ELSEVIER

27 March 1995

PHYSICS LETTERS A

Physics Letters A 199 (1995) 241–244

The Landau equation including memory and energy conservation

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Received 3 November 1994; accepted for publication 18 January 1995
Communicated by L.J. Sham

Abstract

In the context of the reduced density operator technique the derivation of non-Markovian kinetic equations is briefly reviewed. It is shown that the time retardation in the collision integrals leads to total energy conservation, while the ordinary quantum Boltzmann equation provides only kinetic energy conservation.

The derivation of generalized quantum Boltzmann equations is widely known in the literature [1–3]. The general starting point in deriving kinetic equations is the coupled set of equations of motion for the reduced density operators. This set was first derived by Irving and Zwanzig [4]. Their formal structure is similar to the so-called BBGKY hierarchy [5] for reduced distribution functions in classical statistical physics. The first to use this BBGKY hierarchy in deriving kinetic equations were Bogoljubov [6], Born and Green [7] and Kirkwood [8]. The quantum Boltzmann equation differs from the classical one in the collision term, which takes into account that the final scattering states can be occupied and consequently blocked by the Pauli exclusion principle. Moreover, the quantum mechanical transition rate is used, rather than the classical one. Of the various other extensions proposed for the ordinary Boltzmann equation, the work of Klimontovich and Kremp [9] and McLennan [10] should be mentioned, which treats quantum gases with bound states. For a comprehensive review see Ref. [11] and for a review of the development of the kinetic theory during the last fifty years see Ref. [12].

Whereas the ordinary Boltzmann equation yields conservation of density, momentum and *kinetic* energy, it is a challenging question what the kinetic equation should look like in order to conserve the *total* energy, i.e. kinetic and interaction energy. Different procedures are suggested in the literature. Starting from the general considerations of the symmetries in the two-particle correlation functions [13], many attempts have been made to establish approximations, which ensure these symmetries and therefore conserve the total energy [1–3,11,14].

In this Letter it is shown directly how the total energy conservation is connected with the retardation effects or non-Markovian collision integrals. It is apparently not widely known that even in the Born approximation the total energy conservation can be obtained. The equivalence between retardation or memory and energy conservation thus becomes obvious. For the case of simplicity it has been restricted here to non-degenerate spatially homogeneous systems.

Starting from the conserving BBGKY hierarchy of the reduced density operators,

$$\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial t}F_{1\ldots s}=[F_{1\ldots s},H_s]+nTr_{s+1}[F_{1\ldots s+1},V_{s,s+1}]\,, \tag{1}$$

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SSDI 0375-9601(95)00061-5

with the renormalization to a volume $\Omega^s = Tr_{1\ldots s} F_{1\ldots s}$, we want to consider the binary collision approximations, i.e. to neglect the influence of density operators higher than F_{12}. Then the equation for the two-particle density operator (1) is easily solved,

$$F_{12}(t) = \exp\left(\frac{\mathrm{i}}{\hbar} H_2^0(t-t_0)\right) F_{12}(t_0) \exp\left(\frac{\mathrm{i}}{\hbar} H_2^0(t-t_0)\right)$$
$$+ \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} \exp\left(-\frac{\mathrm{i}}{\hbar} H_2^0(t-t')\right) [F_{12}(t'), V_{12}] \exp\left(\frac{\mathrm{i}}{\hbar} H_2^0(t-t')\right) \mathrm{d}t' . \tag{2}$$

