

# Time evolution of a weakly interacting Bose system, with or without condensate

Oliver Penrose

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## 1 The classical Boltzmann equation and Lanford’s proof

The Boltzmann equation for a classical hard-sphere gas is (p. 78 of [6])

$$\begin{aligned} \frac{\partial}{\partial t} f_t(\mathbf{q}, \mathbf{p}_1) = & -\frac{\mathbf{p}_1}{m} \frac{\partial}{\partial \mathbf{q}} f_t(\mathbf{q}, \mathbf{p}_1) + \\ & + \rho a^2 \int_{\boldsymbol{\omega} \cdot (\mathbf{p}_1 - \mathbf{p}_2) > 0} d\mathbf{p}_2 d\boldsymbol{\omega} \boldsymbol{\omega} \cdot \left(\frac{\mathbf{p}_1 - \mathbf{p}_2}{m}\right) [f_t(\mathbf{q}, \mathbf{p}_1') f_t(\mathbf{q}, \mathbf{p}_2') - f_t(\mathbf{q}, \mathbf{p}_1) f_t(\mathbf{q}, \mathbf{p}_2)] \end{aligned} \quad (1)$$

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Here  $\rho$  is the overall number density,  $\rho f_t(\mathbf{q}, \mathbf{p})$  is the distribution function in one-body phase space (i.e. the expected number of particles per unit phase-space volume near the point  $\mathbf{p}, \mathbf{q}$  in one-body phase space) at time  $t$ ,  $m$  is the mass of each particle,  $a$  is the diameter of one of the hard spheres  $\mathbf{p}_1', \mathbf{p}_2'$  are the post-collision momenta of two particles with pre-collision momenta  $\mathbf{p}_1, \mathbf{p}_2$  and  $\boldsymbol{\omega} \in \mathbf{R}^3$ , is a unit vector in the direction from  $\mathbf{p}_1$  to  $\mathbf{p}_2$  at the moment of collision. The explicit formula for  $\mathbf{p}_1', \mathbf{p}_2'$  is ([6] p. 75) is

$$\begin{aligned} \mathbf{p}_1' &= \mathbf{p}_1 - \boldsymbol{\omega} \boldsymbol{\omega} \cdot (\mathbf{p}_1 - \mathbf{p}_2) \\ \mathbf{p}_2' &= \mathbf{p}_2 + \boldsymbol{\omega} \boldsymbol{\omega} \cdot (\mathbf{p}_1 - \mathbf{p}_2) \end{aligned} \quad (2)$$

Lanford gave a proof that this equation holds in the limit where  $a \rightarrow 0$  at fixed  $\rho a^2$ , for times less than about 0.2 of the mean free time, provided the particles are completely independent at the initial time.

The work described here is part of an attempt to obtain results similar to Lanford’s for a quantum mechanical system. I shall give a formal derivation of a quantum version of eqn (1) which takes into account the effect of Bose (or Fermi) statistics and in particular the possibility of a Bose-Einstein condensate. For simplicity, the hard spheres have been replaced by a “soft” interaction. I believe that essentially the same method can be used for hard spheres, but the

notation is more complicated. The derivation is certainly not a proof, but I hope that it may have the potential to form the basis for such a proof. (For other work on the problem of deriving a quantum Boltzmann equation see [1], [2, 10] and [3].)

## 2 Length and time scales

From smallest to largest, the relevant classical length scales are:

- $a$ , the hard-sphere diameter
- $\rho^{-1/3}$  a typical nearest-neighbour separation
- $\lambda := \hbar/\sqrt{m\kappa T}$  the thermal de Broglie wavelength ( $\kappa :=$  Boltzmann's constant,  $T =$  temperature, meaning that the mean kinetic energy per particle is of order  $\kappa T$ )
- $1/\rho a^2$  the classical mean free path
- $|\Omega|^{1/3}$ , the size of the container, assumed much larger than all other lengths in the problem.

