On the Quantum Boltzmann equation

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Outline

- 1. The particle system. Lanford result (quick)
- 2. Scaling limits (low-density and weak-coupling)
- 3. Formal derivation for Q. particle systems. MB statistics
- 4. FD and BE statistics

I my opinion this is an important and still largely unsolved problem.

Unfortunately in my talk no new results....only hopes.

I will not discuss Linear problems, Kinetic picture for waves, Mean-Field limits, models..... But I do not forget the many facets!

The Quantum Boltzmann equation (QBE) was introduced by Uehling and Uhlembeck (U-U) in 1933 (after similar considerations by Nordheim in 1928). Now it was necessary to use the Wigner transform (Wigner 1932).

Considering that the Schroedinger equation appeared in 1926 one can say that, at the time, real progresses were produced with a much quicker speed.

Personal consideration. When reading the U-U paper I tried to understand whether the authors believe QBE is a consequence of a scaling limit or not. Then I realized it was a stupid question: the community of physicists had the same attitude as for the classical B. eq.n. If it works and it is reasonable, with respect to the first principles, it is ok.

Some years later H. Grad (but also C. Cercignani, G. Gallavotti, Bogolyubov......) changed in a sense this perspective. Scaling limit and rigorous derivation.

Boltzmann derived his famous equation in 1872 for N hard spheres of diameter ε . (x, v) position and velocity.

$$(\partial_t + \mathbf{v} \cdot \nabla_x) f(x, \mathbf{v}) = Q(f, f)(x, \mathbf{v}).$$

Q is a bilinear operator which will be discussed later on. $\int_{\Delta} f(x, v, t) dx dv$ is either the probability of finding a given particle in Δ at time t, or the fraction of molecules in Δ at time t. Statistical description and l.l.n.

Collision: v' and v'_1 are the outgoing velocities. $n \cdot (v - v_1) > 0$.



The real equation from mechanics is

$$(\partial_t + \mathbf{v} \cdot \nabla_x) f_1^N = (N-1) \varepsilon^2 C_{1,2}^{\varepsilon} f_2^N$$

where

$$C_{1,2}^{\varepsilon}f_2^N = (N-1)\varepsilon^2 \int dv_2 \int_{S^2} dn f_2^N(x,v,x+n\varepsilon,v_2)(v_2-v)\cdot n$$

and f_1^N , f_2^N is the one and two particle marginals. Assuming propagation of chaos (namely factorization) before the collision (criticism), after a short manipulation we obtain the B. eq.n in the limit $N \to \infty$ and $\varepsilon \to 0$ with $N\varepsilon^2 = 1$

$$Q(f,f)(x,v) = \int dv_2 \int_{S_+} dn (v-v_2) \cdot n [f(x,v')f(x,v'_2) - f(x,v)f(x,v_2)].$$

$$S_+ = \{n | (v-v_2) \cdot n \ge 0\}.$$



 $\partial_t f + v \cdot \nabla_x f = Q(t, f)$ H = $\int f \log f dx dv \lambda dt$

Important remark.

Assuming initially (an almost) chaotic state. Chaoticity at time t > 0? I am looking whether particle 1 and 2 are uncorrelated. Yes, if they have not collided. Indeed the probability of such a collision is $C\varepsilon^2$ thus very small.

But this is not really true because 1 and 2 could be correlated by a chain of collisions (in (0, t)).

Too bad: this means that propagation of chaos is not a Markovian property. One has to analyze all the history of the system in (0, t). Indeed the only validity result we have, makes use of a Cauchy-Kovalevsky kind of argument. Actually O. Lanford (1975) proved the validity of the B.eq.n for short times.

Lanford.

N identical hard spheres of unitary mass in all the space \mathbb{R}^3 (or in a bounded domain Λ).

