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Nonlinear transport laws for low density fluids

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Abstract

Hydrodynamics equations derived directly from Boltzmann's equation and specialized to sheared planar flow are shown to yield approximate nonlinear laws of heat transport and of viscous flow. The law of viscous flow predicts non-Newtonian effects including shear thinning and the law of heat transport is more general than Fourier's law: it is not linear and it implies heat flow parallel to the isotherms. These nonlinear transport laws are faithfully corroborated by molecular dynamic simulations based on straightforward Newtonian dynamics. © 1998 Elsevier Science B.V. All rights reserved.

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1. Gas-dynamics: No local thermodynamic equilibrium

Transport in dilute systems subjected to strain is quite nontrivial. The assumption behind the Navier–Stokes equations that changes in a fluid take place smoothly so that the system can be considered in a state of local thermodynamic equilibrium, does not hold when the length scales associated to gradients are comparable to the mean free path of the molecules.

To reassess the form of the transport laws in the case of low density systems far from equilibrium, it is most convenient to go back to kinetic theory. A quite complex hydrodynamics, that we shall call *Boltzmann–Grad gas-dynamics*, describing gases subject to gradients that far exceed the applicability of Navier–Stokes formalism, is obtained making a formal moment expansion of the distribution function $f(r,c,t)$ and solving self-consistently for the coefficients of the expansion [1].

Boltzmann–Grad gas-dynamics involve, besides the density, velocity and temperature fields, two additional hydrodynamic fields: the pressure tensor $\mathbb{P}$ and the heat flux

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vector q. Since the whole framework is derived from Boltzmann's equation – the relationship between the energy density per unit mass, u, and T in dimension d is simply $u=(d/2m)k_BT$ and the pressure equation is that for ideal gases: $p=n\,k_BT$. The *dynamic equations* for $\mathbb{P}$ and q are nonlinear and they fully substitute the usual *static linear constitutive equations* used in standard hydrodynamics.

The resulting gas-dynamic equations are found in Grad's article and specialized to the d-dimensional fluid of hard disks ($d=2$ or 3) are in [2,3]. In [3] we were able to find a closed solution to this hydrodynamics in the case of a laminar planar Couette flow. It was shown, for example, that since the system heats up, there is heat flux q and this flux vector has not only a component orthogonal to the isotherms but also has a component *parallel* to them. The corresponding thermal conductivities were found in a closed form. They depend not only on temperature and density but also on the shear rate. In the same article we found a closed and nonlinear law of viscous flow that can be forced to look like Newton's law but with a shear viscosity coefficient which again depends on the shear rate and presents shear thinning.

The above reference was written before we knew about similar results derived from the BGK approximation to Boltzmann's equation [4]. These authors too derive the existence of a longitudinal component of the heat flux. The Couette flow of a dilute system of Maxwell particles under strong strain has also been studied theoretically in [5,6] using the BGK equation.

The approximate law of heat transport presented in this article for the normal component q_y resembles expressions already known for *dense fluids*, as one can see, for example in [7] and references therein.

In Boltzmann's equation the walls of the gas container should either be considered as external forces acting about the boundaries of the system or, if walls are idealized as rigid geometric objects, they can be included as boundary conditions. The description given above does not include walls in any of these variants, therefore we cannot expect that the present theoretical framework will give a fine description near the walls.

Section 2 presents Boltzmann–Grad's gas-dynamic equations in the bidimensional planar case. In Section 3 the transport laws implied by these gas-dynamic equations are approximated up to the third order. Section 4 makes some comparisons with our own molecular dynamic simulations.

From now on we choose temperature units such that $k_B=1$.