Lanford's proof uses the so-called Boltzmann-Grad limit, in which we take  $a \rightarrow 0$  and  $\rho \rightarrow \infty$  at fixed  $\rho a^2$  i.e. at fixed mean free path (for more detail about his proof, see [6] and chapter 4 of [11]). In quantum mechanics, however, taking  $\rho$  to infinity at fixed  $\hbar$  and  $m$  would have the effect of taking us to the zero-temperature limit, since in this limit the actual temperature  $T$  would be much less than the Einstein condensation temperature  $\text{const.} \hbar^2 \rho^{2/3} / m\kappa$ . To preserve finite-temperature quantum effects we should keep the ratio  $\lambda/\rho^{-1/3}$ , which is proportional to  $(T_{\text{cond.}}/T)^{1/2}$ , fixed. Instead of the B-G limit I will therefore use a limit in which  $a \rightarrow 0$  at fixed  $\rho$  and  $\lambda$ . In Spohn's[11] terminology, this is the *weak coupling limit*

In this limit, the mean free path tends to infinity and so does the mean free time, which is (mean free path)/(mean particle speed), so that time variation becomes very slow. To make this time variation visible after the limit  $a \rightarrow 0$  has been taken, we can define a re-scaled time variable proportional to  $t$ /(mean free time), viz.

$$\tau := a^2 t \quad \boxed{\text{tau}} \quad (3)$$

Measured in terms of  $\tau$  rather than  $t$ , the time evolution should approach a useful limit as  $a \rightarrow 0$ . This way of scaling the time appears to be due to van Hove[13]. It was used by Hugenholtz[5] in a rigorous derivation of the quantum Boltzmann equation for a Fermi gas on a lattice.

To get the full Boltzmann equation a similar re-scaling in space is also necessary. However this is more complicated because we have to separate out the macroscopic part of the space variation, which is on a scale comparable with the mean free path and should therefore be re-scaled, from the microscopic part, which should not. To avoid these complications, for the purpose of this talk I

assume translational invariance; then there is no macroscopic space variation and so no space re-scaling is necessary.

### 3 Dynamics and the BBGKY hierarchy

We consider a system of  $N$  particles in a 3-dimensional periodic box  $\Omega$ , so that its Hilbert space is  $L^2(\Omega^N)$ . The Hamiltonian

$$H := \frac{1}{2m} \sum_{i=1}^N \mathbf{p}_i^2 + \sum_{i < j \leq N} V_{ij} \quad (4)$$

where  $V_{ij}$  (or alternatively  $V_{i,j}$ ) is the interaction between the  $i$ th and  $j$ th particles. To mimic the  $a$ -dependence of the hard-sphere interaction, we can take the interaction to be

$$V_{ij} := aU_{ij} := aU(\mathbf{q}_i - \mathbf{q}_j) \quad \boxed{U} \quad (5)$$

where  $U$  is an even function on  $\mathbf{R}^3$  with positive integral, scaled in such a way (cf [7, 8]) that

$$\int U(\mathbf{x}) d^3\mathbf{x} = 4\pi\hbar^2/m \quad \boxed{U_{\text{int}}} \quad (6)$$

and  $\mathbf{p}_i, \mathbf{q}_i$  are the momentum and position operators for the  $i$ th particle. The motivation for this formula (which is essentially a definition of  $a$ ) is that the effective scattering length of the interaction as defined is  $a$ , so that in some sense this system will behave like a gas of hard spheres. In particular, according to first-order perturbation theory, the ground-state energy per particle of the Hamiltonian  $H$  is  $2\pi\hbar^2 a/2m$ , which is the same as the ground-state energy of a gas of hard spheres to lowest order in  $a$  [8].

These operators act in an abstract Hilbert space  $\mathcal{H}^N := \bigotimes_{i=1}^N \mathcal{H}_i$ , which is the direct product of the Hilbert spaces  $\mathcal{H}_i = L^2(\Omega)$  of the individual particles. At this stage there is no need to restrict to the Bose (or Fermi) subspace of  $\mathcal{H}^N$ . (In the case where the particles are hard spheres of diameter  $a$ , a different Hilbert space would be used, namely  $L^2(\Omega^N)_a$  where  $(\Omega^N)_a$  means the part of  $\Omega^N$  in which all the inter-particle separations are at least  $a$ , but here only 'soft' interactions are considered).

