Revista Mexicana de Física 23 (1974) 321-326

GENERALIZED HYDRODYNAMICS AND RELAXATION TIMES

R.M. Velasco* and E. Piña*

Escuela Superior de Física y Matemáticas, I. P. N.
México, D. F.

(Recibido: julio 10, 1973)
(Versión revisada: junio 13, 1974)

ABSTRACT: A comparison between different aspects of generalized hydrodynamic equations, when one considers a relaxation time to solve difficulties of ordinary hydrodynamics is made from three different points of view, both macroscopic and microscopically.

It is well known that the linearized hydrodynamic equations are satisfactory to describe the behavior of a system near its equilibrium state (long times), however, if we extend their range for shorter times, we find some phenomenological difficulties as well as microscopic ones. In this note we show that the introduction of a relaxation time enables us to solve these difficulties.

We consider three aspects of the problem: a) Firstly, the results obtained in experiments on dispersion of sound have shown that the dispersion relation obtained from the linearized hydrodynamic equations is in disagreement with experimental data for short times. Consider the linearized

---

* Also at Instituto Mexicano del Petróleo.

equations for a one component system.

$$\rho_0(\partial/\partial t)\begin{pmatrix} v(\boldsymbol{r},t) \\ s(\boldsymbol{r},t) \\ \mathbf{v}(\boldsymbol{r},t) \end{pmatrix} = \begin{pmatrix} 0 & 0 & \nabla \\ 0 & (\lambda/T_0)\nabla^2 & 0 \\ \nabla & 0 & \eta\nabla^2 + (\tfrac{1}{3}\,\eta + \eta_v)\nabla\nabla \end{pmatrix}\begin{pmatrix} -p(\boldsymbol{r},t) \\ T(\boldsymbol{r},t) \\ \mathbf{v}(\boldsymbol{r},t) \end{pmatrix} , \tag{1}$$

where ρ_0 is the equilibrium density, $v(\boldsymbol{r},t)$, $s(\boldsymbol{r},t)$, $p(\boldsymbol{r},t)$ and $T(\boldsymbol{r},t)$ are specific volume, specific entropy, pressure and temperature deviations from equilibrium values, $\mathbf{v}(\boldsymbol{r},t)$ is the hydrodynamic velocity; λ, η_v and η are the thermal conductivity and the volumetric and shear viscosities. Fourier transformation of eq. (1) enables us to obtain the classical Kirchhoff[1] dispersion equation, and a comparison with experimental data about sound dispersion shows a discrepancy for large frequencies[2]. Recently some people[3, 4] suggested a modification of eq. (1) by the introduction of a relaxation time for each constitutive equation flux-thermodynamic force; M. Carrasi and A. Morro[3] suggested the phenomenological relations:[*]

$$\tau_v(\partial/\partial t)\,\mathbf{P}_{\alpha\beta} = -\left[\eta(\partial v_\beta/\partial x_\alpha) + (\partial v_\alpha/\partial x_\beta) + (\eta_v - \tfrac{2}{3}\eta)\,\mathrm{div}\,\mathbf{v}\,\delta_{\alpha\beta} + \mathbf{P}_{\alpha\beta} - p\,\delta_{\alpha\beta}\right]$$

$$\alpha,\beta = 1,2,3. \tag{2}$$

$$\tau_q(\partial/\partial t)\,\boldsymbol{J}_q = -(\lambda\nabla T + \boldsymbol{J}_q) , \tag{3}$$

where $\mathbf{P}_{\alpha\beta}$ and $\boldsymbol{J}_q$ are the pressure tensor and the heat flux, τ_v and τ_q are the relaxation times associated with these fluxes. Substituting the constitutive equations (2) and (3) in the balance equations for the momentum density and entropy, we obtain, after linearization, the generalized hydrodynamic equations

---

[*] Actually Carrasi and Morro used a slightly different constitutive equation for the pressure tensor, however this does not modify essentially any of these results.