2. Bidimensional laminar flow

In the following we specialize Boltzmann–Grad gas-dynamics to the 2D laminar and stationary case when the movement of a 2D hard disk fluid is between two walls separated by a distance L_y, parallel to the X-axis. There is gravity $g=(g,0)$ in the X-direction. In this case there is x-translation invariance and therefore the only coordinate that plays a role is the transversal coordinate y. The only nontrivial velocity component is $v_x(y)$ and only its derivative v_x' appears in the equations, but we eliminate it in favor

Table 1
On the left are the values of the parities I_g of the different hydrodynamic fields as defined in the text. On the right are the I_y parities for the Couette and Poiseuille flows, y is the coordinate transversal to the flow

	I_g		I_y^{Couette}	$I_y^{\text{Poiseuille}}$
γ	$-$	γ	$+$	$-$
T	$+$	T	$+$	$+$
P_{xy}	$-$	P_{xy}	$+$	$-$
P_{yy}	$+$	P_{yy}	$+$	$+$
q_x	$-$	q_x	$-$	$+$
q_y	$+$	q_y	$-$	$-$

of the adimensional shear rate γ,

$$\gamma(y) = \tau(y) v_x', \quad \tau(y) \equiv \frac{1}{2\sigma p(y)} \sqrt{\frac{mT(y)}{\pi}}\,, \tag{1}$$

where τ is the free flight time. The diameter and mass of the particles are σ and m, respectively. The origin of coordinates is chosen in the middle of the channel so that $-L_y/2 \leqslant y \leqslant L_y/2$.

The mass balance equation is identically satisfied. The momentum and energy balances imply that P_{yy} is uniform and

$$P_{xy}' = mg\frac{p}{T}, \qquad \tau q_y' = -\gamma P_{xy}\,. \tag{2}$$

The balance equations associated to the pressure tensor are two:

$$p(y) = P_{yy} - \tfrac{3}{2}\gamma(y) P_{xy}(y), \quad \frac{\tau}{2} q_x' = -P_{xy} - \gamma P_{yy}\,. \tag{3}$$

Finally, the balance equations associated to q are

$$-\frac{6\tau}{m} P_{xy} T' = 2g\tau P_{yy} + q_x + 3\gamma q_y\,, \tag{4}$$

$$-\frac{\tau}{m}[4P_{yy}T' + 3(\gamma P_{xy} T)'] = -2g\tau P_{xy} + q_y + \gamma q_x\,. \tag{5}$$

These is a set of five coupled nonlinear ordinary differential Eqs. (2a), (2b), (3b), (4) and (5) for the hydrodynamic fields γ, T, P_{xy}, q_x and q_y. Furthermore, one has to determine the constant P_{yy} while, by definition, $P_{xx} = P_{yy} - 3\gamma P_{xy}$. The hydrostatic pressure is determined from Eq. (3a).

As it is seen from Eq. (2), P_{xy} is not uniform only when $g \neq 0$.

One can convince oneself that the above hydrodynamic equations are invariant under the inversion $g \to -g$ provided γ, P_{xy} and q_x are inverted too. We will say that these three hydrodynamic fields have negative I_g *parity*. In cases when there is also invariance with respect to the inversion of the transversal coordinate y it is possible to define the I_y parity. Table 1 gives the value of these parities for our hydrodynamic fields.

To analyze the above equations we could choose quite general boundary conditions compatible with x-translation invariance. We could fix temperatures T_0 and $T_0 + \Delta$ at the bottom and top walls, and fix the tangential velocities to be $-v_b$ and v_t at these walls. Furthermore, choosing periodic boundary conditions in the x-direction (periodicity length L_x) it is natural to require that the integral of the number density be the number of particles or $\int \frac{p}{T}\, dy = N/L_x$. A quite trivial exercise is to integrate the above system of equations when $g=0$ and $v_b=v_t=0$ (hence $\gamma=0$). It is a purely conductive case and one can derive the analytic form of the temperature profile parameterized by Δ. This case is so simple that it can be studied in a wider context as in [8].

In the general case, we could take g, Δ, v_b and v_t as first order quantities in the sense that simple adimensional quantities proportional to them are much smaller than unity. This would imply that γ, P_{xy} and dT/dy are first order while T and P_{yy} are finite (zero order). Obtaining a first order solution for our hydrodynamic equations is then a simple exercise. At this order, for example, q_x is a nontrivial constant.

In the usual Couette and Poiseuille cases $\Delta=0$ and dT/dy is a second order quantity. These two quite important cases will be considered in the following section to write down transport laws. We reported an early study of Poiseuille flow for a dense fluid in [9].

