The thermohydrodynamical picture of a charged Brownian particle

L.A. Barreiro, J.R. Campanha and R.E. Lagos
Departamento de Física, IGCE UNESP
CP 178, 13500-970 *Rio Claro, SP, Brazil*
monaco@rc.unesp.br

Recibido el 18 de enero de 2001; aceptado el 18 de julio del 2001

We study a charged Brownian gas with a non uniform bath temperature, and present a thermohydrodynamical picture. Expansion on the collision time probes the validity of the local equilibrium approach and the relevant thermodynamical variables. For the linear regime we present several applications (some novel).

Keywords: Thermodynamics, brownian motion.

Estudiamos un gas browniano con carga y presentamos el cuadro termohidrodinámico considerando una temperatura de contenerdor no uniforme. Con una expansión en el tiempo de colisión exploramos la validez de la hipótesis de equilibrio local y las posibles variables termodinámicas relevantes. En el régimen lineal presentamos varias aplicaciones (algunas inéditas).

Descriptores: Termodinámica, movimiento browniano.

PACS: 05.40.Jc; 05.70.Ln; 82.20.Mj

We generalize previous work [1], considering a magnetic field [2] and a non uniform bath temperature $T(\mathbf{x},t)$. Following the Ref. 1 we write down Kramers equation for the probability distribution $P(\mathbf{x},\mathbf{v},t)$ in phase space for the Brownian particle (mass m charge e) under an external force $\mathbf{F}$:

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\frac{\partial}{\partial \mathbf{x}}+\frac{1}{m}\mathbf{F}\frac{\partial}{\partial \mathbf{v}}\right)P=J, \tag{1}$$

$$J=\frac{1}{\tau}\frac{\partial}{\partial \mathbf{v}}\left(\mathbf{v}+v_T^2\frac{\partial}{\partial \mathbf{v}}\right)P-\frac{1}{\tau_0}\left(P-\mathbf{n}_0 f_0(\mathbf{v})\right). \tag{2}$$

The Fokker-Planck collision time τ is the inverse of the friction coefficient and the thermal velocity v_T is given by $mv_T^2=T$ (hereinafter $k_B=1$). The diffusion coefficient D and the mobility $\xi=\tau/m$ are related via the celebrated Einstein relation D$=\xi T=\tau v_T^2$. In the collision term J we include a generalized BGK collision mechanism [3]. The latter is characterized by a relaxation time τ_0 and a prescribed referential particle density $n_0(\mathbf{x},t)$ (for example the actual Brownian particle density $n(\mathbf{x},t)$). f_0 is the usual equilibrium distribution function. The external force (not necessarily uniform) includes a mechanical part $-\nabla V_{\text{mec}}$, an electric field $\mathbf{E}=-\nabla\phi$ and a magnetic field $\mathbf{B}$. Let us define a potential function $V=V_{\text{mec}}+e\phi$ and a covariant derivative $\mathbf{D}=\nabla+\mathbf{\Gamma}$, where

$$\nabla=\frac{\partial}{\partial \mathbf{x}} \quad and \mathbf{\Gamma}=T^{-1}\nabla V.$$

Also define the vector ω (notice the cyclotron frequency is $|\omega|=\omega_c$) by $mc\omega=e\mathbf{B}$. Thus the external force $\mathbf{F}$ is given by $\mathbf{F}(\mathbf{x},\mathbf{v})=-\nabla V-m\omega\times\mathbf{v}$. We generalize our previous ansatz [1] as:

$$P=f_0(\mathbf{v})\sum_{n_i=0}^{\infty}\Psi_{\mathbf{n}}(\mathbf{x},t)\prod_{k=1}^{3}\left(\frac{\Phi_{n_k}(w_k)}{\Phi_0(w_k)}\right), \tag{3}$$

where $\Phi_{n_k}(w_k)$ are the orthonormal Hermite functions with $\sqrt{2}v_T w_k=v_k$ and with $\mathbf{n}=(n_1,n_2,n_3)$. As before, we require the density of Brownian particles to be

$$n(\mathbf{x},t)=\int d\mathbf{v}P(\mathbf{x},\mathbf{v},t).$$

By direct substitution of the ansatz into (1), and as in Ref. 1 a set of differential recursive (difference) equations for the $\Psi_n's$ are readily obtained. After a partial integration we obtain

$$\frac{\tau}{\tau_0}n_0\delta_{\mathbf{n},\mathbf{0}}+\tau\omega\cdot\mathbf{A}^{\star}\times\mathbf{A}Z_{\mathbf{n}}=(\mathbf{A}^{\star}\mathbf{A}+\tau R)Z_{\mathbf{n}}, \tag{4}$$