$$\rho_0 (\partial/\partial t)\, v(\mathbf{r}, t) = \nabla \cdot \mathbf{v}(\mathbf{r}, t)$$

$$\rho_0 \left(\tau_q (\partial/\partial t) + 1\right)(\partial/\partial t)\, s(\mathbf{r}, t) = (\lambda/T_0)\, \nabla^2 T(\mathbf{r}, t) \qquad (4)$$

$$\rho_0 \left(\tau_v (\partial/\partial t) + 1\right)(\partial/\partial t)\, \mathbf{v}(\mathbf{r}, t)$$

$$= - \nabla p(\mathbf{r}, t) + \left[(\eta_v + \tfrac{1}{3}\,\eta)\, \nabla\nabla \cdot \mathbf{v}(\mathbf{r}, t) + \eta \nabla^2 \mathbf{v}(\mathbf{r}, t)\right] ,$$

these new equations yield to a generalized Kirchhoff's equation which agrees with experimental data for large frequencies when $\tau_v = \tau_q \simeq 10^{-9}$ sec, which is of the same order of magnitude as the collision time. It is clear that equations (4) reduce to the usual linearized equations (1) when the relaxation time goes to zero. We remark that eq. (3) has been proposed by several authors to explain the fact of non instantaneous temperature changes in the system[4].

b) From a fluctuation theory point of view, R. Zwanzig[5] showed that the Langevin equation yields to contradictions when the transport processes are not slow, and he proposed a generalized Langevin equation

$$(\partial/\partial t)\, \overline{a}_i(\mathbf{k}, t) = - \int_0^t dt'\, K_{ij}(\mathbf{k}, t')\, \overline{a}_j(\mathbf{k}, t - t') , \qquad (5)$$

where the $\overline{a}_i(\mathbf{k}, t)$ are the Fourier transform in $\mathbf{r}$ of the average deviation from the equilibrium values of the dynamical variables which describe the system, and $K_{ij}(\mathbf{k}, t)$ is the memory function. Equation (5) and a parameter of slowness drop out the difficulties presented by the Langevin equation, furthermore, we obtain the relationships between the time-correlation functions and the transport coefficients. We propose the simplest memory function for the generalized Langevin equation[6]

$$K_{ij}(\mathbf{k}, t) = \left(L_{is}(\mathbf{k})\, g_{sj}/\tau_i\right) \exp\,(- t/\tau_i) , \qquad (6)$$

where g_{sj} is the matrix corresponding to the second derivatives of entropy, the τ_i are the relaxation time for each flux $J_i(\mathbf{k}, t) = (\partial/\partial t)\, a_i(\mathbf{k}, t)$ and $L_{is}(\mathbf{k})$ is the transport coefficients matrix which in the case of a simple one component fluid reduces to

$$L_{is}(\boldsymbol{k}) = (T_0/\rho_0) \begin{pmatrix} 0 & 0 & -ik \\ 0 & -(\lambda/T_0)\boldsymbol{k}^2 & 0 \\ -ik & 0 & -\eta\boldsymbol{k}^2 - (\eta_v + \tfrac{1}{3}\eta)\,kk \end{pmatrix} \tag{7}$$

Substituting eq. (6) in the generalized Langevin equation (5) we can write the flux-force generalized relationships which have the following form

$$\tau_i(\partial/\partial t)\, J_i(\boldsymbol{k},t) = L_{ij}(\boldsymbol{k})\, X_j(\boldsymbol{k},t) - J_i(\boldsymbol{k},t) \ , \tag{8}$$

where the $X_j(\boldsymbol{k},t) = -g_{js}\,\overline{a}_s(\boldsymbol{k},t)$ are the Fourier transforms in $\boldsymbol{r}$ of the generalized thermodynamic forces.

Moreover taking into account that the $\boldsymbol{r}$-Fourier transform of the linearized hydrodynamic equation (1) is related to the Langevin equation[6], we can establish the relationship between the generalized hydrodynamic equations and the generalized Langevin equation. In particular we immediately see that the constitutive equations (8) have the same form that the relations (2) and (3) which have been proposed from purely phenomenological arguments.

c) Lastly, L. P. Kadanoff and P.C. Martin[8] have used the susceptibilities (Fourier-Laplace transform of the response function), obtained from the linearized hydrodynamic equations to calculate sum rules. This procedure leads to discrepancies with the calculation of the same rules based on the continuity equations satisfied by the quantum-mechanical operators associated with the dynamical variables of interest. Such discrepancies appear because one extrapolates to large frequencies the information contained in the linearized hydrodynamic equations.