3. The symmetric Couette and Poiseuille flows: third order transport laws

In the case when there is no temperature difference between the two walls ($\Delta=0$) and $v_b=v_t=v_0$ the system has a symmetry with respect to inverting y provided also γ is inverted, since it comes from a derivative with respect to y. Considering again g and γ as first order quantities the hydrodynamic fields can be expanded as sums of even (odd) order contributions if I_g is even (odd). The only fields with zero order contributions are the temperature ($T\approx T_0$) and the constant P_{yy}. Since T is even, dT/dy is of second order. One can check, for example from the first order integration suggested in Section 2, that q_x has a first order *uniform* term.

Hence, both for the Couette and Poiseuille flows q_x' is a third-order quantity which implies through Eq. (2) that $P_{xy}+\gamma P_{yy}$ is of third order even though both terms are first order. Taking all this into consideration and solving algebraically Eqs. (4) and (5) for q_x and q_y one derives that up to second order (the remainder is of fourth order),

$$q_y = -\frac{4\tau P_{yy}}{m}\, T' + \frac{3\tau P_{yy} T}{2m}(\gamma^2)' - 3\tau p g \gamma\,, \tag{6}$$

while q_x up to the third order is

$$q_x = -2g\tau P_{yy} + \frac{18\tau P_{yy}}{m}\gamma T' - \frac{3\tau P_{yy} T}{m}(\gamma^3)' + 9\tau p \gamma^2 g\,. \tag{7}$$

In the case of the planar laminar Couette flow $g=0$ (we should rename I_g as I_γ), and we have shown in [3] that P_{xy} and γ are uniform, therefore, q takes the form $-\mathbb{K}\nabla T$ which looks like Fourier's law but $\mathbb{K}$ is a matrix of thermal conductivity which not only depends on the density and temperature but also depends on the shear rate. The components of $\mathbb{K}$ were given analytically and there values coincided with what was measured for small values of the shear rate [3].

In the case of the Poiseuille flow, as we see from the expressions given above, q does not take the form $-\mathbb{K}\nabla T$ as other gradients come into play.

The law of viscous flow this time is

$$P_{xy} = -\gamma P_{yy} + \frac{\tau^2 P_{yy}}{2}\left(\frac{3mg^2}{T}\gamma + \left\{(\ln T)' - \frac{21}{2}(\gamma^2)'\right\} g - \frac{18}{m}(\gamma T')' + \frac{3T}{m}(\gamma^3)''\right). \tag{8}$$

In the case of the Poiseuille flow the shear rate, to first order, is linear in y, its gradient is uniform and its second derivative is of third order. In the case of the Couette flow we have $g = 0$ and γ uniform, as shown in [3], and the above approximate expression for P_{xy} is

$$P_{xy}^{\text{Couette}} \approx -\gamma P_{yy} - \frac{9\tau^2 P_{yy}}{m}\gamma T'', \tag{9}$$

but we know that the exact expression, within Boltzmann–Grad's gas-dynamics is [3]

$$P_{xy}^{\text{Couette}} = \frac{4 + 3\gamma^2 - \sqrt{16 + 120\gamma^2 - 63\gamma^4}}{3(4 - 3\gamma^2)\gamma} P_{yy}\,. \tag{10}$$

In spite of the heating up of the system and hence its nonuniform temperature, and density fields, P_{xy}^{Couette} is uniform. Our simulations show this to be true even near the walls where our formalism breaks down and in particular γ does not turn out to be uniform.

In the above transport laws we have written q_y, q_x and P_{xy} in terms of ($I_g = +$, $I_y = +$) quantities – like T and P_{yy} – multiplying terms odd in γ, d/dy and, in the case of the Poiseuille flow, g as well. We notice that in both cases (Couette and Poiseuille flows) q_y has the same parity as d/dy and $\gamma\, g$ (obviously terms proportional to g exist only in the Poiseuille case); q_x has the same parity as $\gamma\, d/dy$ and as g; P_{xy} has the same parity as γ and as $g\, d/dy$. Therefore, the expressions for the transport laws at any order will have forms similar to the ones found up to the third order, but the $(+,+)$ factor in each term will be more complex as we go up to higher orders.

4. Theory versus simulations

We have solved perturbatively the Poiseuille case up to the sixth order [10] and have integrated, as we have repeatedly emphasized, in a closed form the Couette case [3]. In this section we compare these theoretical results with our own molecular dynamic simulations [11,12] using a dilute fluid of hard disks.

