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A convergent virial expansion for the quantum Lorentz gas with point interactions

C Carvalho

CFMC, Av. Gama Pinto 2, 1699 Lisboa Codex, Portugal
Fakultat für Physik, Universität Bielefeld, D-4800 Bielefeld, Federal Republic of Germany

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Abstract. We study the quantum Lorentz gas with point interactions. We use the explicit form of the resolvent of this system to set up an expansion for the pressure and the central limit theorem to sum the many random contributions to the scattering of the light particle due to the heavy particles. We also discuss the convergence of our expansion.

1. Introduction

The purpose of this paper is to use a novel expansion and a central limit argument to study virial coefficients for the quantum Lorentz gas with point interactions with finitely many centres. We begin by describing the model and establishing our notation.

We consider a cubic box of volume $V = L^3$ in $\mathfrak{R}^3$ where there are N fixed 'heavy' scatterers fixed at positions $R_1, \ldots, R_N$. These positions will be random, independently and uniformly distributed in the box. There are also M identical 'light' particles at positions $r_1, \ldots, r_M$. The only interaction will be a point interaction between the light particles and the heavy particles. We assume that the light particles are independent, distinguishable and not interacting with each other, so that it suffices to consider a single light particle moving around the heavy particles. Thus we will study the single particle Hamiltonian formally given by

$$H_{(R,\lambda)} = -\Delta + \sum_{j=1}^{N} \lambda_j \delta(\cdot - R_j) \tag{1}$$

where $-\Delta$ is the kinetic energy of the light particle and the λ_j are the coupling constants.

Before giving the precise definition of the Hamiltonian (1) in section 2 we will discuss the statistical mechanics of this system.

We have to calculate the partition function Z. Following the well known results in [1] we may express Z in terms of the Watson transform $\mathscr{L}^{-1}$ [2] of the spatial average $\langle \cdot \rangle$ over the positions of the heavy particles of the trace of the resolvent difference

$$ZZ_0^{-1} = 1 + Z_0^{-1} \mathscr{L}^{-1} \langle \mathrm{Tr}(G - G_0) \rangle. \tag{2}$$

Here Z is $\langle \mathrm{Tr}\, \mathrm{e}^{-\beta H_{(R,\lambda)}} \rangle$ with $\beta = 1/KT$ and $Z_0 = V\Lambda^{-3}$, with $\Lambda = (4\pi\beta)^{1/2}$, is the free gas partition function. G and G_0 are, respectively, the resolvents of H and H_0, the free Hamiltonian.

The standard procedure in corresponding problems with bounded interactions instead of the above delta interaction is to introduce the Born expansion for the resolvent difference $G-G_0$. This leads directly to the usual virial expansion for the pressure P. The pressure is of course given by

$$P=-(\partial F/\partial V)_T \tag{3}$$

where the free energy F is $-KT\ln Z$. For the free gas $P_0=KT/V$. Introducing the Born expansion into (2) and applying (3) yields a series expansion for P as a function of the density. The coefficients of the various powers of $\rho=N/V$ in this expansion are the virial coefficients.

We cannot, however, use the Born expansion to study the pressure in the Lorentz gas with point interactions since our potential is extremely singular [3, 4]. We therefore use a different expansion starting from the explicit form for the resolvent difference for point interactions in order to obtain an expansion for

$$\frac{\operatorname{Tr} e^{-\beta H_{(R,\lambda)}}}{\operatorname{Tr} e^{-\beta H_0}}. \tag{4}$$

There remains to take the spatial averaging. Here we observe that in order for equilibrium to exist we must have a lower limit $2r$ on the distance between the heavy scatterers. This is not a matter of mathematical convenience but a physical necessity, because of the singular attractive interaction, some sort of exclusion mechanism is required to prevent the system from collapsing. The minimal distance which ensures dilution and Boltzmann statistics which we use here provide a useful approximation to a more physically realistic Fermi system. To make the spatial averaging we use a central limit theorem argument to do the average in the large N limit and we obtain conditions for the convergence of this new expansion for the pressure. Though our expansion is different from the usual virial expansion, by studying the density dependence of the coefficients in our expansion, we can determine the usual virial coefficients. We will see that to leading order in our expansion

$$P=P_0+\rho(B+\rho C). \tag{4}$$

Since all higher-order corrections contain at least a factor of ρ^2, B is the second virial coefficient.