A state of the system is a sequence $Z_N = z_1 \dots z_N = (X_N, V_N)$ where $z_i = (x_i, v_i)$ denotes position and velocity of the i - thparticle. We describe the system from a statistical point of view: we introduce a probability measure $W^N(Z_N)dZ_N$ (absolutely continuous with respect to the Lebesgue measure) on the phase space of the system. W^N is symmetric in the exchange of particles. The time evolved measure is defined by

$$W^N(Z_N;t)=W^N(\Phi^{-t}(Z_N)).$$

Here $\Phi^t(Z_N)$ denotes the the dynamical flow. The *j*-particle marginals

$$f_j^N(Z_j;t) = \int dz_{j+1} \dots dz_N W^N(Z_j, z_{j+1} \dots z_N;t), \qquad j = 1 \dots N.$$

The Lanford's proof

Looking for an evolution equation for $f_j^N(t)$. H-S hierarchy. We have (Cercignani 1973)

$$(\partial_t + \mathcal{L}_j^{\varepsilon})f_j^N = (N-j)\varepsilon^2 C_{j+1}^{\varepsilon}f_{j+1}^N, \quad j = 1 \dots N$$

where $\mathcal{L}_{j}^{\varepsilon}$ is the generator of the dynamics of j hard-spheres of diameter ε :

$$S_{\varepsilon}(t)f(Z_j) = f(\Phi^{-t}Z_j) = e^{-t\mathcal{L}_j^{\varepsilon}}f(Z_j)$$

and

$$C_{j+1}^{\varepsilon}f_{j+1}^{N}(x_{1},v_{1},\ldots x_{j},v_{j}) = -\sum_{k=1}^{j}\int dn\int dv_{j+1}n\cdot(v_{k}-v_{j+1})$$

$$f_{j+1}^N(x_1,v_1,\ldots,x_k,v_k,\ldots,x_k+\varepsilon n,v_{j+1})$$

where *n* is the unit vector.

 $f_j^N = 0$ if j > N and hence, for j = N, we have nothing else than the Liouville equation.

Therefore, by the Dyson (Duhamel) expansion:

$$f_j^N(t) = \sum_{n=0}^{N-j} \alpha_n^{\varepsilon}(j) \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n$$

$$S_{\varepsilon}(t-t_1) C_{j+1}^{\varepsilon} \dots S_{\varepsilon}(t_{n-1}-t_n) C_{j+n}^{\varepsilon} S_{\varepsilon}(t_n) f_{0,n+j}^N.$$

$$\alpha_n^{\varepsilon}(j) = \varepsilon^{2n}(N-j)(N-j-1)\dots(N-j-n+1).$$

For $f_j(t) = f(t)^{\otimes j}$

$$f_j(t) = \sum_{n \ge 0} \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n$$

$$S(t-t_1)C_{j+1} \dots S(t_{n-1}-t_n)C_{j+n}S(t_n)f_{n+j}(0).$$

Lanford's approach

i) Uniform bound on both series (for short times)

ii) term by term convergence.

i) Cauchy-Kovalevski kind of argument. ii) almost obvious by direct inspection, but crucial. I am cheating. As regards i): $C_j = O(j)$, then the generic term is bounded by (neglecting large velocities)

$$j(j+1)\cdots(j+n-1)C^{j+n-1}rac{t^n}{n!}$$

so that both series are absolutely convergent but only for a short time.

Theorem (Lanford 1975) Under suitable assumptions on the initial data, there exists $t_0 > 0$ s.t., for $t \le t_0$ and for all j = 1, 2, ... ($N\varepsilon^2 = 1$)

$$\lim_{\varepsilon\to 0} f_j^N(t) = f_j(t) \quad a.e.$$

Moreover

$$f_j(t) = f(t)^{\otimes j}$$
 a.e.,

where f(t) solves the Boltzmann equation.

What happened after 1/2 century? Old papers by Spohn, Lebowitz, Lanford...(fluctuations, linearized eq.n...), Illner, P. (global result for a very special situation), King's thesis (smooth potentials, but incomplete). Recently the french group (Bodineau, Gallagher, Saint-Raymond, Simonella, Texier) (fluctuations, linearized eq.n., large deviation), Ayi (long range).

Weak-coupling limit

Let ε be a small scale parameter denoting the ratio between the macroscopic and microscopic scale. Then scale by ε the space and time in the equation of motion. $N \approx \varepsilon^{-2}$. Low density or B-G limit.