$$R=\partial+\nabla\mathbf{A}^{\star}+v_T^2\left(\mathbf{D}\mathbf{A}+\mathbf{A}^2\left(\frac{\partial g}{\partial t}+\mathbf{Q}\nabla g\right)\right), \tag{5}$$

where

$$\sqrt{n_1!n_2!n_3!}Z_{\mathbf{n}}=v_T^{n_1+n_2+n_3}\Psi_{\mathbf{n}},$$

$$\partial=\frac{\partial}{\partial t}+\tau_0^{-1}, 2g=\ln \mathrm{T}.$$

The asymmetric lowering and raising operators $\mathbf{A}$ and $\mathbf{A}^*$ are defined respectively by

$$A_1Z_{\mathbf{n}}=Z_{n_1-1,n_2,n_3} \quad and \quad A_1^{\star}Z_{\mathbf{n}}=(1+n_1)Z_{n_1+1,n_2,n_3}$$

(similarly for the remaining components), and with $\mathbf{Q}=v_T^2\mathbf{A}+\mathbf{A}^{\star}$.

The particle number balance equation (Eq.4 with $|\mathbf{n}| = 0$) defined here as the generalized Smoluchowsky equation, is given by

$$\frac{\partial n}{\partial t} + \nabla \mathbf{J} = -\frac{1}{\tau_0}\left(n - n_0\right), \tag{6}$$

with $\mathbf{J} = (Z_{100}, Z_{010}, Z_{001})$. The passage to hydrodynamics is performed as before [1] defining the particle flux, the charge flux, the pressure tensor and the energy flux, respectively by:

$$\mathbf{J} = \int d\mathbf{v}\mathbf{v}P(\mathbf{x},\mathbf{v},t),$$

$$\mathbf{J}_e = e\mathbf{J}, \quad \mathbf{\Pi}(\mathbf{x},t) = m\int d\mathbf{v}\mathbf{v}\mathbf{v}P(\mathbf{x},\mathbf{v},t) \quad \text{and}$$

$$2\mathbf{J}_E(\mathbf{x},t) = m\int d\mathbf{v}\mathbf{v}\mathbf{v}^2P(\mathbf{x},\mathbf{v},t).$$

We also define the energy density E and the nonequilibrium temperature Θ as before [1]; $2E(\mathbf{x},t) = \mathrm{Tr}\mathbf{\Pi} = 3p = 3n\Theta$. Again from Eq. (4), this time with $|\mathbf{n}| = 1$, we derive the balance equation for the charge flux (generalized Ohm law [4]):

$$\tau^\star \frac{\partial \mathbf{J}_e}{\partial t} + \mathbf{J}_e = \sigma^\star \mathbf{W}, \tag{7}$$

$$\mathbf{W} = \mathbf{E} + R_H \mathbf{J}_e \times \mathbf{B} - \frac{1}{e}\nabla V_{\mathrm{mec}} - \frac{1}{en}\nabla \mathbf{\Pi}, \tag{8}$$

where $\tau^{*-1} = \tau^{-1} + \tau_0^{-1}$, $\sigma^\star = m^{-1}e^2\tau^* n$ and $R_H^{-1} = nec$. With the additional definitions $\varepsilon = mnv_T^2$ and $\varepsilon_0 = mn_0v_T^2$ we obtain for the energy flux balance equation [Eq.(4), with $1 < |\mathbf{n}| \leq 3$]

$$\frac{\partial E}{\partial t} + \nabla \mathbf{J}_E = -\mathbf{J}\nabla V - \frac{2}{\tau}(E - \varepsilon) - \frac{1}{\tau_0}(E - \varepsilon_0). \tag{9}$$

We perform the passage to thermodynamics [1] with the definition for the entropy density

$$S = \int d\mathbf{v} \quad S^*(\mathbf{x},\mathbf{v},t) = -\int d\mathbf{v}$$

$P(\mathbf{x},\mathbf{v},t)\ln\lambda\ P(\mathbf{x},\mathbf{v},t)$(with $\lambda = \mathrm{e}^{-1}\left(h/m\right)^3$, $\ln \quad \mathrm{e} = 1$, so in the appropriate limit we retrieve the usual thermodynamical entropy [1]). The entropy flux is defined as

$$\mathbf{J}_S = \int d\mathbf{v}\mathbf{v} \quad S^*(\mathbf{x},\mathbf{v},t),$$

then the entropy density balance equation is given by

$$\frac{\partial S}{\partial t} + \nabla \mathbf{J}_S = -\int d\mathbf{v} J\left(1 + \ln\lambda P\right). \tag{10}$$