The paper is organised as follows. Section 2 is devoted to a careful definition of $H_{(R,\lambda)}$. In section 3 we introduce the expansion for $G-G_0$ and we study its convergence, in particular how this depends on r. In section 4 we use an appropriate lower limit on the distance between the scatterers and apply the central limit theorem argument to compute the average over allowed positions of the scatterers. This yields our expansion which we discuss in the final section 5.

2. The model

We give precise meaning to our formal Hamiltonian $H_{(R,\lambda)}$ appearing in (1) by prescribing [5, 6] that its ground-state wavefunction has the form

$$\phi(x)=\sum_{j=1}^{N}\frac{e^{-\kappa|x-R_j|}}{4\pi|x-R_j|} \tag{2.1}$$

for a fixed $\kappa > 0$. This amounts to choosing the infinitesimal coupling constant in order to have a prescribed binding energy for the interaction. This is a choice made when a particular ground state is chosen.

As discussed in [3] this is not the only way of making sense of the Hamiltonian (1). The complete relation between the two methods is developed in the author's thesis. We know that the general form of the resolvent for point interactions is [3]

$$(H-k^2)^{-1}(x,y) = G_0(x-y) + \sum_{m,n=1}^{N} [\Gamma_\alpha(k)^{-1}]_{mn} G_0(R_m - x) G_0(R_n - y) \tag{2.2}$$

for $\operatorname{Im} k > 0$. Here the $N \times N$ matrix $\Gamma_\alpha(k)$ has entries

$$[\Gamma_\alpha(k)]_{mn} = \left(\alpha_m - \frac{\mathrm{i}k}{4\pi}\right)\delta_{mn} - (H_0 - k^2)^{-1}(R_m - R_n)(1-\delta_{mn}) \tag{2.3}$$

and

$$(H_0 - k^2)^{-1}(x,y) = G_0(x-y) \qquad G_0(x) = \frac{\mathrm{e}^{\mathrm{i}k|x|}}{4\pi|x|}. \tag{2.4}$$

We must at this point identify the particular values of α_m in (2.3) which correspond to the dynamics generated by the ground state ϕ. To this end we first determine the boundary condition obeyed by ϕ at the scattering sites. We need only consider the s-wave relative to this site [7]. Denoting the s-wave component of ϕ by ϕ_0, one has

$$c_j = \left.\frac{\phi_0'}{\phi_0}\right|_{x=R_j} = -\kappa + \sum_{m\neq j} \frac{\mathrm{e}^{-\kappa|R_m - R_j|}}{4\pi|R_m - R_j|}. \tag{2.5}$$

Call H_α the Hamiltonian with resolvent (2.2). We determine for which α H_α has the ground state ϕ by checking boundary conditions.

For ψ in the domain of H_α, we have from [3] the representation:

$$\psi(x) = \varphi_k(x) + \sum_j a_j G_0(x - R_j) \tag{2.6}$$

where

$$a_j = [\Gamma_\alpha^{-1}(k)]_{jm} \varphi_k(R_m)$$

or for short

$$a = \Gamma^{-1}\varphi \qquad \text{and} \qquad \varphi_k \in D(-\Delta).$$

Now ψ obeys the same boundary conditions as ϕ at $x = R_j$, i.e.