The two-particle Hamiltonian was split into $H_2 = H_2^0 + V_{12}$. In the first Born approximation, the solution reads

$$F_{12}(t) = F_1(t)F_2(t) + \frac{\mathrm{i}}{\hbar} \int_{t_0}^{t} \exp\left(-\frac{\mathrm{i}}{\hbar} H_2^0(t-t')\right) [F_1(t')F_2(t'), V_{12}] \exp\left(\frac{\mathrm{i}}{\hbar} H_2^0(t-t')\right) \mathrm{d}t' + \mathrm{o}(V_{12}^2) \tag{3}$$

where at the artificial time t_0 the two-particle density can be factorized into $F_{12}(t_0) = F_1(t_0)F_2(t_0)$. This is also known as weakening of the initial correlation. Further, an analogous equation for the one-particle density is used to propagate $F_1(t_0)$ to $F_1(t')$. In this way additional terms linear in V would arise, but they vanish when inserted into the collision integral of Eq. (1) due to the double commutator structure. Substituting Eq. (3) back into the first equation of (1), one obtains the kinetic equation for the one-particle density operator. For spatially homogeneous systems, which will be considered in the following, the momentum representation of the operator F_1 is the appropriate choice. The resulting equation for the one-particle distribution function is

$$\frac{\partial}{\partial t} f(p_1) = \frac{1}{\hbar^2} \int \frac{\mathrm{d}p_2 \mathrm{d}p_1' \mathrm{d}p_2'}{(2\pi\hbar)^9} V(|p_1 - p_1'|)^2 (2\pi\hbar)^3 \delta(p_1 + p_2 - p_1' - p_2')$$
$$\times \int_0^{\infty} \mathrm{d}\tau \, [f(p_1', t-\tau) f(p_2', t-\tau) - f(p_1, t-\tau) f(p_2, t-\tau)] \times 2\cos\left(\frac{1}{\hbar}(\epsilon_1 + \epsilon_2 - \epsilon_1' - \epsilon_2')\tau\right). \tag{4}$$

Here we used the normalization $\int [\mathrm{d}p_1/(2\pi\hbar)^3] f(p_1) = n$ and $\epsilon = p^2/2m$. Further, we assumed a potential $\langle p_1 p_2 | V | p_1' p_2' \rangle = (2\pi\hbar)^3 V(p_1 - p_1') \delta(p_1 + p_2 - p_1' - p_2')$. This form of kinetic equation is well known in the literature [1,15–17] and plays an important role in considerations of large-field problems [18,19,15]. An alternative approach for the quantum case has been given in Ref. [20]. If one neglects the time retardation in the distribution functions, one obtains the usual quantum Boltzmann collision integral using the identity $\int_0^{\infty} \mathrm{d}\tau \cos(a\tau) = \pi\delta(a)$. The influence of retardation in Eq. (4) can be calculated numerically. This leads to a diminishing of the influence of collisions on the temporal development of the distribution function [21]. For transport problems in electric fields it can be shown that Eq. (4) reproduces precisely the Debye–Onsager relaxation effect, which diminishes the applied electric field through the moving screening cloud [22].

Now we will turn to the interesting question of conservation laws. Multiplying Eq. (4) by 1 or $\boldsymbol{p}$ and integrating over p_1, one obtains the density or momentum conservation,

$$\frac{\partial}{\partial t} n = 0 , \qquad \frac{\partial}{\partial t} \langle p_1 \rangle = 0 ,$$

where the momentum-conserving δ distribution function is used in the manner known from the treatment of the ordinary Boltzmann equations. The total energy conservation is more interesting. While the ordinary quantum Boltzmann equation conserves only the kinetic energy it will be shown now that Eq. (4) leads to total energy conservation. This can be elaborated by multiplying Eq. (4) by $p^2/2m$ and integrating over p_1. The right-hand side of the resulting equation can be written as a time derivation and one finally obtains

$$\frac{\partial}{\partial t}\left(\left\langle\frac{p_1^2}{2m}\right\rangle+\langle V_{12}\rangle\right)=0\,, \tag{5}$$

with

$$\langle V_{12}\rangle=\frac{1}{2\hbar}\int\frac{\mathrm{d}p_1\,\mathrm{d}p_2\,\mathrm{d}p_1'\,\mathrm{d}p_2'}{(2\pi\hbar)^{12}}\,V(|p_1-p_1'|)^2(2\pi\hbar)^3\delta(p_1+p_2-p_1'-p_2')$$

$$\times\int_0^\infty \mathrm{d}\tau\,[f(p_1',t-\tau)f(p_2',t-\tau)-f(p_1,t-\tau)f(p_2,t-\tau)]\,\sin\left(\frac{1}{\hbar}\,(\epsilon_1'+\epsilon_2'-\epsilon_1-\epsilon_2)\tau\right). \tag{6}$$