The system consists of N particles inside a rectangular box of $L_x \times L_y$. The collisions among particles are perfectly elastic. The vertical walls (along the Y-direction) are treated as periodic boundaries while the collisions with the horizontal walls impose a temperature $T_0 = 1$ on the fluid as well as a velocity v_0 at the top wall and $-v_0$ at the bottom wall in the case of Couette flow, but $v_0 = 0$ in the case of Poiseuille flow. One has to bear in mind though that, for finite systems such as the present one, there are velocity and temperature jumps which cannot be neglected, implying that the limits of $T(y)$ and $v_x(y)$ do not give exactly the values externally imposed.

The fraction of area covered by the disks is chosen to be 1% (the nonideal corrections to the equation of state are less than 2%). The size of the system is large enough that the ratio $\mathscr{B}$ between the *mean free path* ℓ and the width L_y of the channel is about 0.018.

4.1. Poiseuille flow

For Poiseuille flow simulations we consider a system of $N = 7056$ particles in a box of size $L_y = L_x/4 = 1488.83\sigma$ and also a larger system with $N = 30\,000$ and $L_y = L_x = 1488.83\sigma$. The external acceleration has been chosen as $g = 0.119T_0/mL_y = 0.00008$. We report here results for the smaller system.

As T_0 is the only free parameter that enters the sixth-order expansions of the hydrodynamics field profiles, we use the simulational results for P_{yy} to determine its effective value which is $T_0 = 1.10$ near the walls through the sixth-order expansion of the P_{yy} constant. The other theoretical profiles obtained using this value for T_0 are then compared with the simulational results. We found very good agreement.

In Fig. 1 (at the top) is a comparison between the simulational results and the theoretical predictions (first and third order) for the γ profile. It can be seen that better agreement is obtained when considering third order corrections.

Theory predicts a non vanishing heat flux q_x parallel to the isotherms as it is indeed observed in the simulations. At the bottom, Fig. 1 compares simulational results with theory. First order gives a uniform negative value which describes well the profile in the central part of the channel. To take account of the observations by the walls, third order theoretical predictions must be considered.

4.2. Couette flow

Results for a system of $N = 7680$ particles are in [3]. Here we report results for a larger system of $N = 29\,538$ particles with $L_y = L_x = 1524.31\sigma$ and wall velocities of $v_0 = 1.0\sqrt{T/m}$. The results confirm the theoretical predictions and a better agreement with theory is found in the case of the larger system since boundary effects are smaller.

Most profiles show discrepancies with theoretical results at the boundaries but very good agreement is found in the bulk of the system. From the simulational values of P_{xx} and P_{yy} an effective value for γ is obtained through the theoretical expressions. The free parameter T_0 is fixed using the theoretical expressions for $T(y)$ and the simulational values of the temperature at the center of the channel. Using these values for γ and T_0 the other theoretical profiles are built. Very good agreement with theory is found.