$$c_j = \left.\frac{\psi_0'}{\psi_0}\right|_{x=R_j} = \mathrm{i}k + a_j^{-1} 4\pi \left(\sum_m (1-\delta_{jm}) G_0(R_j - R_m) a_m + \varphi_k(R_j)\right) \tag{2.7}$$

or, for short, after multiplication by a_j

$$ca = \mathrm{i}ka + 4\pi(Ga + \varphi) \tag{2.8}$$

with

$$G_{jm} = (1-\delta_{jm}) G_0(R_j - R_m).$$

Inserting $\varphi = \Gamma a$, this yields

$$ca = 4\pi\alpha a \qquad \text{i.e.} \qquad c_j = 4\pi\alpha_j. \tag{2.9}$$

As a consequence all we need to do to determine the resolvent of the Hamiltonian given in terms of the ground state ϕ, is to insert the specific boundary values c_j, i.e. the values of α

$$\alpha_j = \frac{1}{4\pi}\left(-\kappa + \sum_{m \neq j} \frac{e^{-\kappa|R_m - R_j|}}{-\kappa|R_m - R_j|}\right) \tag{2.10}$$

into the definition of the resolvent operator.

3. The expansion

In this section we will study an expansion for the resolvent difference and its convergence.

From (2.2) we see that we only need to invert the matrix Γ in order to have an explicit expression for the resolvent.

We write A for the diagonal part of $\Gamma_\alpha(k)$

$$A_{mn} = \left(\alpha_m - \frac{ik}{4\pi}\right)\delta_{mn} \tag{3.1}$$

and B for the off-diagonal part, with

$$B_{mn} = (H_0 - k^2)^{-1}(R_m - R_n)(1 - \delta_{mn}). \tag{3.2}$$

Our expansion is based on the observation that

$$\Gamma_\alpha(k)^{-1} = [I - A^{-1}B]^{-1}A^{-1} = \left(\sum_{p=0}^{\infty} (A^{-1}B)^p\right)A^{-1} \tag{3.3}$$

whenever

$$\|A^{-1}B\| < 1 \tag{3.4}$$

Here $\|\cdot\|$ denotes the matrix norm. Physically (3.3) corresponds to writing the physical propagator $(H - z)^{-1}$ as a sum over intermediate scattering events, in which the vertex corresponding to scattering on the heavy particle at R_m leads to the insertion of a factor

$$[A^{-1}]_{mn} = 4\pi\left(-\kappa + \sum_{m \neq j} \frac{e^{-\kappa|R_m - R_j|}}{-\kappa|R_m - R_j|} - ik\right)^{-1}\delta_{mn}. \tag{3.5}$$

Notice that, because of the term

$$\sum_{j \neq j} \frac{e^{-\kappa|R_m - R_j|}}{-\kappa|R_m - R_j|}$$

the other scatterers also contribute to the scattering at R_m. This collective behaviour results from the choice (2.1) of the ground-state wavefunction. With respect to the convergence of the series (3.3) we have to discuss for which values of k, given values for κ, $a_1, \ldots, a_N$, the condition (3.4) is satisfied. This can be easily done, having fixed a positive real number r, under the additive hypothesis that the configuration $(R_1, \ldots, R_N)$ of the scatterers is in the set S_r defined by

$$\min_{m,n}|R_m - R_n| \geq 2r \tag{3.6}$$

for some $r>0$. As

$$\|A^{-1}B\| \leqslant \|A^{-1}\| \, \|B\| \tag{3.7}$$

we start by estimating $\|A^{-1}\|$, observing that in S_r the following inequality holds.

With $k=t+\mathrm{i}s$, $s>0$

$$\|A^{-1}\| \leqslant \left|\frac{6}{4\pi r^3\kappa^2}-\frac{\kappa}{4\pi}\right|^{-1} \tag{3.8}$$

when

$$s \leqslant \frac{3}{r^3\kappa^2} \qquad \text{and} \qquad \kappa \geqslant \frac{6^{1/3}}{r}.$$

Also for all $k=t+\mathrm{i}s$

$$\|A^{-1}\| \leqslant \frac{4\pi}{|t|}.$$

The proof, given in appendix A, is based on the subharmonocity of the function

$$\frac{\mathrm{e}^{-\kappa|x|}}{|x|}$$

which leads to the inequalities

$$-\frac{\kappa}{4\pi} \leqslant \alpha_m \leqslant -\frac{\kappa}{4\pi}+\frac{3}{4\pi r^3\kappa^2} \tag{3.9}$$

the proof of which is also given in appendix A. We should remark that as r increases to infinity, the last result reduces to the obvious result in the one-centre case.