If the system has probability  $p_\alpha$  of being in quantum state  $\psi_\alpha \in \mathcal{H}^N$ , where  $\alpha$  goes over some index set, then the statistical operator (or density operator or density matrix)  $D$  is defined by

$$D\phi = \sum_{\alpha} p_{\alpha} \psi_{\alpha}(\psi_{\alpha}, \phi) \quad \forall \phi \in \mathcal{H}^N \quad (7)$$

or, in Dirac notation,

$$D := \sum_{\alpha} |\psi_{\alpha}\rangle p_{\alpha} \langle \psi_{\alpha}| \quad (8)$$

It is positive semidefinite and its trace is 1. Moreover, it must have the same symmetry under particle permutations as the wave function, i.e. (for Bose statistics)

$$PD = DP = D, \quad \boxed{\text{permsym}} \quad (9)$$

for all of the  $N!$  permutation operators  $P$  permuting the  $N$  particles. For simplicity I'll only give the formulas for Bose statistics, but the modification for Fermi statistics is obvious.

By virtue of Schrödinger's equation  $i\hbar\psi = H\psi$ , the time evolution of the statistical operator is given by the quantum Liouville equation

$$i\hbar D = HD - DH \quad \boxed{\text{Liouv}} \quad (10)$$

The  $s$ -particle reduced statistical operator  $D_s$ , an operator on the Hilbert space  $\mathcal{H}^s := \bigotimes_{i=1}^s \mathcal{H}_i$ , is defined by

$$D_s = N(N-1)\dots(N-s+1) \text{tr}_{s+1}\dots\text{tr}_N D \quad \boxed{\text{Ds}} \quad (11)$$

where  $\text{tr}_{s+1}$  means that the trace over the component  $\mathcal{H}_{s+1}$  of the direct product defining the Hilbert space  $\mathcal{H}_{s+1}$ . The reduced statistical operator  $D_s$  is positive semidefinite, has trace  $N(N-1)\dots(N-s+1)$ , and has the same symmetry as  $D$ , i.e. it obeys an equation analogous to (9). Successive reduced statistical operators are related by

$$(N-s+1)D_s = \text{tr}_{s+1} D_{s+1} \quad (12)$$

so that, for example,  $D_1 = (N-1)^{-1} \text{tr}_2 D_2$ .

The quantum BBGKY hierarchy is obtained by taking the trace of the Liouville equation (10) over the component one-body Hilbert spaces  $\mathcal{H}_{s+1}\dots\mathcal{H}_N$  and then dividing by  $N(N-1)\dots(N-s+1)$ ; it is

$$i\hbar \frac{dD_s}{dt} = [H_s, D_s] + \sum_{i=1}^s \text{tr}_{s+1}[V_{i,s+1}, D_{s+1}] \quad \boxed{\text{QBBGKY}} \quad (13)$$

where  $[H_s, D_s]$  denotes the commutator  $H_s D_s - D_s H_s$ .

## 4 The $a \rightarrow 0$ limit of the first BBGKY eqn

The first equation in the BBGKY hierarchy can be written

$$i\hbar \frac{dD_1}{dt} = [K_1, D_1] + \text{tr}_2[V_{12}, D_2] \quad \boxed{\text{hier1}} \quad (14)$$

where  $K_1 := \mathbf{p}_1/2m$  is the kinetic energy of particle number 1. Since we are assuming translational invariance,  $D_1$  commutes with  $\mathbf{p}_1$  and so the first term on the right vanishes. Dividing by  $a^2$  and using the notations defined in (3) and (5) we get, in the limit,

$$i\hbar \frac{dD_1}{d\tau} = \lim_{a \rightarrow 0} a^{-1} \text{tr}_2[U_{12}, D_2] \quad \boxed{\text{proto}} \quad (15)$$

To evaluate the right side we need a way of calculating  $D_2$  to order  $a$ .

## 5 The small- $a$ formulas for $D_2$ and $D_3$ .

The hierarchy equation for  $D_2$ , eqn (13) with  $s = 2$ , can be written

$$i\hbar a^2 \frac{dD_2}{d\tau} = [(K_1 + K_2 + aU_{12}), D_2] + \text{tr}_3[a(U_{13} + U_{23}), D_3] \quad \boxed{\text{hier2}} \quad (16)$$

where  $K_i := \mathbf{p}_i^2/2m$  denotes the kinetic energy of the  $i$ th particle. Expanding  $D_2$  in powers of  $a$ , let us denote the zero-order term by  $\bar{D}_2$  and the first-order one by  $a\tilde{D}_2$ , so that

$$D_2 = \bar{D}_2 + a\tilde{D}_2 + O(a^2). \quad \boxed{\text{D2expn}} \quad (17)$$