 $N \approx \varepsilon^{-3}$ particles but the particles are weakly interacting: rescale the two-body potential ϕ by $\sqrt{\varepsilon}$. Since ϕ varies on a scale ε (in macro unities), the force is $\approx (\frac{1}{\sqrt{\epsilon}})$ but acts on the time interval $\approx \varepsilon$. The momentum variation due to the single scattering is therefore $\approx \sqrt{\varepsilon}$. The number of particles met by a test particle is $\approx \frac{1}{\epsilon}$. Hence the total momentum variation for unit time is $\approx \frac{1}{\sqrt{\epsilon}}$. However this variation, in case of homogeneous gas and symmetric force, should be zero in the average. The variance should be $\approx \frac{1}{2}(\sqrt{\varepsilon})^2 = O(1)$. As a consequence of this central limit type of argument we expect that the kinetic equation which holds in the limit (if any), should be a diffusion equation in the velocity variable. Formally one obtains

$$(\partial_t + \mathbf{v} \cdot
abla_x) f = Q_L(f, f)$$
 $Q_L(f, f) = \int d\mathbf{v}_1
abla_{\mathbf{v}} a(
abla_{\mathbf{v}} -
abla_{\mathbf{v}_1}) ff_1,$

where a = a(V) is

$$a_{i,j}(V) = \frac{B}{|V|}(\delta_{i,j} - \hat{V}_i \hat{V}_j).$$

 Q_L is called the Landau equation (sometimes Landau-Fokker-Planck).

No rigorous results even for short times. Bobylev, P., Saffirio (2013) and Winter (2021) essentially consistency or partial results. For quantum systems we should have a B. type eq.n because of the tunnel effect.

Weak-coupling limit for quantum systems

Schrödinger equation for the same system

$$i\partial_t\Psi(X_N,t)=-rac{1}{2}\Delta_N\Psi(X_N,t)+U(X_N)\Psi(X_N,t),$$

where $\Delta_N = \sum_{i=1}^N \Delta_i$, Δ_i is the Laplacian with respect to the x_i variables.

Potential energy

$$U(x_1 \ldots x_N) = \sum_{i < j} \phi(x_i - x_j).$$

Rescale in a W-C way

$$iarepsilon\partial_t \Psi^arepsilon(X_N,t) = -rac{arepsilon^2}{2} \Delta_N \Psi^arepsilon(X_N,t) + \sqrt{arepsilon} U_arepsilon(X_N,t),$$

where:

$$U_{\varepsilon}(x_1 \dots x_N) = \sum_{i < j} \phi\left(\frac{x_i - x_j}{\varepsilon}\right)$$

We want to analyze the limit $\varepsilon \to 0$ in the above equations, when $N = \varepsilon^{-3}$. It is not a semiclassical (or high frequency) limit.

For Q systems no diffusion, due to the tunnel effect, but jumps: a given particle has a finite prob. to find another one (among ε^{-3} choices) to perform a collision (finite angle). All the others are transparent. Then we can also consider the statistics: M-B, F-D, B-E.

No complete results for genuine particle systems.

Term by term convergence for the hierarchy of Wigner functions Benedetto, Castella, Esposito, P. (2008).

A derivation program in collaboration with P. Butta'.

A special situation: superposition of plane waves, yielding the homogeneous B. eq.n. Steps:

1) M-B statistics. Control of the leading order contribution (for short times).

2) Full control: estimate of the error.

3) Statistics (F-D) by means of the initial quasi-free states.

N particles in \mathbb{T}_L 3-D torus of side $L = 2\pi\varepsilon^{-1}$, $N = \varepsilon^{-3}$. Heisemberg equation in rescaled variables

$$i\partial_t \rho(X_N, Y_N) = -\frac{\varepsilon}{2} (\Delta_{X_N} - \Delta_{Y_N}) \rho +$$

 $\varepsilon^{-1/2} [U_{\varepsilon}(X_N) - U_{\varepsilon}(Y_N)] \rho$

$$U_{\varepsilon}(X_N) = \sum_{i < j} \phi_{\varepsilon}(x_i - x_j), \ \phi_{\varepsilon}(x) = \phi(\frac{x}{\varepsilon}).$$

Pass in Fourier.

