BBGKY hierarchy for hard spheres

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Key result in equilibrium has been virial expansion convergence → complete very detailed equilibrium rarefied gases at high temperature in Gibbs states.

It is highly desirable to achieve a similar understanding in systems in stationary states out of equilibrium.

Difficulty: in equilibrium systems enclosed in finite containers have a probability distribution and correlation with a density on phase space.

This is no longer true for systems in steady non equilibrium: however correlations exist up to a large fraction of the number of degrees of freedom (hence all in infinite systems).

Existence of stationary states of flowless hard spheres gas with $T_{\pm\infty}$ different.
Which are the equations for the correlations? (Cercignani, Spohn)

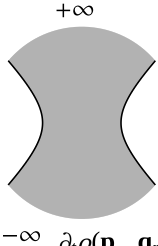


Fig.1: *A hyperboloid-like container* Ω.
Shape is symbolic (d=3)

Stationary regular BBGKY hierarchy (hard core):

$$\partial_t \rho(\mathbf{p}_n, \mathbf{q}_n) = 0 = \sum_{i=1}^{n} \Big(-p_i \cdot \partial_i \rho(\mathbf{p}_n, \mathbf{q}_n)$$

$$+ \int_{\sigma(q_i, \mathbf{q}'_n)} \omega \cdot (\pi - p_i)\, \rho(\mathbf{p}_n, \mathbf{q}_n, \pi, q_i + r\omega) d\sigma_\omega\, d\pi \Big)$$

$$+ \int_{\Omega} \omega \cdot (\pi - \pi')\, \rho(\mathbf{p}_n, \mathbf{q}_n, q, \pi, q + r\omega, \pi')\, dq\, d\sigma_\omega\, d\pi\, d\pi'$$

$$+ \int_{\partial\Omega} \omega \cdot \pi\, \rho(\mathbf{p}_n, \mathbf{q}_n, q, \pi)\, d\sigma_q\, d\pi$$

$\rho(\mathbf{q}_n, \mathbf{p}_n)$ differentiable in $|q_i - q_j| > r$ with continuous derivs in $|q_i - q_j| \ge r$.

The “blue” terms are set to 0: as derived under the strong continuity assumption. Let

$$p_i' = p_i - \omega \cdot (p_i - p_j)\,\omega, \quad p_j' = p + \omega \cdot (p_i - p_j)\,\omega \qquad \omega\,(p_i - p_j) > 0$$

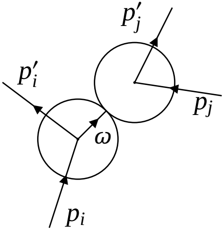
with $q_j = q_i + r\omega$ be a pair collision.

Let $(\mathbf{q}_n, \mathbf{p}_n)$, $(\mathbf{q}_n, \mathbf{p}_n')$ with

$\mathbf{p}_n' = (p_1 \ldots p_i' \ldots p_j' \ldots)$

$\mathbf{p}_n = (p_1 \ldots p_i \ldots p_j \ldots)$

be incoming and outgoing momenta



Strong continuity is

$$\rho(\mathbf{q}_n, \mathbf{p}_n') = \rho(\mathbf{q}_n, \mathbf{p}_n)$$

It can be shown (Marchioro-Pellegrinotti-Presutti, Spohn) that strong continuity is conserved outside a set of 0 phase volume if

(a) system is finite
(b) it is true initially

Furthermore the blue terms vanish identically.

Notations

Reference state: activity=z_0, temperature =β_0^{-1}. Maxwellian:

$$G_{\mathbf{q}_n}(\mathbf{p}_n) \stackrel{def}{=} \frac{e^{-\frac{1}{2}\beta(\mathbf{q}_n)\,\mathbf{p}_n\cdot\mathbf{p}_n}}{\sqrt{(2\pi)^{nd}\det\beta(\mathbf{q}_n)^{-1}}},$$

If x is a Gaussian v., $C \stackrel{def}{=} \langle x^2 \rangle$, then Wick's (*i.e.* Hermite's) monomials are

$$: x^k : \stackrel{def}{=} (2C)^{k/2} H_k(\frac{x}{\sqrt{2C}})$$

and $\rho(\mathbf{p}_n, \mathbf{q}_n)$ can be expanded in Wick's (Hermite's) monomials:

$$: \mathbf{p}_n^A : \stackrel{def}{=} \prod_{k=1}^{n} \prod_{\alpha=1}^{d} : p_{k\,\alpha}^{a_\alpha^k} :, \qquad A = (\mathbf{a}^1, \ldots, \mathbf{a}^n)$$

where $\mathbf{a} = (a_1, a_2, a_3) \in Z_+^3$ are integers.
Let $A_{i\alpha}^{\pm 1} = (\mathbf{a}'^1, \ldots, \mathbf{a}'^n)$ be $A = (\mathbf{a}^1, \ldots, \mathbf{a}^n)$ with

$$\mathbf{a}^i = (a_1^i, a_2^i, a_3^i) \Rightarrow \mathbf{a}'^i, \quad \text{with} \quad a'^i_\alpha = a^i_\alpha \pm 1$$