The zero-order and first-order parts of (16) are then

$$[K_1 + K_2, \bar{D}_2] = 0 \quad \boxed{\text{D2eq0}} \quad (18)$$

$$[K_1 + K_2, \tilde{D}_2] + [U_{12}, \bar{D}_2] + \text{tr}_3[(U_{13} + U_{23}), \bar{D}_3] = 0 \quad \boxed{\text{D2eq1}} \quad (19)$$

where  $\bar{D}_3$  denotes the lowest-order term in the expansion for  $D_3$  analogous to (17). By the zero-order part of the  $s = 3$  equation analogous to (16),  $\bar{D}_3$  should satisfy

$$[K_1 + K_2 + K_3, \bar{D}_3] = 0 \quad \boxed{\text{D3eq0}} \quad (20)$$

To choose the appropriate solution of (19), we can use an ansatz analogous to Boltzmann's classical *Stosszahlansatz*. His ansatz is a product formula for the pre-collision distribution of two particles. The analogous quantum ansatz has two parts: (i) the zero-order part of the two-body density matrix can be calculated from a product formula (to be elaborated below) and (ii) the order- $a$  part of the two-body density matrix can be calculated by the methods of scattering theory and it corresponds to outgoing waves rather than incoming waves.

Dealing first with part (ii), let's write eqn (19) in the form

$$\mathcal{K}_{12}\tilde{D}_2 = -\{[U_{12}, \bar{D}_2] + \text{tr}_3[(U_{13} + U_{23}), \bar{D}_3]\} \quad \boxed{\text{D2eq1a}} \quad (21)$$

where  $\mathcal{K}_{12}$  denotes a 'super-operator', that is to say an operator which acts in the algebra of operators in the two-particle Hilbert space  $\mathcal{H}_1 \otimes \mathcal{H}_2$ , and is defined by

$$\mathcal{K}_{12}A = (K_1 + K_2)A - A(K_1 + K_2) \quad \boxed{\text{cK}} \quad (22)$$

Despite appearances,  $\mathcal{K}_{12}$  is a Hermitian super-operator, if we define the inner product between two operators  $A, B$  to be  $(A, B) := \text{tr}(A^*B)$  where the star denotes a Hermitian conjugate.

The recipe provided by scattering theory for picking out the solutions of equations similar to (21) which correspond to outgoing scattered waves is (see, for example, [4]) to replace the kinetic energy-type super-operator  $\mathcal{K}_{12}$  by  $\mathcal{K}_{12} - i\epsilon\mathcal{I}$  where  $\mathcal{I}$  is the identity super-operator and  $\epsilon$  is a small positive number which is to be set equal to 0 at the end of the calculation. The new super-operator

is manifestly non-singular and so the modified version of (22) has the unique solution

$$\tilde{D}_2 = -(\mathcal{K}_{12} - i\epsilon\mathcal{I})^{-1}\{[U_{12}, \bar{D}_2] + \text{tr}_3[(U_{13} + U_{23}), \bar{D}_3]\} \quad \boxed{\text{scat}} \quad (23)$$

Substituting this into (15) we get

$$i\hbar \frac{dD_1}{d\tau} = \text{tr}_2[V_{12}, \bar{D}_2 - (\mathcal{K}_{12} - i\epsilon\mathcal{I})^{-1}([U_{12}, \bar{D}_2] + \text{tr}_3[(U_{13} + U_{23}), \bar{D}_3])] \quad \boxed{\text{raw}} \quad (24)$$

which will give a kinetic equation for  $D_1$  if we can express  $\bar{D}_2$  and  $\bar{D}_3$  in terms of  $D_1$ .

## 6 Plausible assumptions about $\bar{D}_2, \bar{D}_3$ , etc.

If the particles obey Boltzmann statistics, the obvious assumption about  $\bar{D}_2$  and  $\bar{D}_3$  is the product formula

$$\left. \begin{aligned} \bar{D}_2 &= \bar{D}_1 \otimes \bar{D}_2 \\ \bar{D}_3 &= \bar{D}_1 \otimes \bar{D}_2 \otimes \bar{D}_3 \end{aligned} \right\} \quad \boxed{\text{Boltzprod}} \quad (25)$$

This assumption obviously satisfies the conditions (18,19), because of the assumed translational invariance of  $\bar{D}_1$ .

