Stationary BBGKY hierarchy for hard spheres: problems and heat equation

by Guido Gentile, Alessandro Giuliani, GG

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 with a density on phase space.

This is no longer true for systems in steady non equilibrium: need infinite

Study existence of stationary states of a hard spheres gas with temperatures at $\pm\infty$ different: $\rho_{\pm\infty}(\mathbf{q}_n)$ correspond to $\rho_\pm$ and $\beta_\pm^{-1} = \langle p_i^2 \rangle$.

Joel (1959): We try to find Γ-space ensembles that will represent systems not in equilibrium in the same way that microcanonical, canonical, g.c. ensembles represent systems in equilibrium ... And there is of course no *priori* assurance that such a parallel can be made

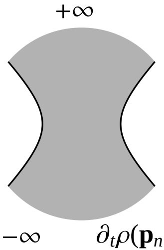


Fig.1: *A hyperboloid-like container* Ω. *Shape is symbolic (d=3)*

Stationary regular BBGKY hierarchy (hard core):

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

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

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

Representation (reference state activity=z_0, temperature $=\beta_0^{-1}$):

$$G_{\mathbf{q}_n}(\mathbf{p}_n) \stackrel{def}{=} \frac{e^{-\frac{1}{2}\beta(\mathbf{q}_n)\mathbf{p}_n\cdot\mathbf{p}_n}}{\sqrt{(2\pi)^{nd}\det\beta(\mathbf{q}_n)^{-1}}}, \qquad :x^k: \stackrel{def}{=} (2C)^{k/2}H_k(\frac{x}{\sqrt{2C}})$$

Look for BBGKY solution expanded in Wick (Hermite) monomials:

$$\rho(\mathbf{p}_n,\mathbf{q}_n) = G_{\mathbf{q}_n}(\mathbf{p}_n)\sum_A \rho_A(\mathbf{q}_n)\ :\mathbf{p}_n{}^A:$$

$$:\mathbf{p}_n^A: \stackrel{def}{=} :\prod_{k=1}^{n}\prod_{\alpha=1}^{d}(\overline{p}_{k\,\alpha})^{a_\alpha^k}:, \qquad \overline{p}_k \stackrel{def}{=} -\sqrt{\beta(q_i)}p_k$$

Regular BBGKY $\Rightarrow$ hierarchy in the coefficients $\rho_A(\mathbf{q}_n)$.

Result 0: *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 $|A'| = |A|, |A|+2, |A|+4$.*

Key cancellation: $|A|+6$ is missing

Up to boundary conditions: Even A and odd A are independent

Ansatz: $\overline{p}_k \overset{def}{=} -\sqrt{\beta(q_i)}p_k$: then $\rho_A(\mathbf{q}_n) = 0$ if $|A| = 1, 2$ and

$$\Big(\rho_\emptyset(\mathbf{q}_n) + \sum_{a^1,\ldots,a^n} z_0^n \frac{(-1)^{a^j}}{2^{a_j} a^j!} F_{2a^1,\ldots,2a^n}(\mathbf{q}_n) : \prod_{i=1}^{n} (\overline{p}_i^2)^{a^i} :$$

$$+ \sum_{a^1,\ldots,a^n} \sum_{i,\alpha} z_0^n \frac{(-1)^{a^j}}{2^{a_j} a^j!} \partial_{i\alpha} \widetilde{F}_{2a^1,\ldots,2a^n}(\mathbf{q}_n) : \partial_{\overline{p}_{i\alpha}} \prod_{i=1}^{n} (\overline{p}_i^2)^{a^i} : \Big)$$

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.

Eqs. simplify: *e.g.* let $\Delta_{a^1;a^2,\ldots,a^n} \overset{def}{=} F_{2a^1,\ldots,2a^n} - F_{2(a^1+1),\ldots,2a^n}$ then:

$$\partial_{1\alpha}\Delta_{a^1;\ldots}(\mathbf{q}_n)+\frac{\partial_{1\alpha}\beta(q_1)}{\beta(q_1)}\Big(a^1\Delta_{2(a^1-1);\ldots}(\mathbf{q}_n)-(a^1+1)\Delta_{a^1;\ldots}(\mathbf{q}_n)\Big)$$

$$+\,z_0\int_{s(q_i;\mathbf{q}_n)} d\sigma_\omega\omega_\alpha\Big(\Delta_{a^1;\ldots,a^n,0}(\mathbf{q}_n,q_1+r\omega)\Big)=0$$