$$\begin{split} i\partial_t \hat{\rho}(K_N, H_N) &= -\frac{1}{2\varepsilon} (K_N^2 - H_N^2) \hat{\rho} + \frac{1}{\sqrt{\varepsilon}} T_N \hat{\rho}(K_N, H_N). \\ T_N &= \sum_{i < j} T_{i,j}, \end{split}$$

$$T_{i,j}\hat{\rho}(K_N;H_N) = \int dp \hat{\phi}(p) [\hat{\rho}(\dots k_i + p,\dots k_j - p\dots;H_N) - \hat{\rho}(K_N;\dots h_i + p,\dots h_j - p\dots)]$$

$$=\int dp\hat{\phi}(p)\sum_{\sigma=0,1}(-1)^{\sigma}\hat{
ho}(\ldots k_i+(1-\sigma)p,\ldots k_j-(1-\sigma)p\ldots;$$

 $\dots h_i + \sigma p, \dots h_j - \sigma p \dots).$ $\int F(p) dp = \sum_{p \in \mathbb{Z}^3_{\varepsilon}} F(p) \varepsilon^3. \text{ Initially}$ $\hat{\rho}_0(K_N; H_N) = f_0^{\otimes N}(K_N) \delta_{K_N, H_N}, \quad f_0 \ge 0, \int f_0 = 1.$

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A superposition of plane waves.

Partial traces (equivalent of the marginals)

$$\hat{\rho}_j^N(K_j; H_j) = \int dK_{N-j} \ \hat{\rho}_N(K_j, K_{N-j}; H_j, K_{N-j}).$$

Hierarchy (skip N)

$$\partial_t \hat{\rho}_j = -\frac{i}{2\varepsilon} T_j^0 \hat{\rho}_j - \frac{i}{\sqrt{\varepsilon}} T_j \hat{\rho}_j - \frac{i(N-j)}{\sqrt{\varepsilon}} C_{j+1} \hat{\rho}_{j+1},$$

where

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$$T_{j}^{0} = (\mathcal{K}_{j}^{2} - \mathcal{H}_{j}^{2})$$

 $C_{j+1} = \sum_{\ell} C_{\ell,j+1},$
 $C_{\ell,j+1} = \int dk_{j+1} \int dp \hat{\phi}(p) \sum_{\sigma=0,1} (-1)^{\sigma}$
 $k_{\ell} + (1 - \sigma)p, \dots k_{j+1} - (1 - \sigma)p; \dots h_{\ell} + \sigma p, \dots h_{j+1} - \sigma p).$

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Heuristics. Compute the derivative on the initial datum. First $C_{j+1}\hat{\rho}_{0,j+1} = 0$ (diagonality implies p = 0, $\sum_{\sigma} (-1)^{\sigma} = 0$. Good: the coefficient if front is $= O(\varepsilon^{-7/2})$. Also the diagonal part of $T_j^0 \hat{\rho}_{0,j}$ and $T_j \hat{\rho}_{0,j}$ are vanishing. Only the off-diagonal part starts to increase. But it is small. The interplay between the diagonal and off-diagonal part generates the O(1) contribution in an algebraically complicated way. We expect that the diagonal part is O(1) and the off-diagonal part small, strongly oscillating, but with many terms.

The hierarchical equations do not seem appropriate to work with. Therefore we introduce a closed equation for the diagonal part.

If $\hat{\rho}^d = P^d \hat{\rho}$, P^d projection on the diagonal part, then

$$\partial_t \hat{\rho}^d(t) = -\frac{1}{\varepsilon} \int_0^t dt_1 P^d T_N U_N(t-t_1) T_N \hat{\rho}^d(t_1)$$

$$U_N(t)=e^{P^0(-\frac{t}{2\varepsilon}T_N^0-\frac{t}{\varepsilon^{1/2}}T_N)t},$$

and $P^0=1-P^d$ the projection over the off-diagonal part. Then we also recover $(\hat{\rho}^0(t)=P^0\hat{\rho}(t))$

$$\partial_t \hat{\rho}^0(t) = -rac{i}{\sqrt{arepsilon}} \int_0^t dt_1 U_N(t-t_1) T_N \hat{
ho}^d(t_1).$$

Note that they are delay eq.ns!