In the case of Bose statistics, the assumption (25) will not do, however. An assumption which does give the right symmetry properties is

$$\left. \begin{aligned} \bar{D}_2 &= \sum^{2!} P \bar{D}_1 \otimes \bar{D}_2 \\ \bar{D}_3 &= \sum^{3!} P \bar{D}_1 \otimes \bar{D}_2 \otimes \bar{D}_3 \end{aligned} \right\} \quad \boxed{\text{Boseprod}} \quad (26)$$

where the sum in the first line goes over the  $2!$  permutations of two particles and the one in the second goes over the  $3!$  permutations of three particles. There is no need to put a symmetrizing sum on the right as well as on the left, because the products  $\bar{D}_1 \otimes \bar{D}_2$ , etc., commute with all permutation operators.

For simplicity I am going to assume the product ansatz (25) or (26) for all times. A better but somewhat more complicated method would be to assume the product ansatz only for the initial time and then to verify that the equations of motion for the diagonal parts of the  $s \geq 2$  density matrices imply that the ansatz continues to hold at later times. (At item (c) on page 98 of [6], Lanford describes the analogous calculation for the classical case.)

The kinetic equation that results when (25) or (26) is substituted into the formula (24) can be simplified by expressing it in the wave-number (momentum) representation. For conceptual simplicity, consider a system in a finite periodic box  $\Omega$ . The Dirac-type formula for going between the position and wave-number representations is

$$\langle \mathbf{x} | \mathbf{k} \rangle = |\Omega|^{-1/2} \exp(i\mathbf{k} \cdot \mathbf{x}) \quad \boxed{\text{Dirac}} \quad (27)$$

It has the properties

$$\begin{aligned} \int_{\mathbf{R}^3} d^3\mathbf{x} \langle \mathbf{k}' | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{k}'' \rangle &= \delta(\mathbf{k}', \mathbf{k}'') \\ \sum_{\mathbf{k}} \langle \mathbf{x}' | \mathbf{k} \rangle \langle \mathbf{k} | \mathbf{x}'' \rangle &= \delta(\mathbf{x}' - \mathbf{x}'') \end{aligned} \quad \boxed{\text{deltas}} \quad (28)$$

where  $\delta(\cdot, \cdot)$  is the Kronecker delta and  $\delta(\cdot)$  is a Dirac delta-distribution.

Let us define  $n_{\mathbf{k}}$  to be the expected number of particles with wave number  $\mathbf{k}$ . It is a diagonal element of the one-body density matrix in the wave-number representation, a matrix which is diagonal because of translational invariance. This matrix can therefore be written

$$\langle \mathbf{k} | D_1 | \mathbf{l} \rangle = n_{\mathbf{k}} \delta(\mathbf{k}, \mathbf{l}) \quad (29)$$

We shall also need the diagonal elements of the two- and three-body density matrices. Under the ‘Boltzmann’ ansatz (25) they are very simple:

$$\begin{aligned} n_{\mathbf{k}_1, \mathbf{k}_2} &= n_{\mathbf{k}_1} n_{\mathbf{k}_2} \\ n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} &= n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} \end{aligned} \quad \boxed{\text{nprod}} \quad (30)$$

where  $n_{\mathbf{k}_1, \mathbf{k}_2} := \langle \mathbf{k}_1, \mathbf{k}_2 | D_2 | \mathbf{k}_1, \mathbf{k}_2 \rangle$  and the definition of  $n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3}$  is analogous. For the ‘Bose’ ansatz, the corresponding formulas are

$$\begin{aligned} n_{\mathbf{k}_1, \mathbf{k}_2} &= n_{\mathbf{k}_1} n_{\mathbf{k}_2} \theta(\mathbf{k}_1, \mathbf{k}_2) \\ n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} &= n_{\mathbf{k}_1} n_{\mathbf{k}_2} n_{\mathbf{k}_3} \theta(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \end{aligned} \quad \boxed{\text{Bosenprod}} \quad (31)$$

where  $\theta(\mathbf{k}_1, \mathbf{k}_2)$  is defined to equal 1 if  $\mathbf{k}_1$  and  $\mathbf{k}_2$  are different and 2 if they are the same, while  $\theta(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$  is defined to equal 1 if  $\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3$  are all different, 2 if two are the same and 6 if all three are the same.