Next we turn to $\|B\|$. For $k=t+\mathrm{i}s$, $s>0$ we have

$$\|B\| \leqslant \frac{3}{2\pi r^3 s^2} \tag{3.10}$$

(see appendix B).

Therefore we conclude that provided the configuration of the scatterers is in S_r the expansion (3.3) holds for $k=t+\mathrm{i}s$ satisfying in the region

$$\left\{k \,\middle|\, \frac{6}{2s-\kappa}\frac{1}{r^3 s^2}<1-\varepsilon,\ s>\kappa\right\} \cup \left\{k \,\middle|\, \frac{6}{r^3}\frac{1}{|t|s^2}<1-\varepsilon,\ s>0\right\}$$

for any positive ε.

4. An application of the central limit theorem

To leading order in the convergent expansion studied in the last section

$$(H-k^2)^{-1}(x,x)-(H_0-k^2)^{-1}(x,x) = \sum_{m=1}^{N}\left(\alpha_m-\frac{\mathrm{i}k}{4\pi}\right)^{-1}((H_0-k^2)^{-1}(x-R_m))^2. \tag{4.1}$$

Hence to leading order

$$\mathrm{Tr}[(H-k^2)^{-1}-(H_0-k^2)^{-1}] = \sum_{m=1}^{N}\left(\alpha_m-\frac{\mathrm{i}k}{4\pi}\right)^{-1}\left(\frac{1}{4\pi}\right)^2\int \mathrm{d}^3x\,\frac{\mathrm{e}^{2\mathrm{i}k|R_m-x|}}{|R_m-x|^2} \tag{4.2}$$

which gives us

$$\mathrm{Tr}(H-k^2)^{-1}-\mathrm{Tr}(H_0-k^2)^{-1}=\sum_{m=1}^{N}\left(\alpha_m-\frac{\mathrm{i}k}{4\pi}\right)^{-1}\left(-\frac{1}{8\pi\mathrm{i}k}\right). \tag{4.3}$$

According to (2) we must now average this over the positions of the scatterers $R_1,\ldots,R_N$ on which $\alpha_1,\ldots,\alpha_N$ depend.

Recall that

$$\left(\alpha_m-\frac{\mathrm{i}k}{4\pi}\right)^{-1}=4\pi\left(-\kappa+\sum_{n\neq m}\frac{\mathrm{e}^{-\kappa|R_m-R_n|}}{|R_m-R_n|}-\mathrm{i}k\right)^{-1}. \tag{4.4}$$

The region where the scatterers are distributed is taken to be a cubic box of edge length $N^{1/3}L$. The volume is then $NL^3=V(N)$. The admissible configurations of the scatterers are N-tuples $(R_1,\ldots,R_N)$ where each R_m is in the box and

$$\min_{m,n}|R_m-R_n|\geqslant 2r. \tag{4.5}$$

Let $\Omega\subset\Re^{3N}$ be this set of points. We will average over Ω with uniform measure. So that we have to compute for fixed m (say $m=1$)

$$\frac{1}{|\Omega|}\int_\Omega \mathrm{d}^3R_1\ldots\mathrm{d}^3R_n\,4\pi\left(-\kappa+\sum_{n\neq m}\frac{\mathrm{e}^{-\kappa|R_m-R_n|}}{|R_m-R_n|}-\mathrm{i}k\right)^{-1}. \tag{4.6}$$

To rewrite this in a form useful for computation, we introduce

$$F(R)=\begin{cases}\dfrac{\mathrm{e}^{-\kappa|R|}}{|R|} & R>r\\ 0 & R\leqslant r.\end{cases} \tag{4.7}$$

We introduce the new variables R_1, $R_{12},\ldots,R_{1N}$ by

$$R_{1n}=R_n-R_1.$$

Clearly the Jacobian of this transformation is unity. Let

$$\tilde{\Omega}(R_1)=\{(R_{12},\ldots,R_{1N}):(R_1,\ldots,R_N)\in\Omega\}. \tag{4.8}$$