Expansion:

$$\rho(\mathbf{p}_n, \mathbf{q}_n) = G_{\mathbf{q}_n}(\mathbf{p}_n)\Big(\rho_\emptyset(\mathbf{q}_n) + \sum_{A\neq\mathbf{0}} \rho_A(\mathbf{q}_n)\ :\mathbf{p}_n{}^A:\Big), \qquad A = (\mathbf{a}^1, \ldots, \mathbf{a}^n)$$

Look for BBGKY solution $\Rightarrow$ smooth coefficients $\rho_A(\mathbf{q}_n)$ for $|q_i - q_j| > r$.

Possibly ordering them in terms of the sizes of

$$\varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1 \text{ (temperature difference)},\ \ \varepsilon(q) \stackrel{def}{=} \frac{\beta(q)}{\beta_+} - 1,\ \text{ and } z_0 \text{ (density)}$$

An involved hierarchy of equations is derived with

(a) *For each* $\rho_A(\mathbf{q}_n)$ *the hierarchy involves* $\rho_{A'}(\mathbf{q}_m)$ *with* $m = n+1, |A'| = |A|$ *or* $\rho_{A'}(\mathbf{q}_n)$ *with* $|A'| = |A|, |A|+2, |A|+4$.

(b) Cancellation: $|A| + 6$ is missing

Up to boundary conditions: odd A and even A are independent.

For completeness the equations with no “blue terms” are explicitly written:

BBGKY: Red = terms expected to yield all contributions of $O(\varepsilon_0)$:

$$\#1 \ \sum_{i\alpha}\Big\{\Big[\partial_{i\alpha}\rho_{B^{-1}_{i\alpha}} + \beta(q_i)^{-1}(b^i_\alpha + 1)\partial_{i\alpha}\rho_{B^{+1}_{i\alpha}}\Big]$$

$$\#2 \ -\frac{1}{2}\partial_{i\alpha}\beta(q_i)\sum_{\alpha'}\Big[\rho_{(B^{-2}_{i\alpha'})^{-1}_{i\alpha}}(\mathbf{q}_n)$$

$$\#3 \ +\beta(q_i)^{-1}\Big(2\rho_{B^{-1}_{i\alpha'}}(\mathbf{q}_n)\delta_{\alpha\alpha'}$$

$$\#4 \ +(b^i_\alpha + 1 - 2\delta_{\alpha\alpha'})\rho_{(B^{-2}_{i\alpha'})^{+1}_{i\alpha}}(\mathbf{q}_n)$$

$$\#5 \ +2(b^i_{\alpha'} - \delta_{\alpha\alpha'})\rho_{(B^{-1\,-1}_{i\alpha\, i\alpha'})^{+1}_{i\alpha'}}(\mathbf{q}_n)\Big)$$

$$\#6 \ +\beta(q_i)^{-2}\Big(2\delta_{\alpha\alpha'}(b^i_{\alpha'} + 1)\rho_{B^{+1}_{i\alpha'}}(\mathbf{q}_n)$$

$$\#7 \ +2(b^i_\alpha + 1)\, b^i_{\alpha'}\rho_{(B^{-1}_{i\alpha'})^{+1+1}_{i\alpha i\alpha'}}(\mathbf{q}_n)\Big)\Big]$$

$$\#8 + \int_{s(q_i;\mathbf{q}_n)}\omega_\alpha\Big[-\beta(q_i + r\omega)^{-1}\rho_{(BA')^{+1}_{(n+1)\,\alpha}}(\mathbf{q}_n, q_i + r\omega)$$

$$+\rho_{(BA')^{-1}_{i\alpha}}(\mathbf{q}_n, q_i + r\omega)$$

$$+\beta(q_i)^{-1}(b^i_\alpha + 1)\rho_{(BA')^{+1}_{i\alpha}}(\mathbf{q}_n, q_i + r\omega)\Big]\, d\sigma_\omega\Big\} = 0$$

Of course we have to check that the "blue" terms vanish identically in the solutions: this will be strictly required.