We also need the momentum representative of the interaction. It is

$$\begin{aligned} \langle \mathbf{k}_1, \mathbf{k}_2 | U | \mathbf{l}_1, \mathbf{l}_2 \rangle &:= \int_{\Omega^2} d^3\mathbf{x}_1 d^3\mathbf{x}_2 \langle \mathbf{k}_1, \mathbf{k}_2 | \mathbf{x}_1, \mathbf{x}_2 \rangle U(\mathbf{x}_1 - \mathbf{x}_2) \langle \mathbf{x}_1, \mathbf{x}_2 | \mathbf{l}_1, \mathbf{l}_2 \rangle \\ &= |\Omega|^{-1} \delta(\mathbf{k}_1 + \mathbf{k}_2, \mathbf{l}_1 + \mathbf{l}_2) U_{\mathbf{k}_1 - \mathbf{l}_1} \end{aligned} \quad \boxed{\text{Umat}} \quad (32)$$

where  $\langle \mathbf{k}_1, \mathbf{k}_2 | \mathbf{x}_1, \mathbf{x}_2 \rangle := \langle \mathbf{k}_1 | \mathbf{x}_1 \rangle \langle \mathbf{k}_2 | \mathbf{x}_2 \rangle$  and  $U_{\mathbf{k}} := \int_{\Omega} d^3\mathbf{r} U(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{x}}$ .

## 7 The kinetic equation for Boltzmann statistics

For Boltzmann statistics, the result of substituting (25) into (24) using the momentum representation is

$$i\hbar \frac{dn_{\mathbf{k}_1}}{d\tau} = \sum_{\mathbf{k}_2} \sum_{\mathbf{l}_1} \sum_{\mathbf{l}_2} |\langle \mathbf{k}_1, \mathbf{k}_2 | U | \mathbf{l}_1, \mathbf{l}_2 \rangle|^2 \frac{2i\epsilon(n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2})}{\epsilon^2 + (\hbar^2/2m)^2(\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2)^2} \quad \boxed{\text{KE(B3)}}$$

Using (32) the right-hand side can be written

$$\frac{1}{|\Omega|^2} \sum_{\mathbf{k}_2} \sum_{\mathbf{l}_1} |U_{\mathbf{k}_1 - \mathbf{l}_1}|^2 \frac{2i\epsilon(n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2})}{\epsilon^2 + (\hbar^2/2m)^2(\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2)^2} \quad (\mathbf{l}_2 := \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{l}_1) \quad (34)$$

In the limit  $\Omega \rightarrow \mathbf{R}^3$ , the sums can be replaced by integrals using the standard recipe  $\sum_{\mathbf{k}} \rightarrow |\Omega|(2\pi)^{-3} \int_{\mathbf{R}^3} d^3\mathbf{k}$  and the formula becomes

$$\frac{1}{(2\pi)^6} \int_{\mathbf{R}^6} d^3\mathbf{k}_2 d^3\mathbf{l}_1 |U_{\mathbf{k}_1 - \mathbf{l}_1}|^2 \frac{2i\epsilon(n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2})}{\epsilon^2 + (\hbar^2/2m)^2(\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2)^2} \quad (\mathbf{l}_2 := \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{l}_1) \quad (35)$$

On taking the limit  $\epsilon \searrow 0$  as specified in the formulation of (23) the formula becomes

$$\frac{1}{(2\pi)^6} \int_{\mathbf{R}^6} d^3\mathbf{k}_2 d^3\mathbf{l}_1 |U_{\mathbf{k}_1 - \mathbf{l}_1}|^2 (n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2}) 2\pi i \delta \left( \frac{\hbar^2}{2m} (\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2) \right) \quad (\mathbf{l}_2 := \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{l}_1) \quad (36)$$

so that

$$\frac{dn_{\mathbf{k}_1}}{d\tau} = \frac{2m}{(2\pi)^5 \hbar^3} \int_{\mathbf{R}^6} d^3\mathbf{k}_2 d^3\mathbf{l}_1 |U_{\mathbf{k}_1 - \mathbf{l}_1}|^2 (n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2}) \delta(\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2) \quad \boxed{\text{QBE}} \quad (37)$$