Then (4.6) becomes

$$\frac{1}{|V(N)|}\int \mathrm{d}^3R_1\left(\frac{1}{|\tilde{\Omega}(R_1)|}\int_{\tilde{\Omega}(R_1)}\mathrm{d}^3R_{12}\ldots\mathrm{d}^3R_{1N}\frac{4\pi}{-\kappa+\Sigma_{n=2}^N F(R_{1n})-\mathrm{i}k}\right). \tag{4.9}$$

Because of the rapid exponential decay of F, the integrand is nearly constant in R_1. It differs significantly from its value at $R_1=0$ only when R_1 is close to the boundary of the box. Note that of course $V(N)|\tilde{\Omega}(R_1)|=|\Omega|$ and hence $|\tilde{\Omega}(R_1)|\equiv|\tilde{\Omega}|$ is independent of R_1. So we can replace the integration over R_1 in (4.9) by the evaluation at $R_1=0$ and (4.9) becomes

$$\frac{1}{|\tilde{\Omega}|}\int_{\tilde{\Omega}(0)}\mathrm{d}^3R_{12}\ldots\mathrm{d}^3R_{1N}\frac{4\pi}{-\kappa+\Sigma_{n=2}^N F(R_{1n})-\mathrm{i}k}. \tag{4.10}$$

Clearly $|\tilde{\Omega}|=(V(N)-(N-1)\frac{4}{3}\pi r^3)^{N-1}$ up to a negligible error. Now consider the integration in the variable R_{12}. Again we use the exponential decay of F; This guarantees us that, as a function of R_{12}

$$\frac{4\pi}{-\kappa+\Sigma_{n=2}^N F(R_{1n})-\mathrm{i}k} \tag{4.11}$$

is nearly constant outside a ball of fixed (independent of N) radius. Now of course, if we integrate a constant over some region, we do not care about the shape of the region; all that concerns us is its volume. Therefore we may freely deform the region of integration in R_{12} to a ball of volume

$$(V(N)-(N-1)\tfrac{4}{3}\pi r^3)^{N-1} \tag{4.12}$$

and we do not change the value of the integral (4.10). Repeating this procedure for the remaining variables, we have replaced the region of integration by an $(N-1)$-fold Cartesian product of sphere of volume $V(N)-\frac{4}{3}\pi r^3(N-1)$. Making the substitution, (4.10) becomes

$$\frac{1}{V(N)^{N-1}}\int \mathrm{d}^3R_{12}\ldots\mathrm{d}^3R_{1N}\frac{4\pi}{-\kappa+\Sigma_{n=2}^{N}F(R_{1n})-\mathrm{i}k}. \tag{4.13}$$

This is the expectation value

$$E\left(\frac{4\pi}{-\kappa+\Sigma_{n=2}^{N}X_n-\mathrm{i}k}\right) \tag{4.14}$$

where $X_1(N),\ldots,X_N(N)$ are independent, identically distributed random variables with mean

$$M(N)=EX_1(N)=\frac{4\pi}{V(N)}\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r} \tag{4.15}$$

up to an exponential error. The main term is $\mathrm{O}(1/N)$.

The second moment is given by

$$E(X_1(N))^2=\frac{2\pi}{V(N)}\frac{1}{\kappa}\mathrm{e}^{-2\kappa r} \tag{4.16}$$

up to a term $\mathrm{O}(\mathrm{e}^{-N})$.

