Diffusion equation for semiclassical bosons and fermions

1979 J. Phys. A: Math. Gen. 12 541

(http://iopscience.iop.org/0305-4470/12/4/013)

J. Phys. A: Math. Gen., Vol. 12, No. 4, 1979. Printed in Great Britain

Diffusion equation for semiclassical bosons and fermions

S Harris

College of Engineering and Applied Sciences, State University of New York at Stony Brook, Stony Brook, New York 11794, USA

Received 31 July 1978, in final form 4 October 1978

Abstract. We derive the equation of evolution in the configuration space for a system of semiclassical bosons or fermions starting from the recently derived nonlinear Kramers–Chandrasekhar equation for such particles. The latter equation does not contract to the corresponding Fokker–Planck equation in the velocity space; however, we show that in the context of a Chapman–Enskog approximation the contraction to the physical space leads to the diffusion equation with the classical relationship between the self-diffusion coefficient and the friction coefficient maintained.

1. Introduction

The classical Kramers–Chandrasekhar (KC) equation (Chandrasekhar 1943, equation (249)) provides a description of Brownian particle motion in the full μ space. Contracted descriptions, in either the momentum or configuration space, are also of interest and are frequently all that are required for dealing with a given situation, e.g. spatial homogeneity or relaxation on the macroscopic time scale. In the former case the Fokker–Planck (FP) equation can be obtained easily by direct integration over the spatial variable, but in the latter case some care is necessary if a closed equation for the density is to be obtained. A variety of approximate techniques have been employed in reducing the KC equation to the diffusion equation, but in our opinion the Chapman–Enskog method (Resibois 1965) is the most direct of these.

The situation described above becomes less clear when the Brownian particles obey the exclusion principle, i.e. are bosons or fermions. A semiclassical theory of such systems has recently been developed by Balazs (1978), who has obtained both the KC and FP equations. As might be expected, the collision terms in both of these equations are nonlinear, reflecting the effects of the exclusion principle, and in this respect these equations are similar to the semiclassical generalisation of the Boltzmann equation obtained some time ago by Uehling and Uhlenbeck (1933). As a result of this nonlinearity, the KC equation does not contract into the FP equation after integration over the spatial coordinate, which indicates that the contraction to a diffusion equation may encounter similar problems. This uncertainty has a further basis in that the streaming term in the generalised KC equation is also nonlinear, and this term plays an important role in the reduction to the diffusion equation. As we shall see, however, it is just this nonlinear form which is required to obtain the diffusion equation. Our specific purpose here will be to show that, in the context of a Chapman–Enskog-like theory, the generalised KC equation does reduce to the diffusion equation with a diffusion coefficient which depends on the friction coefficient in the usual (classical) manner.

0305-4470/79/040541+03$01.00

2. Chapman–Enskog approximation

The generalised KC equation derived by Balazs (1978) is

$$\frac{\partial f}{\partial t}+\boldsymbol{p}\cdot\frac{\partial}{\partial \boldsymbol{q}}f(1-af)=\zeta\frac{\partial}{\partial \boldsymbol{p}}\cdot\left[\boldsymbol{p}f(1-af)+\frac{1}{2}\frac{kT}{\zeta}\frac{\partial f}{\partial \boldsymbol{p}}\right]$$
$$\equiv \zeta\Omega f \tag{1}$$

where, in the semiclassical description, $f=f(\boldsymbol{q},\boldsymbol{p},t)$, $a=h^3/\beta$ for fermions with β the Brownian particle statistical weight, ζ is the friction coefficient, and the particle mass has been set equal to unity. For bosons the sign of a is negative.

The Chapman–Enskog solution (Resibois 1965) is found by expanding f in a parameter ϵ of the same order of smallness as the spatial gradients in the system. Thus, each $\partial/\partial\boldsymbol{q}$ on the LHS of equation (1) is considered to $O(\epsilon)$. Further, the time dependence of f on the macroscopic time scale is assumed to be through $n(\boldsymbol{q},t)=\int \mathrm{d}\boldsymbol{p}\, f(\boldsymbol{q},\boldsymbol{p},t)$ so that $\partial f/\mathrm{d}t\rightarrow(\delta f/\delta n)(\partial n/\partial t)$ on this time scale. Then $\partial f/\partial t$ (as well as $\partial f/\partial\boldsymbol{q}$) will be at least of $O(\epsilon)$ since $\partial n/\partial t$ contains spatial gradients. Writing $f=\Sigma_i\,\epsilon^i f^{(i)}$, with the constraint $n=\int\mathrm{d}\boldsymbol{p}\, f^{(0)}$, and substituting this into equation (1) we obtain the following equations by equating terms of order ϵ^0 and ϵ':