A closed kinetic equation for  $n_{\mathbf{k}}$  can now be obtained by using the formula (30) to express  $n_{\mathbf{l}_1, \mathbf{l}_2}$  and  $n_{\mathbf{k}_1, \mathbf{k}_2}$  in terms of  $n_{\mathbf{k}}$ , etc:

To bring out the analogy with the classical Boltzmann equation more clearly, we consider the case where the range of the interaction potential is small enough in comparison with the thermal wavelength to justify replacing  $U_{\mathbf{k}_1 - \mathbf{l}_1}$  by  $U_{\mathbf{0}}$ , which by (6) is equal to  $4\pi\hbar^2/m$ . We also define  $\mathbf{u} := \mathbf{l}_1 - \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2)$  so that  $\mathbf{l}_1 = \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2) - \mathbf{u}$ ,  $\mathbf{l}_2 = \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2) + \mathbf{u}$ , and  $\mathbf{k}_1^2 + \mathbf{k}_2^2 - \mathbf{l}_1^2 - \mathbf{l}_2^2 = 2\mathbf{u}^2 - \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)^2$ . Then eqn (37) becomes

$$\begin{aligned} \frac{dn_{\mathbf{k}_1}}{d\tau} &= \frac{2m}{(2\pi)^5 \hbar^3} \left( \frac{4\pi\hbar^2}{m} \right)^2 \int_{\mathbf{R}^6} d^3\mathbf{k}_2 d^3\mathbf{u} (n_{\mathbf{l}_1} n_{\mathbf{l}_2} - n_{\mathbf{k}_1} n_{\mathbf{k}_2}) \delta \left( 2\mathbf{u}^2 - \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)^2 \right) \\ &= \frac{\hbar}{8\pi^3 m} \int_{\mathbf{R}^3} d^3\mathbf{k}_2 \int_{S^2} d^2\mathbf{w} |\mathbf{k}_1 - \mathbf{k}_2| (n_{\mathbf{l}_1} n_{\mathbf{l}_2} - n_{\mathbf{k}_1} n_{\mathbf{k}_2}) \quad \boxed{\text{QBE2}} \quad (38) \end{aligned}$$

where  $\mathbf{w}$  is defined by  $\mathbf{u} = \mathbf{w} \frac{1}{2} |\mathbf{k}_1 - \mathbf{k}_2|$  and  $S^2$  denotes the surface of the unit sphere in  $\mathbf{R}^3$ . Since  $\hbar|\mathbf{k}_1 - \mathbf{k}_2|/m$  is the magnitude of the relative velocity of two particles with wave numbers  $\mathbf{k}_1, \mathbf{k}_2$  eqn (38) is analogous to the classical Boltzmann equation (1). A factor  $a^2$  appears in (1) but not in (37); this is because of the  $a^2$  in the definition of  $\tau$ . The remaining major discrepancy between the two kinetic equations is an extra factor  $8\pi^3\rho$  in (1), which arises from the different normalizations used for  $f$  and for  $n_{\mathbf{k}}$ : the integral of  $f$  over momentum space is 1, but the integral of  $n_{\mathbf{k}}$  over  $\mathbf{k}$  space is  $8\pi^3\rho$ . This last statement can be checked by considering the infinite-volume limit of the finite-system sum rule  $\sum_{\mathbf{k}} n_{\mathbf{k}} = N$ , viz.

$$\rho = \lim_{\Omega \rightarrow \mathbf{R}^3} \frac{1}{\Omega} \sum_{\mathbf{k}} n_{\mathbf{k}} = \frac{1}{8\pi^3} \int n_{\mathbf{k}} d^3\mathbf{k} \quad (39)$$



## 8 The kinetic equation for Bose statistics

In the case of Bose statistics, a tedious calculation based on (26) and (24) shows that formula (33) is now replaced by a similar formula in which the factor

$$n_{\mathbf{k}_1, \mathbf{k}_2} - n_{\mathbf{l}_1, \mathbf{l}_2} \quad (40)$$

is replaced by

$$n_{\mathbf{k}_1, \mathbf{k}_2} + n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{l}_1} + n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{l}_2} - n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{l}_1, \mathbf{l}_2, \mathbf{k}_1} - n_{\mathbf{l}_1, \mathbf{l}_2, \mathbf{k}_2} \quad (41)$$