Kadanoff and Martin studied the spin diffusion problem and solved these difficulties through the *ad hoc* introduction of a relaxation time. The same problem appears in the hydrodynamic equations for a simple one component fluid, *i. e.* , one can calculate the commutation relations corresponding to the sum rules, from the conservation equations satisfied by the operators such as density, momentum and energy; in fact the third sum rule (second derivative of the Fourier transform in $\boldsymbol{R} = \boldsymbol{r} - \boldsymbol{r}'$ of the relaxation function) is proportional to $\boldsymbol{k}^2$ when the operators satisfy conservation laws. Thus

$$[(\partial^2/\partial t^2)\int dR\, \exp(-i\boldsymbol{k}\cdot \boldsymbol{R})\Big(\int_t^{\infty} d\tau\, (1/i\hbar)\, \big\langle [A(\boldsymbol{r}',t'), B(\boldsymbol{r},t)]\big\rangle_{\mathrm{eq}}\Big)]_{t=0}\ \alpha \boldsymbol{k}^2 \tag{9}$$

where $A(\boldsymbol{r},t)$ and $B(\boldsymbol{r},t)$ are any of such operators and $\tau = t - t'$.

The same sum rule[10] calculated from the susceptibilities obtained from the linearized hydrodynamic equations is proportional to $\boldsymbol{k}^4$, which shows that the linearized hydrodynamic results do not satisfy the microscopic requirements imposed by the commutation relations.

Then, it is straightforward to use generalized hydrodynamic equations the simplest set being obtained with flux-force relationships which contain a relaxation time as in eqs. (8), (2), (3) and give us the correct $\boldsymbol{k}^2$ dependence in the sum rule.

Furthermore, using the value which results from the calculation of the sum rule using the generalized hydrodynamic equations in terms of relaxation times, it is possible to compare with the sum rule value in eq. (9), which can be calculated from a microscopic model. This procedure determines directly the value of the relaxation time. In this form some rule calculations[11] lead us to associate with the momentum density a relaxation time

$$\tau_v = (\eta/\rho_0 c^2) \simeq 10^{-9}\,\mathrm{seg}$$

where c^2 is given in reference (11) and contains only microscopic parameters associated with the intermolecular potential and the pair distribution function

Now, we ask about the relationship between different aspects of this problem. First of all, we know that the phenomenological relations which contain relaxation times of the order of magnitude of collision times give some agreement with experimental data on sound dispersion. Secondly, if we interpret the linearized equations as Langevin ones, it is remarked that the inconsistencies pointed out can be eliminated by introduction of generalized equations (time-dependent transport coefficients), and the simplest generalization yields the flux-force relation we mentioned before. Finally, the microscopic restrictions imposed by the sum rules lead us to the same generalized hydrodynamic equations. Thus we can say that this simplest generalization enables us to solve the problem in the phenomenological level consistently with the microscopic one.

Furthermore, we are proposing a method to evaluate the relaxation time which appears in the phenomenological relaxations. In fact we point out that the order of magnitude of τ_v is that needed to have a good agreement with the experimental data. Moreover these times give us the order of magnitude of frequencies in which it is possible to neglect non-Markoffian contributions to the generalized Langevin equation.

ACKNOWLEDGMENT

The authors sincerely wish to thank Prof. L. García-Colín for helpful suggestions during the preparation of this manuscript.

REFERENCES

1. S.R. de Groot, P. Manzur, *Non-Equilibrium Thermodynamics*, (North Holland, 1962).
2. J.D. Foch, G.W. Ford, ***Studies in Statistical Mechanics***, Vol. V, ed. by J. de Boer, G.E. Uhlenbeck, (North Holland, 1970).
3. M. Carrasi, A. Morro, Il Nuovo Cimento, 9B (1972) 321.
4. P. Vernotte, Compt. Rend., 246 (1958) 3154.
5. R. Zwanzig, J. Chem. Phys., 40 (1964) 2527.
6. B. Robertson, Phys. Rev., 160 (1967) 175,
   B.J. Berne, D. Forster, Ann. Rev. Phys. Chem., 22 (1971) 563.
7. B.U. Felderhoff, I. Oppenheim, Physica, 31 (1965) 1441.
8. L.P. Kadanoff, P.C. Martin, Ann. Phys. 24 (1963) 419.
9. R. Kubo, *Lectures Theor. Phys.*, (Boulder), 1 (1958) 120.
10. R.M. Velasco, *The theory of linear response and its applications to chemically reactive media* (Ph.D. Thesis, University of México, 1973) unpublished.
11. D. Forster et.al., Phys. Rev., 170 (1968) 155.

RESUMEN

Usando tres diferentes puntos de vista, tanto macroscópicos como microscópicos, se hace una comparación de diversos aspectos de las ecuaciones hidrodinámicas generalizadas considerando un tiempo de relajamiento para eliminar dificultades en la hidrodinámica ordinaria.