Key example: the equation for $\rho_\emptyset(\mathbf{q}_n)$ is, simply,

$$-\partial_{i\alpha}\rho_\emptyset(\mathbf{q}_n) + \frac{\partial_{i\alpha}\beta(q_i)}{\beta(q_i)}\rho_\emptyset(\mathbf{q}_n) - \int_{\sigma(q_i,\mathbf{q}'_n)} \omega_\alpha d\sigma_\omega \, \rho_\emptyset(\mathbf{q}_n q_i + r\omega) = 0$$

Eq. admits exact solution, close to the reference state z_0, β_0^{-1}: *i.e* the hard spheres gas equilibrium correlations with activity $z(q) \stackrel{def}{=} z_0 \, \frac{\beta(q)}{\beta_0}$

Special case: Then up to $O(\varepsilon_0^2)$ and $O(z_0^2)$ it is

$$\beta_0^{-1}\partial_q\Big(12\rho_{400} - 4\rho_{220} + \rho_{211}\Big) = -\frac{1}{2}\rho_\emptyset(q)\partial_q\varepsilon(q)$$

Impossible unless $\rho_\emptyset(q)$ is a function of β: true up to $O(z_0^2)$.
Next order in z_0 would require

$$\rho_\emptyset(q) = z_0\frac{\beta(q)}{\beta_0}(1 - z_0 c_2 \int_{s(q)\cap\Omega} \frac{\beta(q')}{\beta_0} \, dq')$$

= function $\beta(q)$: away from $\partial\Omega$ true if $\beta(q)$ is harmonic

Illusory (see below) BUT $\Rightarrow$ idea: harmonicity $\equiv$ solubility condition

Open problem: is a function $f(q)$ in Ω with the *property of the mean*

$$f(q) = \int_{s(q)\cap\Omega} f(q')\frac{dq'}{c_2}, \qquad c_2 = \frac{4\pi}{3}r^3$$

for all balls $s(q) \subset \Omega$ of fixed radius r, harmonic at least "far from $\partial\Omega$"?

Even if yes this cannot be used here because, to $O(z_0^2)$, $\rho_2(q_1, q_2)$ contributes and the argument is not conclusive!

From the theory of the Mayer expansion $\rho_\emptyset(q)$ would be a function of $\beta(q)$ even up to $O(z_0^3)$. Yet: the argument is really incorrect, as shown by

Ansatz: $\rho_A(\mathbf{q}_n) = 0$ if $|A| = 1, 2$ and

$$\Big(\rho_\emptyset(\mathbf{q}_n) + \sum_{a^1,\ldots,a^n} \rho_{a^1,\ldots,a^n}(\mathbf{q}_n) \prod_{i=1}^{n} \frac{:(\beta(q_i)p_i^2)^{a^i}:}{(2a^i)!!}$$

$$+ \sum_{i,\alpha}\sum_{a^1,\ldots,a^n} \rho_{i,\alpha;a^1,\ldots,a^n}(\mathbf{q}_n)\frac{1}{\sqrt{\beta(q_i)}}\partial_{p_{i\alpha}} \prod_{i=1}^{n} \frac{:(\beta_{q_i}p_i^2)^{a^i}:}{(2a^i)!!}\Big)$$

i.e.

Even correlations functions of the $\prod_i :(p_i^2)^{a^i}:$ only.

Odd correlations functions of first derivatives $\partial_{p_{j\alpha}}\prod_i(p_i^2)^{a^i}$ only.

Fundamental solution, from the ansatz:

Even correlations: exact by recurrence, $\varepsilon(q) \stackrel{def}{=} \frac{\beta(q)}{\beta_0} - 1$, $\varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1$,

$$\rho_{even}(\mathbf{q}_n, \mathbf{p}_n) = \rho_\emptyset(\mathbf{q}_n) \prod_{i=1}^{n} \varphi(q_i, p_i) \quad \text{with}$$

$$\varphi(q,p) \stackrel{def}{=} G_{\beta(q)}(p) \frac{\beta_0}{\beta(q)} \Big(\sum_{k=0}^{\infty} \frac{(\varepsilon(q)^k + \varepsilon(q)\,(-1)^k)}{(2k)!!} : (\beta(q)p^2)^k : \Big)$$

Odd correlations: exact

$$\rho_{odd}(\mathbf{q}_n, \mathbf{p}_n) G_{\beta_0}(\mathbf{p}_n) = z_0^n \, \delta_{n>1} \sum_{i=1}^{n} G_{\beta_0}(\mathbf{p}_n)$$

$$\cdot \Big(r\, \partial_i F(q_i) \cdot \partial_{p_i} \sum_{k=0}^{\infty} \frac{(-\beta_0)^k : p_i^{2k} :_{\beta_0}}{(2k)!!} \Big) \prod_{j \neq i} K(p_j)$$

where $K(p) \stackrel{def}{=} \sum_{a=1}^{\infty} C(a) : p^{2a} :_{\beta_0}$ with the $C(a)$'s arbitrary, AND

$$-\Delta F(q) = 0, \quad \text{in } \Omega, \quad \partial_n F(q) = 0, \quad \text{in } \partial\Omega$$

So far no approximation. But $\beta(q)$ arbitrary!