Also as in Ref. 1 we define the generalized free energy densities F and G, and the intrinsic and total chemical potentials respectively as $F = E - \Theta S$, $G = F + p = n\mu_{\mathrm{int}}$ and $\mu = \mu_{\mathrm{int}} + V$. Here we introduce no a priori assumptions on the functional dependence of the entropy (as in the local equilibrium approach, LEQ) nor do we assume relevant variables as is extended irreversible thermodynamics (EIT, [5]). As in Ref. 1, all fluxes (including the ones not computed here), Θ, μ, S, in fact all thermodynamic potentials can be expanded in powers of τ (adequate at least in the overdamped limit and with $\tau_0 \gg \tau$), formally rendering all variables universal functions of the set $\{\nabla, \mathbf{D}, n, T, \mathbf{B}\}$. Thus, at any given τ expansion stage, the only relevant variables are n and T. For Brownian motion, the universal equation for the particle density is the generalized Smoluchowsky equation plus a set of boundary conditions (BC). This picture is distinct but not inconsistent with EIT [5], where incorporating the BC to the fluxes, the latter may be interpreted as relevant variables. LEQ is satisfied only to first order in τ, where

$$\Theta = T(1 - \tau\frac{\partial \ln g}{\partial t}).$$

Hereafter we consider the linear (first order in τ) case and a stationary temperature $T = \Theta$. Then the particle flux is cast as (with $\mathbf{B} = B\hat{z}$)

$$\mathbf{J} = -\xi\mathbf{K}n\nabla V - \mathbf{K}\nabla(\mathrm{D}n), \tag{11}$$

$$\mathbf{K} = \frac{1}{1+\theta^2}\begin{pmatrix} 1 & \theta & 0 \\ -\theta & 1 & 0 \\ 0 & 0 & 1+\theta^2 \end{pmatrix}, \tag{12}$$

with

$$\theta = \mathrm{D}\mathrm{D}_B{}^{-1}$$

and where Bohm's diffusion coefficient is

$$D_B = cT(eB)^{-1}.$$

Notice that

$$\theta = \sigma_0 B R_H = \tau\omega_c \quad where \quad \sigma_0 = m^{-1}e^2\tau n.$$

The scope of the Brownian motion scheme is highlighted with some direct applications of Eq. (11):

a)If diffusion is disregarded ($\nabla n = 0$, say electrons in a metal) and with $\nabla T = 0$ we retrieve the classical magnetoresistance and Hall effect models [6]

b) If we consider two Brownian gases, say electrons and holes (inhomogeneous semiconductors), with the n_0's the equilibrium carriers' densities and the τ_0's generation-recombination times, then (6) together with (11) constitute generalized transport equations [6]

c)The diffusive part has the 'correct Fick law' for nonuniform temperature [7]

d) Equation (11) can also de cast as

$$\mathbf{J} = -\xi\mathbf{K}(n\nabla\mu + S\nabla T) \tag{13}$$

in agreement with Ref. 8 for the $\nabla T = 0$ case, suggesting that diffusive mass transport is solely convective transport of both mass and entropy; and finally

e)In the high magnetic field regime and with $\nabla T = 0$ the cross diffusion current is driven by $D_B \sim B^{-1}$ the anomalous Bohm coefficient, never derived but proposed to explain the observed B^{-1} behavior instead of the expected B^{-2} term [9].

Work in progress includes illuminated systems [10], chemical reactions [11], the non linear regime in earnest, transport and entropy production general properties, and the validity of any Onsager-like scheme.

Acknowledgments

This work was supported by *FAPESP, SP* Brazil.

1. L.A. Barreiro, J.R. Campanha and R.E. Lagos, arXiv: cond-mat/9910405; *Physica A* **283** (2000) 160.
2. R. Czopnik and P. Garbaczewsky, arXiv: cond-mat/0005353.
3. P.L. Bathnagar, E.P. Gross and M. Krook, *Phys. Rev.* **94** (1954) 511.
4. D.R. Nicholson, *Introduction to Plasma Theory* (John Wiley & Sons, 1983)
5. D. Jou, J. Casas-Vásquez and G. Lebon, *Rep. Prog. Phys.* **62** (1999) 1035.
6. N.W. Ashcroft and N.D. Mermin, *Solid State Physics* (Holt, Rinehart and Winston, 1976).
7. N.G. van Kampen, *Z. Phys. B* **68** (1987) 135.
8. R. Landauer, *Helvetica Physica Acta* **56** (1983) 847.
9. F.C. Chen, *Introduction to Plasma Physics* (Plenum Press, NY & London, 1974).
10. R.E. Lagos, H. Suhl and T. Tiedje, *J. Appl. Phys.* **54** (1983) 3951.
11. R.E. Lagos, T.P. Simões and A.L. Godoy, *Physica A* **257** (1998) 401.