For $a^i = 0$ $(A=\emptyset)$ this is, with $m=1$, $z_0^n\Delta_{1;0,\ldots,0}\equiv\rho^{\{1\}}(\mathbf{q}_n)$ with

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

$\Rightarrow$ solved by Kirkwood-Salsburg eq. in ext. field!!, i.e. activity

$$z(q)\overset{def}{=}z_0\cdot\Big(\frac{\beta(q)}{\beta_0}\Big)^m$$

Odd correlations

Look for solutions ≠ 0 of the odd correlations. Exact solutions can be found (disregarding boundary conditions at collisions)

$$\rho_{odd}(\mathbf{q}_n, \mathbf{p}_n) = \delta_{n>1} \sum_{i\alpha} C_{n,i}\, \partial_{i\alpha} \widetilde{F}(\mathbf{q}_n) \cdot \partial_{\overline{p}_{i\alpha}} \frac{: \overline{\mathbf{p}}_n^A :}{\mathbf{a}^i!}$$

with $\widetilde{F}(\mathbf{q}_n) = \prod_{i=1}^n \widetilde{F}(q_i)$ and with $C_{n,i}(A_1, \ldots, A_n)$ depending only on A_j, $j \neq i$ and arbitrary provided

$$\Delta\widetilde{F} - \frac{1}{2}\frac{\partial\beta \cdot \partial\widetilde{F}}{\beta} = 0 \text{ in } \Omega, \qquad \partial_n \widetilde{F} = 0 \text{ in } \partial\Omega$$

Any relation between $\widetilde{F}$ and β leads to a nonlinear heat equation which becomes $\Delta T = 0$ upon linearization.

Questions

(1) Are there solutions for the even correlations?
(2) How to determine $\widetilde{F}$ and the arbitrary constants?

There are many exact solutions of the odd hierarchy corresponding to the arbitrary constants $C_n(A_1, \ldots, A_n)$

The even admit also many solutions: one is ($\beta_i \stackrel{def}{=} \beta(q_i)$)

$$F_{2a^1,\ldots,2a^n} \stackrel{def}{=} -\frac{\rho^{\{1\}}(\mathbf{q}_n)}{z_0^n} \prod_{i=1}^{n} \Big[\frac{\beta_0}{\beta_i}(1-\frac{\beta_i}{\beta_0})(1-(1-\frac{\beta_i}{\beta_0})^{a^i-1})\Big]$$

$\rho^{[1]}(\mathbf{q}_n)$ is the Gibbs state of hard spheres at variable activity $z(q) = z_0\frac{\beta(q)}{\beta_0}$.

No apparent freedom.

So far no approximation. Among the solutions are there any satisfying boundary conditions? which B.C.?

Given $\beta_\pm$ (with $\beta_0 = \beta_- > \beta_+ \equiv \beta_0 - \delta$):

Boundary conditions:

(1) **Equilibrium at $\pm\infty$**:

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

(2) **Collision continuity**: if $p_1, p_2 \Rightarrow p'_1, p'_2$ is a collision btwn q_1 and $q_1 + r\omega$ (with $\omega \cdot (p_2 - p_1) < 0$) in the direction ω then

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

i.e. for all 1-particle momentum observ. Q and $q \in \Omega$ this is

$$\sum_{\alpha=1}^{3} \partial_\alpha \int \rho(p,q) p_\alpha Q(p) d^3p =$$

$$\cdot \int_{\omega\cdot(p-\pi)>0} |\omega(\pi - p)| \cdot (Q(p') - Q(p))\, \rho(p,q,\pi,q+r\omega)\, d^3p\, d^3\pi\, d\sigma_\omega$$

if $p, \pi \Rightarrow p', \pi'$ after elastic scattering in the cone $d\omega$

Result: There are (many) solutions up to $O(\delta^2), O(\frac{r}{L})$ (L =width of Ω) which satisfy the boundary conditions $\forall Q \in \mathcal{Q}_{14}$ and

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

Conjecture $14 \to \infty$

Ambiguity is possibly due to lack of b.c. on multiple collisions

The boundary condition equations:

If $\overline{I}_s \stackrel{def}{=} \frac{(2s+3)!!}{3\cdot 2^s s!}$ *i.e.* $\frac{I_s}{2^s s!}$ *l.h.s.* of BC for $p_\alpha p^{2s}$

and $\overline{C}(k) \stackrel{def}{=} C_2(2k)2^k k!$ *r.h.s.* of BC for $p_\alpha p^{2s}$

then the equation for $\overline{C}(k)$ is

$$\overline{I}_s = \sum_{k\geq 1} \overline{\gamma}_{s,k}\overline{C}(k)$$

with $\overline{\gamma}_{s,k}$

$$\overline{\gamma}_{s,k} \stackrel{def}{=} \sum_{\substack{k_0+k_1+k_2=k \\ s_0+s_1+s_2=s}} \sum_{h_0=0}^{k_0} (-1)^{h_0} \frac{(2h_0-1)!!}{2^{h_0} h_0!} \begin{Bmatrix} s_1 \\ k_1 \end{Bmatrix} \begin{Bmatrix} s_2 \\ k_2 \end{Bmatrix} \begin{pmatrix} s_0 + k_0 - h_0 \\ s_0 \end{pmatrix} \begin{bmatrix} k_0 \\ h_0 \end{bmatrix}$$

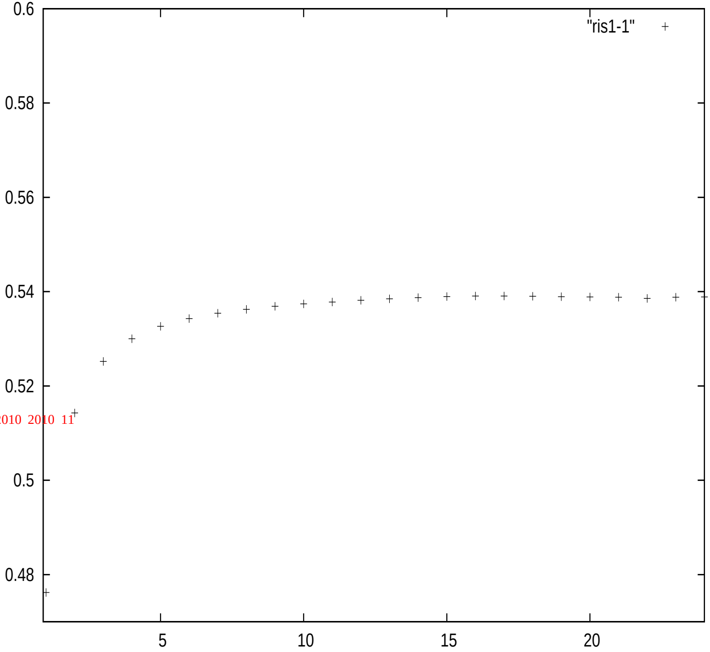
$$+ \text{(same with } s_0 = 0) + \text{(same with } s_1 = s_2 = 0)$$

where, if $a \geq b$,

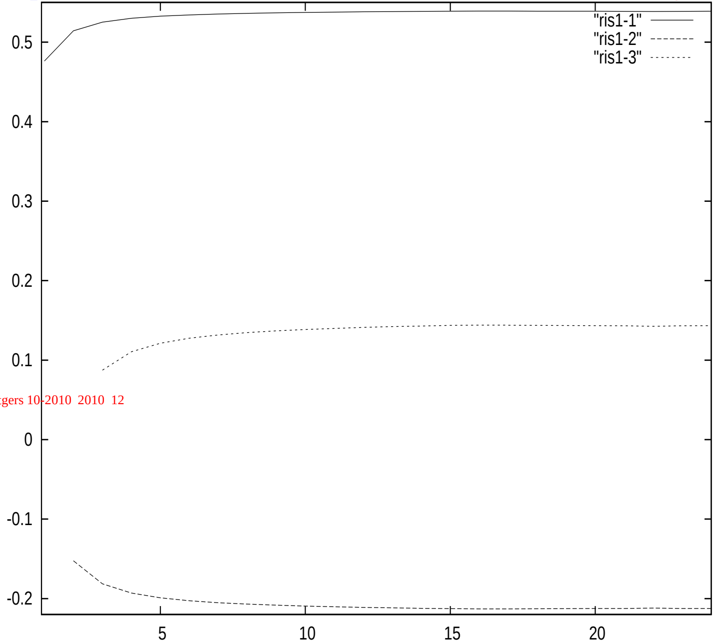
$$\begin{bmatrix} a \\ b \end{bmatrix} \stackrel{def}{=} \frac{(2a-1)!!}{(2b-1)!!\,(2(a-b)-1)!!}, \quad \begin{Bmatrix} a \\ b \end{Bmatrix} \stackrel{def}{=} \frac{(2a-1)!!}{2^a b!(a-b)!}$$

and $\stackrel{def}{=} 0$ if $a < b$.

does it admit a solution?