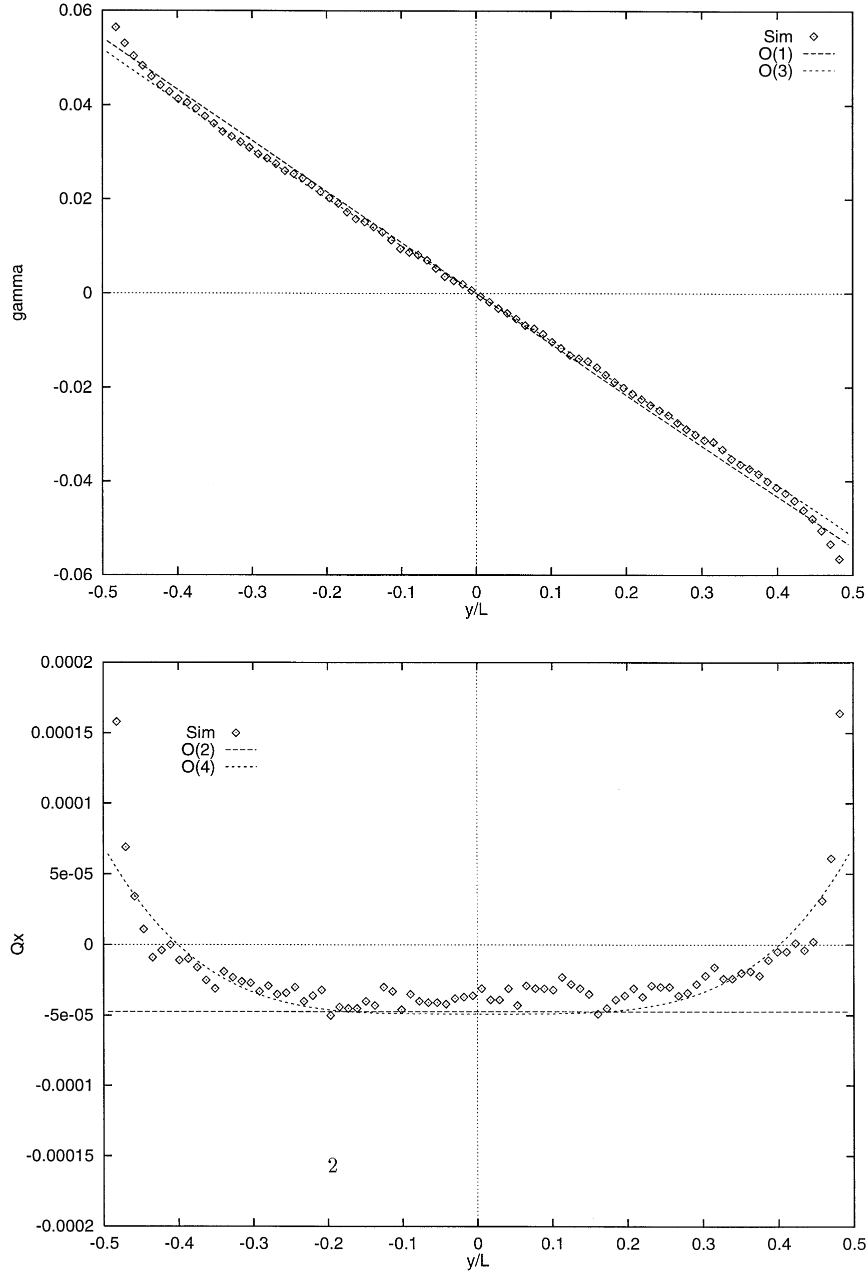

Fig. 1. At the top is the γ profile in the case of Poiseuille flow ($N = 7056$, $mgL_y/k_BT_0 = 0.119$). At the bottom is the q_x profile (heat flux parallel to the isotherms). The squares represent the simulational results. The dashed and dotted lines corresponds to first (second) and third (fourth) order theoretical predictions respectively.

