] L.A. Bunimovich et al., Russian Math. Surveys **46**(4), 47 (106)

[13] G.P. Morriss, C.P. Dettmann and L. Rondoni, Physica A, **240**, 84 (1997)