If we use the simple product formula (30) for  $n_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{l}_1}$  etc. in the above expression, the result is equivalent to replacing the quantum Boltzmann equation arrived at in the previous section by the so-called Boltzmann-Nordheim[9] or Uehling-Uhlenbeck[12] equation for the hard-sphere gas. Strictly speaking, the modified product formula (31) should be used rather than the simple product formula (30); however the modification will make no difference to the final result, because it only affects terms for which either  $\mathbf{k}_1 = \mathbf{k}_2$  or  $\mathbf{l}_1 = \mathbf{l}_2$ ; but the momentum and energy conservation conditions require that if  $\mathbf{k}_1 = \mathbf{k}_2$  or  $\mathbf{l}_1 = \mathbf{l}_2$  holds then all four of  $\mathbf{k}_1, \mathbf{k}_2, \mathbf{l}_1, \mathbf{l}_2$  are equal, so that the factor  $n_{\mathbf{l}_1, \mathbf{l}_2} - n_{\mathbf{k}_1, \mathbf{k}_2}$  is zero and it makes no difference which product formula is used for these terms.

## 9 Bose-Einstein condensation

The modified product formulas (31), and their analogues for higher-order reduced density matrices cannot be used for the condensate. These formulas imply that the  $r$ th factorial moment of the probability distribution of the number of particles with wave number  $\mathbf{k}$  is  $r!$  times the  $r$ th power of the first moment. This formula for the moments is characteristic of an exponential distribution. That is to say, the particles with each individual wave number are distributed grand-canonically, though with (in general) different chemical potentials for different wave numbers.

If a condensate is present, the exponential distribution cannot apply to it, because it would imply a finite probability for the number of particles in the condensate to be larger than the total number of particles in the system. Instead, we would expect the distribution of the number of condensate particles to be concentrated fairly sharply about a single value. Thus, we expect the diagonal elements of the two and three-body density matrices applying to the condensate to be given by the product formula (30) rather than by (31), so that the minor correction to the Boltzmann-Nordheim-Uehling-Uhlenbeck kinetic equation mentioned in the last sentence of the preceding section should not be used for the condensate wave number. However, as explained at the end of the preceding section, the non-zero terms in the kinetic equation are the same whichever product formula is used.

## References

- [1] R Balescu, book on non-equilibrium statistical mechanics, circa 1973?
- [2] D Benedetto, F Castella, R Esposito and M Pulvirenti Some considerations on the derivation of the nonlinear quantum Boltzmann equation. Math Phys Archive, University of Texas (2003) 3-19, to appear in J Stat Phys.
- [3] L Erdős, M Salmhofer and H-T Yau, On the quantum Boltzmann equation, Math Phys Archive 2003
- [4] M Gell-Mann and Goldberger, The formal theory of scattering, Phys. Rev **91** 398 (1953).
- [5] N M Hugenholtz, Derivation of the Boltzmann equation for a Fermi gas, J Stat Phys **32**, 231-254 (1983).
- [6] O Lanford III, Time evolution of large classical systems, pp 1-111 of *Dynamical systems, theory and applications* ed. J Moser. Springer Lecture Notes in Physics **38** (1975).
- [7] T D Lee, K Huang and C N Yang, Phys Rev **106**, 1135 (1957) (I think)
- [8] E H Lieb and J Yngvason, The ground state energy of a dilute Bose gas, AMS/IP studies in advanced mathematics **16**, 295-306 (2000)
- [9] L W Nordheim, On the kinetic method in the new statistics and its application to the electron theory of conductivity. Proc Roy Soc **A119**, 689-698 (1928)
- [10] M Pulvirenti, On the quantum Boltzmann equation. pages 129-138 of *Multiscale methods in quantum mechanics* ed. P Blanchard and G dell'Antonio, Birkhäuser (2003)
- [11] H Spohn, book on dynamics of N-body systems, Springer, circa 1992
- [12] E A Uehling and G E Uhlenbeck, Transport phenomena in Einstein-Bose and Fermi-Dirac gases I, Phys. Rev. **43** 552-561 (1933).
- [13] L van Hove, Physica **21** 517-540 (1955).