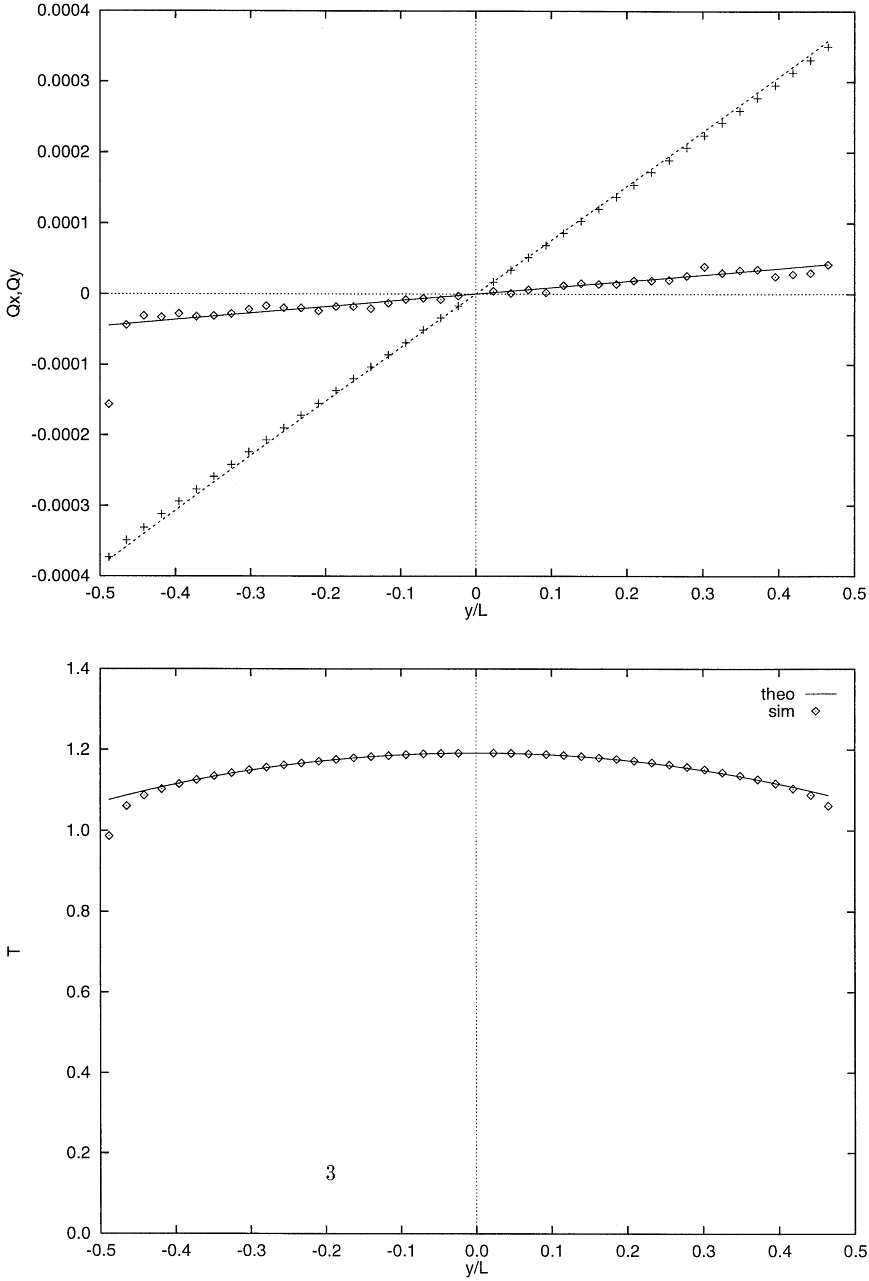

Fig. 2. At the top q_x and q_y profiles for Couette flow ($N = 29\,538$ and $\gamma = 0.06$). At the bottom is the temperature profile. In dots the simulational results. The dashed line corresponds to the theoretical prediction.

Fig. 2 shows at the top both components of the heat flux: the *normal* heat flux orthogonal to the isotherms and the heat flux parallel to the isotherms. The graph at the bottom shows the temperature profile. We see that the theory gives an excellent description of what we observe.

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References

[1] H. Grad, Principle of the kinetic theory of gases, in: S. Flügge (Ed.), Handbuch der Physik, Vol. XII, Springer, New York, 1958.
[2] P. Cordero, D. Risso, Microscopic computer simulation of fluids, in: P.L. Garrido, J. Marro (Eds.), 4th Granada Lectures on Computational Physics, Springer, New York, 1996.
[3] D. Risso, P. Cordero, Phys. Rev. E 56 (1997) 489.
[4] V. Garzó, M. López de Haro, Phys. Fluids 9 (1997) 776.
[5] J.J. Brey, Andrés Santos, Phys. Rev. A 36 (1987) 2842; Ch.S. Kim, J.W. Dufty, A. Santos, J.J. Brey, Phys. Rev. A 40 (1989) 7165.
[6] V. Garzó, J. Chem. Phys. 101 (1994) 1423; V. Garzó, Phys. Rev. E 51 (1995) 3156; V. Garzó, J. Chem. Phys. 103 (1995) 4626.
[7] B.D. Todd, D.J. Evans, Phys. Rev. E 55 (1997) 2800.
[8] D. Risso, P. Cordero, J. Stat. Phys. 82 (1996) 1453.
[9] D. Risso, P. Cordero, in: E. Tirapegui, W. Zeller (Eds.), Instabilities and Nonequilibrium Structures V, Kluwer Academic Publishers, Dordrecht, 1996.
[10] D. Risso, P. Cordero, Phys. Rev. E 58, to be published.
[11] M. Marín, D. Risso, P. Cordero, J. Comput. Phys. 109 (1993) 306.
[12] D. Risso, Ph. D. Thesis, Universidad de Chile, 1994.