Graph of 3 coeff. $(1 \times 1) \to (24 \times 24)$ (to be divided by $2^k k!$)



Also Dirichlet b.c. on $\partial\Omega$ can be considered as well as other geometries can be considered. For instance conic geometry

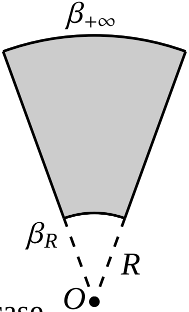


Fig.2: *Ω is a cone with vertex at O truncated at a distance R from its vertex; $T(q) = T_0 + \tau(q)$ solves $\Delta T = 0$ with $\partial_n T = 0$ on $\partial\Omega$ and value τ_- at bottom of Ω and $\tau_+ = 0$ at ∞: i.e. $\tau_- = \frac{\delta}{R}$, $\tau_+ = 0$*

special case

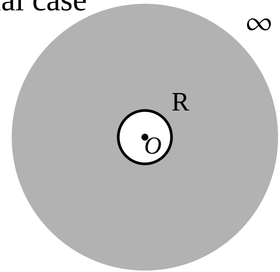


Fig.3: *A special case of Fig.2 the "exterior problem", i.e. the heat conduction outside a ball: a "hot potato" problem. It has an exact solution $T(q)$.*

A geometry with a long cylinder which opens up in two reservoirs

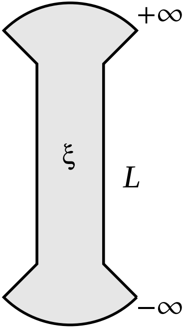


Fig. 4

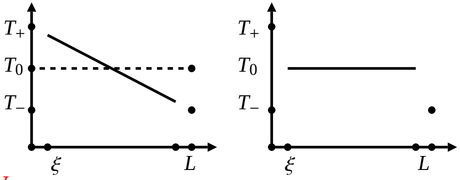
The container Ω is a cylinder of diameter ξ and height $L \gg \xi \gg r$ continued into two cones extending to ∞.

The interpolating inverse temperature $\beta(q)$ will be close to β_+ at the upper end of the cylinder and close to β_- at the bottom.

An essentially 1-dimensional geometry; temperature values at the top and the bottom (dictated by the b.c. at $\pm\infty$ via the heat equation) will be interpolated essentially linearly ("Saint-Venant's principle"), but $\delta T = O(L^{-1})$.

Very different for Dirichlet ($\beta(q) - \beta_0 = const$ on $\partial\Omega$) and Neumann b.c. ($\partial_n \beta = 0$ on $\partial\Omega$)

Consider both Neumann b.c. ($\partial_n \beta = 0$ on $\partial\Omega$) and Dirichlet ($\beta(q) - \beta_0 = const$ on $\partial\Omega$)



respectively.

The transients at the extremes decay exponentially on scale ξ of the cylinder diameter.

Critiques (somewhat negative)

(1) even correlations (exact solutions) can be exactly summed

$$\rho_{even}(\mathbf{q}_n, \mathbf{p}_n) = \rho^{[1]}(\mathbf{q}_n) \prod_{i=1}^{n} \Big(\frac{\beta_0}{\beta(q_i)} \frac{e^{-\frac{1}{2}\beta_0 p_i^2}}{(2\pi\beta_i^{-1})^{3/2}} - (\frac{\beta_0}{\beta(q_i)} - 1)\delta(\overline{p}_i) \Big)$$

Nevertheless $\langle \frac{1}{2}p^2 \rangle = \frac{3}{2}\beta(q)^{-1}$.

(2) The odd correlations with $\widetilde{C}_n(A_2) = 0$ unless $n = 2, |A_2| = 2$ (simplest choice) can also be resummed

$$\rho_{odd}(q_1, q_2, p_2, p_2) = C\, z_0^2 \Big(\partial_{1\alpha}\delta(\overline{p}_1) \cdot e^{-\frac{1}{2}\beta(q_1)\overline{p}_2^2} : \overline{p}_2^2 : + (1 \longleftrightarrow 2) \Big)$$

but not positive. Also $\rho_{odd}(q, p) \equiv 0$.

Way out? more solutions with more arbitrary constants when studying the higher orders (??)