Now it remains to show that (6) is just the interaction part of the energy as we have already indicated. Therefore one calculates the mean correlation energy according to the definition of a two-particle expectation value,

$$\langle V_{12}\rangle=\tfrac{1}{2}n^2Tr_{12}(F_{12}V_{12})\,. \tag{7}$$

On the same level of approximation as used for the derivation of the kinetic equation, one takes the expression for the two-particle density operator (3) and obtains from Eq. (7) in the momentum representation precisely expression (6). Therefore, it is proven that the non-Markovian collision integral (4) leads to complete energy conservation, which makes up for an insufficiency of the ordinary Boltzmann equation.

This represented energy conservation can be extended beyond the Born approximation. The corresponding non-Markovian expressions are given for the T-matrix [23] and for the screened potential approximation [24]. It is interesting that the T-matrix approximation without memory conserves total energy by itself, which is explicitly shown in Ref. [11]. Consequently, the question of the memory effects on the T-matrix approximation will be published elsewhere [23].

Especially for short time scales as in nuclear physics or in nanosecond spectroscopy, total energy conservation should play an important role and therefore this non-Markovian kinetic equation should be used instead of the ordinary quantum Boltzmann equation or Beth–Uhlenbeck equation.

References

[1] Y.L. Klimontovich, Kinetic theory of nonideal gases and nonideal plasmas (Academic Press, New York, 1975).
[2] K. Bärwinkel, in: Proc. 14th Int. Symp. on Rarified gas dynamics (University of Tokyo Press, Tokyo, 1984).
[3] B. Bezzerides and D.F. DuBois, Ann. Phys. (NY) 70 (1972) 10.
[4] J.H. Irving and R.W. Zwanzig, J. Chem. Phys. 19 (1951) 1173.
[5] R. Balescu, Equilibrium and nonequilibrium statistically mechanics, Vol. 2 (MIR, Moscow, 1978) [in Russian].
[6] N.N. Bogoljubov, J. Phys. (USSR) 10 (1946) 256.
[7] M. Born and H.S. Green, Proc. R. Soc. A 188 (1946) 10.
[8] J.G. Kierkwood, J. Chem. Phys. 14 (1946) 180.
[9] Y.L. Klimontovich and D. Kremp, Physica A 109 (1981) 517.
[10] J.A. McLennan, J. Stat. Phys. 28 (1982) 521.
[11] W. Botermans and R. Malfliet, Phys. Rep. 198 (1990) 115.
[12] E.G.D. Cohen, Physica A 194 (1993) 229.
[13] L.P. Kadanoff and G. Baym, Quantum statistical mechanics (Benjamin, New York, 1964).
[14] I.Y. Goncharova, Y.A. Kukharenko and A.S. Lalayan, Kratk. Soobshch. Fiz. 1 (1988) 3.
[15] K. Morawetz and D. Kremp, Phys. Fluids B 1 (1994) 225.
[16] H. Haug and C. Ell, Phys. Rev. B 46 (1992) 2126.
[17] D.B.T. Thoai and H.Haug, Z. Phys. B 91 (1993) 199.
[18] V.P. Seminozhenko, Phys. Rep. 91 (1982) 103.
[19] A.P. Jauho and J.W. Wilkins, Phys. Rev. B 29 (1984) 1919.
[20] M.W. Thomas and R.F. Snider, J. Stat. Phys. 2 (1970) 61.

[21] K. Morawetz, R. Walke and G. Roepke, Phys. Lett. A 190 (1994) 96.
[22] K. Morawetz and D. Kremp, Phys. Lett. A 173 (1993) 317.
[23] K. Morawetz and G. Röpke, Phys. Rev. C (1994), submitted.
[24] K. Morawetz, Phys. Rev. E 50 (1994), to be published.