$$\Omega f^{(0)}=0 \tag{2}$$

$$-\frac{\delta f^{(0)}}{\delta n}\frac{\partial}{\partial\boldsymbol{q}}\cdot\int \mathrm{d}\boldsymbol{p}\,\boldsymbol{p}f^{(0)}(1-af^{(0)})+\boldsymbol{p}\cdot\frac{\partial}{\partial\boldsymbol{q}}f^{(0)}(1-af^{(0)})=\zeta\Omega^{(1)}f^{(1)} \tag{3}$$

where $\Omega^{(1)}f^{(1)}$ denotes the entire $O(\epsilon)$ contribution of Ωf. In equation (3) the first term on the LHS has been obtained by integrating equation (1) over $\boldsymbol{p}$ to obtain

$$\frac{\partial n}{\partial t}-\frac{\partial}{\partial\boldsymbol{q}}\cdot\int\mathrm{d}\boldsymbol{p}\,\boldsymbol{p}f(1-af) \tag{4}$$

and noting that, since the gradient introduces an $O(\epsilon)$, f can be replaced by $f^{(0)}$ in writing $\partial f/\partial t$ to $O(\epsilon)$.

The solution to equation (2) is

$$f^{(0)}=(a+A\exp(p^2/2kT))^{-1} \tag{5}$$

where A is related to $n(\boldsymbol{q},t)$ as follows from normalisation. Expanding the RHS of equation (4) we see that to lowest (non-vanishing) order

$$\frac{\partial n}{\partial t}=-\frac{\partial}{\partial\boldsymbol{q}}\cdot\int\mathrm{d}\boldsymbol{p}\,\boldsymbol{p}[f^{(1)}(1-af^{(0)})+f^{(0)}(1-af^{(1)})]. \tag{6}$$

The RHS of equation (6) can be replaced by an integral depending on the known quantity $f^{(0)}$ only; this follows from operating on equation (3) by $\int\mathrm{d}\boldsymbol{p}\,\boldsymbol{p}$ which allows us to write

$$\frac{\partial n}{\partial t}=-\frac{1}{3\zeta}\frac{\partial^2}{\partial q^2}\int\mathrm{d}\boldsymbol{p}\,p^2f^{(0)}(1-af^{(0)}). \tag{7}$$

The integral on the RHS of equation (7) can be related to $n(\boldsymbol{q},t)$ by an integration by parts. This is perhaps most easily seen by changing the varaible of integration in the intermediate steps to $x = p^2/2kT$. As a result we can write equation (7) in the canonical form

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial q^2} \tag{8}$$

with the classical relationship for the self-diffusion coefficient $D = kT/\zeta$. Although the Einstein relationship $D = kT/\zeta$ still holds, the friction coefficient itself will differ from its classical value. The evaluation of this quantity is a separate problem and, though of interest, will not be considered at this time.

The Chapman–Enskog procedure can also be followed in the case where an external field, $\boldsymbol{K}(\boldsymbol{q})$, is present provided that the field curvature is such that the characteristic distances for the potential and density spatial gradients are the same. The generalized KC equation in this case will include an additional term $\boldsymbol{K}\,.\,(\partial/\partial \boldsymbol{p})f(1-af)$ on the left side (Balazs 1978). Applying the Chapman–Enskog procedure, the equation for $f^{(0)}$ remains unchanged, so that this quantity is again given by equation (5). The equation for $f^{(1)}$ now includes an additional term $\boldsymbol{K}\,.\,(\partial/\partial \boldsymbol{p})f^{(0)}(1-af^{(0)})$ on the left side. With these changes in the basic equations the same procedure as followed above leads to the Smoluchowski equation

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial q^2} - \frac{1}{\zeta}\frac{\partial}{\partial \boldsymbol{q}}\cdot \boldsymbol{K}n. \tag{9}$$

3. Concluding remarks

It is significant to note that the above results are dependent on the altered form of the streaming term appearing in the generalised KC equation; with the usual form of the streaming term, as appears in the Uehling–Uhlenbeck equation (Uehling and Uhlenbeck 1933) the diffusion and Smoluchowski equations will not be recovered. This demonstration is the main object of this paper.

Finally, we might note one further interesting consequence of the particle statistics. In the classical case, $a = 0$, equation (1) can be used to calculate the momentum autocorrelation function directly, but for $a \neq 0$ this no longer appears to be the case. However, since the autocorrelation function can also be calculated from the diffusion equation, our results indicate that the classical exponential behaviour implied by that equation still holds.

References

Balazs N L 1978 *Physica* to be published
Chandrasekhar S 1943 *Rev. Mod. Phys.* **15** 1
Resibois P 1965 *Electrolyte Theory* (New York: Harper and Row)
Uehling E A and Uhlenbeck G E 1933 *Phys. Rev.* **43** 552