The simplified problem (SP)

$$\partial_t \tilde{
ho}(t) = -rac{1}{arepsilon} \int_0^t dt_1 P^d T_N S_N^0(t-t_1) T_N \tilde{
ho}(t_1)$$

 $S_N^0(t) = e^{-rac{i}{2arepsilon} T_N^0 t}$

from which

$$\partial_t \xi_N(t)(K_N) = \varepsilon^3 \sum_{\ell < m} \int dp \hat{\phi}^2(p) \frac{1}{\varepsilon} \int_{-t}^t dt_1 \cos(\frac{\Delta E}{\varepsilon})(t-t_1)$$

 $\{\xi_N(\ldots k_\ell + p \ldots k_m - p \ldots; t_1) - \xi_N(K_N; t_1)\}.$
 $\Delta E = p^2 + p \cdot (k_\ell - k_m).$

Basic estimate

$$|\int dp \hat{\phi}^2(p) rac{1}{arepsilon} \int_{-t}^t d au \cos(rac{\Delta E}{arepsilon}) au| \leq C.$$

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Passing to the marginals:

$$\xi_{j}(t) = \xi_{0,j} + \varepsilon^{3} \int_{0}^{t} dt_{1} L_{j}(t-t_{1}) \xi_{j}(t_{1}) + (N-j)\varepsilon^{3} \int dt_{1} G_{j+1}(t-t_{1}) \xi_{j}(t_{1})$$

where $\xi_j(t)(K_j) = \tilde{\rho}_j(t)(K_j, K_j)$ and *L* and *G* are two suitable operators.

Then, by using the basic estimate

$$\|L_j\xi_j\| \le Cj^2\|\xi_j\|, \ \|G_{j+1}\xi_{j+1}\| \le Cj\|\xi_j\|$$

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At this point one can follow the usual strategy (uniform bound on the series expansion and term by term convergence). The collision operator of the B. eq.n is

$$Q(f,f)(k) = \int dk_1 \int dp \hat{\phi}(p)^2 \delta(\Delta E) \{f(k+p)f(k_1-p) - f(k)f(k_1)\}$$

where

$$\Delta E = \frac{1}{2}(p^2 + p \cdot (k - k_1))$$

and the presence of the δ ensures the energy conservation. Replace sums by integrals (not obvious). Lattice difficulties: oscillations on the same scale.

The full problem should make use of the fact that

$$U_j(t) = S_j^0(t) + O(j^a \sqrt{\varepsilon}).$$

Reasonable, but to be proven.

Statistics.

Canonical \rightarrow Grandcanonical. *N* Poisson intensity ε^{-3} r.v. A state

$$\sigma = \bigoplus_{n} \sigma_{n}$$

where σ_n is a positive *n*-particle operator. Reduced density matrix

$$\rho(X_n; Y_n) = \sum_{M \ge 0} \frac{(n+m)!}{m!} \int dZ_m \sigma_{n+m}(X_n, Z_m; Y_n, Z_m)$$

Require beyond the symmetry in the exchange of particles

$$\rho(X_n; Y_n) = \theta^{s(\phi)} \rho(X_n; \pi(Y_n))$$

where π is a permutation. $\theta = 1$ for Bosons and $\theta = -1$ for Fermions.

Quasi-free states are such that

$$\rho(X_n; Y_n) = \sum_{\pi} \theta^{s(\phi)} \prod_{i=1}^n \rho(x_i; \pi(y_i)).$$

The initial condition. Maximally uncorrelated state which does not violate the statistics.

Evaluate for the determination of the cubic terms $C_2SC_3S = C_{1,2}SC_{1,3} + C_{1,2}SC_{2,3}$ and compare with

 $f' \mathit{ff}_1, \ \mathit{f}_1' \mathit{ff}_1 \ , \mathit{ff}' \mathit{f}_1', \ \mathit{f}_1 \mathit{f}' \mathit{f}_1'$

12 terms (considering the cross-section).

At level of particles permutations we have 6x2x2=24 terms. Some zero, some compensate.

Computation done (but for Wigner) in Benedetto, Castella, Esposito, P. (2004).