References (also in http://ipparco.roma1.infn.it and arXiv)

Lebowitz: Phys. Rev., 114, 1192-1202, 1959
Feynman , Vernon: Annals of Physics, 24, 118–173, 1963
Bonetto, Lebowitz, Rey-Bellet, In Mathematical Physics 2000,
Garrido, Gallavotti: J. Stat. Phys., 126, 1201-1207, 2007
Gallavotti, Presutti: J. Math. Phys., **51**, 015202 (+32), 2010
Gallavotti, Presutti: J. Math. Phys., **51**, 053303 (+9), 2010,
Gallavotti, Presutti: J. Stat. Phys., **139**, 618-629, 10-2010,

Continuity? It is not clear why the correlation functions of a stationary state shoud be continuous at collisions, *e.g.* why

$$\rho(q_1, p_1, q_1 + r\omega, p_2) = \rho(q_1, p_1', q_1 + r\omega, p_2')$$

if $p_1, p_2 \longleftrightarrow p_1', p_2'$ is a collision at q_1 and $q_1 + r\omega$.
True: conserved by dynamics; but no contradiction with initial states in which does not hold. And even if holding at any finite time might fail to hold in the stationary state. Scenario:

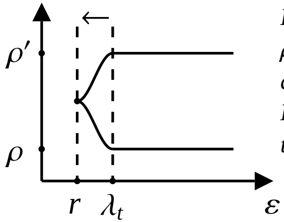


Fig.6: a pair correlations $\rho(\varepsilon)$, $\rho'(\varepsilon)$ discontinuity developing at t large: $\lambda_t \xrightarrow[t\to\infty]{} r$. For $t = +\infty$ $\lambda_t = r$ and discontinuity is sharp.

Which should be appropriate collision b.c. is therefore open: is continuity a required property? are the multiple collisions relevant (notice that they occurr in the hierarchy).

Odd Hierarchy: For $B = (A_1, \ldots, A_n)$ it is

$C_n(A) z_0^n (\prod_{i=1}^n \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!!})(\prod_{i=2}^n \widetilde{F}(q_i))$ times

$$1\#\beta_1^{-\frac{1}{2}}\Big\{\lambda(A,\alpha)\Big[\partial_\alpha^2 \widetilde{F}_{2a^1} + (a^1 - \frac{1}{2}) \cdot \partial_{1\alpha} \widetilde{F}_{2a^1} \frac{\partial_\alpha \beta_1}{\beta_1}\Big]$$

$$\# - \lambda(A_\alpha^{+2},\alpha)\frac{2a_\alpha + 1}{2(a_\alpha + 1)}\Big[\partial_\alpha^2 \widetilde{F}_{2(a^1+1)} + (a^1 + \frac{1}{2})\,\partial_\alpha \widetilde{F}_{2(a^1+1)} \frac{\partial_\alpha \beta_1}{\beta_1}\Big]$$

$$23\# + \frac{\partial_\alpha \beta_1}{\beta_1}\Big[\sum_{\alpha'} \lambda(A_{\alpha'}^{-2},\alpha)\, a_{\alpha'} \partial_\alpha \widetilde{F}_{2(a^1-1)} + \partial_\alpha \widetilde{F}_{2a^1}\Big(- \lambda(A,\alpha)$$

$$4\# - \sum_{\alpha'} \lambda(A_{\alpha\ \alpha'}^{+2\,-2},\alpha)(a_\alpha + \frac{1}{2} - \delta_{\alpha\alpha'})\frac{2(a_{\alpha'} + \delta_{\alpha\alpha'})}{2(a_\alpha + 1)}$$

$$5\# - \sum_{\alpha'} \lambda(A,\alpha)(2a_{\alpha'}^1 - \delta_{\alpha\alpha'})\Big)$$

$$67\# + \partial_\alpha \widetilde{F}_{2(a^1+1),2a^2} \lambda(A_\alpha^{+2},\alpha) \cdot (1 + 2a^1)\Big]\Big\}\frac{2a_\alpha + 1}{2(a_\alpha + 1)}\Big\}$$

$$+ C_{n+1}(A') I_{1\alpha} + \ldots = 0$$

$I_{1,\alpha}$ is $(\prod_{i=1}^{n} \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!})(\prod_{i=1}^{n} \widetilde{F}(q_i))$ times

$$- z_0^{n+1} \int_{s(q_i;\mathbf{q}_n)} d\sigma_\omega \, \omega_\alpha \, \beta_{n+1}^{-\frac{1}{2}} \, \partial_{q_{n+1,\alpha}} \widetilde{F}(\mathbf{q}_n, q_1 + r\omega)$$

with $\beta_{n+1} = \beta(q_{n+1})$, $q_{n+1} \equiv q_1 + r\omega$, $A' = \emptyset$ and the proportionality constant is i, α-independent. Other equations: by symmetry over the selection of the particles positions.

cancellations?