Given $\beta_\pm$ ($\beta_0 = \beta_+ < \beta_- \equiv \beta_0(1+\varepsilon_0)$): which B.C.?

Boundary conditions: $(\varepsilon_0 \stackrel{def}{=} \frac{\beta_-}{\beta_+} - 1,\ \varepsilon(q) \stackrel{def}{=} (\frac{\beta(q)}{\beta_+} - 1))$

(a) Equilibrium at $\pm\infty$ for position correlations: $(\rho_\emptyset(\mathbf{q}_n) = \int \rho(\mathbf{q}_n, \mathbf{p}_n) d\mathbf{p}_n)$

$$\rho_\emptyset(\mathbf{q}_n) \xrightarrow[\mathbf{q}_n \to \pm\infty]{} \text{equilibrium with suitable activity } z_\pm$$

(b) Collision continuity:

$$p_i' = p_i - \omega \cdot (p_i - p_j)\,\omega\,, \quad p_j' = p + \omega \cdot (p_i - p_j)\,\omega \qquad \omega\,(p_i - p_j) > 0$$

However do we have to require continuity?

Not necessarily

Continuity (strong) is generally demanded (Cercignani, Lanford) in the context of Boltzmann-Grad limit (not always, see Spohn).

But no proof available:

(1) at finite volume and out of equilibrium correlations not even defined in SRB states

(2) if the initial state μ has the property (not easy to impose) μ_t keeps it forever (Spohn): however discontinuity might develop at $t = +\infty$

Go back to Maxwell and Boltzmann: their theory is based on the equations

$$\partial_q \int Q(p)\,\rho(q,p)dp = \int_{\omega\cdot(p-\pi)>0} (Q(p') - Q(p))\,\omega\cdot(p-\pi)\,\rho(q,q+r\omega,p,\pi)d\sigma_\omega dp\,d\pi$$

implied by BBGKY + continuity and we call it weak continuity.

Maxwell: uses only for Q = collision invariants or energy flow

$$Q(p) = (1,\ p_a,\ p^2,\ p_a p^2) \stackrel{def}{=} \mathcal{Q}_M$$

(b') **Weak collision continuity**: require it for a family $\mathcal{Q}$ of observables.

To proceed "leave exact world": we are able to impose weak continuity to lowest (non trivial) order in ε_0 and z_0 and away from boundary of Ω: *i.e.* if $\ell(q)$ = distance of $q,\ q+r\omega$ from $\partial\Omega$ up to

$$O(\varepsilon_0^2, \varepsilon_0(z_0 r^3)^3, (z_0 r^3)^{\ell(q)/r})$$

Begin with $Q(p) = p^2$: using the exact solitions **(b')** requires

$$0 = \int_{s(q)\cap\Omega} \rho_{eq}(q, q+r\omega)\,(\beta(q) - \beta(q+r\omega))\,d\omega$$

At distance ℓ from $\partial\Omega$ the $\rho_{eq}(q, q+r\omega)$ is rotation and translation invariant up to $O((z_0 r^3)^{\ell/r})$ by Kirkwood-Salsburg theory of the Mayer expansion.

⇒ Weak continuity for energy true if $\beta(q)$ is harmonic (Fourier).

BUT there are infinitely many other conditions:

"all even" $Q(p) = p_x^{2s_x} p_y^{2s_y} p_z^{2s_z}$ with $s_x + s_y + s_z > 1$ &

"all odd" $Q(p) = p_\alpha p_x^{2s_x} p_y^{2s_y} p_z^{2s_z}$, $s \stackrel{def}{=} s_x + s_y + s_z > 0$:

Remarkably: the free $C(a)$ determined 1-quely by **(b')** for all odd observables for all **s** with $s > 0$ provided $F(q) = \varepsilon(q)$ solving:

$$\frac{(2s+3)!!}{3(s+3)2^s s!} = \sum_{k=1}^{\infty} \overline{\gamma}_{s,k} \frac{(-1)^k}{\sqrt{2\pi}} k! 2^k C(k), \qquad \overline{\gamma}_{s,k} \stackrel{def}{=} \binom{k-(s+\frac{3}{2})}{-(s+\frac{3}{2})}$$

It remains the weak continuity for $Q = p_\alpha, 1$ (momentum and mass transport) and for the even observables of higher degree than 2. For $Q = 1$ it also holds.