Odd hierarchy: For $B = (A^{+\,+1}_{\eta\;\eta'}, A_2, \ldots, A_n)$ it is

$C_n(A) z_0^n \beta_1^{-\frac{1}{2}} \prod_i \frac{(-\beta_i)^{a^i+\delta_{1i}}}{(2\mathbf{a}^i)!!} \frac{\prod_{i=2}^n \widetilde{F}(q_i)}{2(a_{\eta'}+1)2(a_\eta+1)}$ times

$$1\#\ \Big\{\lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1)\partial_{\eta\eta'}\widetilde{F}_{2(a^1+1)} - \lambda(A^{+2\;+2}_{\eta\;\;\eta'}, \eta')2(a_\eta + 1)\partial_{\eta\eta'}\widetilde{F}_{2(a^1+2)}$$

$$+ \frac{\partial_\eta \beta}{\beta}\Big(\lambda(A^{+2}_{\eta'}, \eta')(a^1 + \frac{1}{2})\, 2(a_\eta + 1)\partial_{\eta'}\widetilde{F}_{2(a^1+1)}$$

$$- \lambda(A^{+2\;+2}_{\eta\;\;\eta'}, \eta')(a^1 + \frac{3}{2})2(a_\eta + 1)\partial_{\eta'}\widetilde{F}_{2(a^1+2)}$$

$$2\#\ + \frac{1}{2}\sum_{\alpha'} \lambda(A^{-2\;+2}_{\alpha'\;\eta'}, \eta')2(a_\eta + 1)2(a_{\alpha'} + \delta_{\alpha'\eta'})\partial_{\eta'}\widetilde{F}_{2a}$$

$$345\#\ \ + \partial_{\eta'}\widetilde{F}_{2(a+1)}\Big[- \lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1)$$

$$- \frac{1}{2}\sum_{\alpha'} \lambda(A^{+2\;+2\;-2}_{\eta\;\;\eta'\;\;\alpha'}, \eta')(2a_\eta + 2 - 2\delta_{a'\eta}) \cdot (2a_{\alpha'} + 2\delta_{\alpha'\eta} + 2\delta_{\alpha'\eta'})$$

$$- \lambda(A^{+2}_{\eta'}, \eta')2(a_\eta + 1)\sum_{\alpha'}(2a_{\alpha'} + \delta_{\alpha'\eta'})\Big]$$

$$7\# + \Big[\lambda(A^{+2}_{\eta}{}^{+2}_{\eta'}, \eta')2(a_\eta + 1)\sum_{\alpha'}(2a_{\alpha'} + \delta_{\alpha'\eta} + \delta_{\alpha'\eta'})$$

$$6\# + \lambda(A^{+2}_{\eta}{}^{+2}_{\eta'}, \eta')2(a_\eta + 1)\Big]\partial_{\eta'}\widetilde{F}_{2(a+2)}\Big)\Big\} + (\eta\longleftrightarrow\eta')$$

which must be 0 after adding similar term with $(\eta\longleftrightarrow\eta')$.

For $B = (A_1{}^{+1}_{\eta}, A_2{}^{+1}_{\eta'}, \ldots, A_n)$ it is

$C_n(A_2)z_0^n\beta_2^{\frac{1}{2}} \prod_i \frac{(-\beta_i)^{a^i}}{(2\mathbf{a}^i)!!} \frac{1}{2(a^2_{\eta'}+1)2(a^1_\eta+1)}(\prod_{i>2}^n \widetilde{F}(q_i))$ times an analogous sum

Cancellation

Why do the integrals $\sum_{i,\alpha} I_{i,\alpha}$ vanish?

Realize that sum over *i is an integration over a closed surface* with ω as normal. Then

$$\sum_{\alpha} \int_{\partial} \omega_\alpha \partial_\alpha \beta(q_1 + r\omega)^{-\frac{1}{2}} \partial_\alpha \widetilde{F}(q_{n+1}) d\sigma_\omega$$

$$= \int_{D(\mathbf{q}_n)} \beta(q)^{-\frac{1}{2}} \Big(\Delta\widetilde{F}(q) - \frac{1}{2} \frac{\partial\beta(q) \cdot \partial\widetilde{F}(q)}{\beta(q)} \Big) dq$$

by Green's formula; here Neumann's or Dirichlet b.c. on $\partial\Omega$ is relevant if ∂ contains a part on $\partial\Omega$.

Hence the problem is purely algebraic.