However for the momentum ($s = 0$) it cannot be satisfied (unless $\beta = const$).

Either such continuity is given up or more general solutions are needed. If so weak continuity has to be rediscussed and harmonicity of β may be lost.

This is precisely what happens: other exact solutions can be found which however cntain many more free constants which can be used to impose weak continuity for all observables Q: at the price that the solutions become quite trivial.

Question: should also weak ontinuity for all observables Q (including $(p^2)^{333}$) be given up? if so on which grounds?

Conclusions

0) All solutions are exact but the boundary conditions are imposed only to lowest nontrivial order.

1) There are many “exact” solutions: all of them are compatible with the heat equation without implying it

2) Arbitrary constants are determined by requiring “boundary conditions” or other physical properties

3) Strong continuity might be incompatible with BBGKY stationary in nnequilibrium (*i.e.* “just as the Boltzmann equation is”)

4) Heat conductivity can be expressed in terms of the solutions considered to lowest order:

$$\chi = b\frac{\sqrt{k_B T}}{r^2}k_B$$

It depends on a special combination b of the parameters so far free: it turns out that if $b \neq 0$ then $\beta(q)$ must satisfy the property of the average, “hence” it has to be harmonic.

5) It seems that any progress can come from success in finding more solutions that allow us to impose boundary conditions to higher order in $\beta_+ - \beta_-$. Which are the proper boundary conditions seems not known (are multiple collisions involved?).

6) Smooth potential?: the equation for $\rho_\emptyset$ does not seem easily soluble.

Other solutions: add to the exact solution above any other solution of the BBGKY. Further exact solution is $\rho' + \rho''$:

$$\rho'(q_1,q_2,p_1,p_2) \stackrel{def}{=} \beta_0 z_0^2 \Big(H(q_1)U(p_2)\sum_{k=0}^{\infty}\frac{(-\beta_0)^k : (p_1^2)^k :}{(2k)!!} G_{\beta_0}(\mathbf{p}_2) + (1\longleftrightarrow 2)\Big)$$

$$\rho'(q,p) \stackrel{def}{=} -z_0^2\beta_0\overline{H}(q)U(p)G_{\beta_0}(p), \quad \overline{H}(q) \stackrel{def}{=} \int_{s(q)\cap\Omega} H(q')dq'$$

$$\rho''(\mathbf{q}_2,\mathbf{p}_2) \stackrel{def}{=} \beta_0^{\frac{1}{2}} z_0^2 \Big(\Xi(p_2)\cdot\partial_{q_1}D(q_1)\sum_{k=0}^{\infty}\frac{(-\beta_0)^k : (p_1^2)^k :}{(2k)!!} G_{\beta_0}(\mathbf{p}) + (1\longleftrightarrow 2)\Big)$$

$$\rho''(q,p) \stackrel{def}{=} -\beta_0^{\frac{1}{2}} z_0^2 \Xi(p)\cdot\partial\,\overline{D}(q), \quad \overline{D}(q) = \int_{s(q)\cap\Omega} D(x)\,dx$$

where $U(p) \stackrel{def}{=} \sum_{k=1}^{\infty} u_k : (p^2)^k :_{\beta_0}$, $\Xi(p)_\alpha = \sum_{k=0}^{\infty} x_k : p_\alpha (p^2)^k :_{\beta_0}$ with u_k, x_k arbitrary parameters and $H(q), D(q)$ *harmonic functions* solves for q_1, q_2 at distance $> r$ from $\partial\Omega$.

Weak continuity for $Q = 1, p_a$ can be obtained by fixing $u_1 = 1$, $u_k = 0,\ k \geq 2$.

However the u_k remain undetermined and can be used to obtain continuity for all the Q's: but whenever weak continuity is imposed for all Q's the result is a rather trivial solution and no condition on β arises..

Giving up requiring weak continuity for all Q's can imply that β has to be harmonic: for instance the condition $b \int_{s(q)\cap\Omega}(\beta(q + r\omega) - \beta(q))d\sigma_\omega = 0$ with b a suitable combination of the free constants.

It turns out that the constant b is the same that determines the heat conductivity $\chi = \frac{bk_B}{r^2}\sqrt{k_B T}$: hence "harmonicity" of β would be implied by heat conductivity $\chi \neq 0$.