The variance $\sigma^2(N)$ is then given by

$$\sigma^2(N)=E(X_1(N))^2-(M(N))^2=E(X_1(N))^2+\mathrm{O}(1/N^2)$$

So

$$\sigma^2(N)=\frac{2\pi\rho}{N}\frac{1}{\kappa}\mathrm{e}^{-2\kappa r}. \tag{4.17}$$

Hence $\sigma(N)=\mathrm{O}(\sqrt{1}/N)$. We have

$$\lim_{N\to\infty}(N-1)M(N)=4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\equiv M \tag{4.18}$$

$$\lim_{N\to\infty}\sqrt{N-1}\,\sigma(N)=\sqrt{2\pi\rho}\,\frac{1}{\sqrt{\kappa}}\mathrm{e}^{-\kappa r}\equiv\sigma. \tag{4.19}$$

This is what permits us to apply the central limit theorem [8]. The functions $f_N(x)$ given by

$$f_N(x)=\frac{4\pi}{-\kappa-\sqrt{N-1}\,\sigma(N)X+(N-1)M(N)-\mathrm{i}k} \tag{4.20}$$

converge uniformly to $f(x)$ given by

$$f(x)=4\pi\left(-\kappa-\sqrt{\frac{2\pi\rho}{\kappa}}\,e^{-r\kappa}X+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)e^{-r\kappa}-ik\right)^{-1}. \tag{4.21}$$

Then if we introduce normalised random variables $Y_2(N),\ldots,Y_N(N)$ by

$$Y_n(N)=\frac{X_n(N)-M(N)}{\sigma(N)} \tag{4.22}$$

as $X_n(N)=\sigma(N)+M(N)$, (4.14) has the same large N limit as

$$Ef\left(\sum_{n=2}^{N}\frac{Y_n(N)}{\sqrt{N-1}}\right). \tag{4.23}$$

Application of the central limit theorem should then give

$$\lim_{N\to\infty} Ef\left(\sum_{n=2}^{N}\frac{Y_n(N)}{\sqrt{N-1}}\right)=\int_{-\infty}^{+\infty}dx\,f(x)\,e^{-x^2/2}. \tag{4.24}$$

Actually the distribution of $Y_n(N)$ spreads with N is just such a way that our problem is borderline for the Lindberg condition [8]. Therefore we will not rigorously justify our application of the central limit theorem on *a priori* mathematical grounds. Rather, we will give good *a posteriori* justification of our computation by showing that our results agree with previous independently obtained results for the limiting case.

This last integral is easily computed

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dx\,f(x)\,e^{-x^2/2}=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dx\frac{4\pi}{\sigma x-\gamma}\,e^{-x^2/2} \tag{4.25}$$

where $\gamma=\kappa+ik-M$ and σ given in (4.18) and (4.19). We obtain

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}dx\frac{4\pi}{\sigma x-\gamma}\,e^{-x^2/2}=\frac{\gamma}{\sigma}\left[1-\phi\left(\sqrt{\frac{-\gamma^2}{2\sigma^2}}\right)\right]\frac{\pi}{\sqrt{-\gamma^2}}\,e^{-\gamma^2/2\sigma^2} \tag{4.26}$$

where ϕ is the error function [9].

From the above computations and remarks on surface errors it follows directly that

$$\lim_{N\to\infty}\frac{1}{V(N)}\mathrm{Tr}[(H-k^2)^{-1}-(H_0-k^2)^{-1}]$$

$$=\frac{1}{8\pi ik}\,\rho 2\sqrt{2\pi}\,\frac{\gamma}{\sigma}\left[1-\phi\left(\sqrt{\frac{-\gamma^2}{2\sigma^2}}\right)\right]\frac{\pi}{\sqrt{-\gamma^2}}\,e^{-\gamma^2/2\sigma^2}. \tag{4.27}$$

5. The second virial coefficient and contribution to higher virial coefficients

In this section we combine the previous results to study the virial expansion for our model. Our starting point is the formula

$$ZZ_0^{-1}=1+Z_0^{-1}\mathscr{L}^{-1}\langle\mathrm{Tr}(G-G_0)\rangle \tag{5.1}$$

where $\mathscr{L}^{-1}$ is the Watson transform [2] applied to a function f

$$\mathscr{L}^{-1}f(\beta)=\frac{1}{2\pi i}\int_C dz\,e^{-\beta z}f(z) \tag{5.2}$$

and the contour C is any counter clockwise contour enclosing the poles of the function f. Initially we take any contour staying in the region

$$\left\{k \,\middle|\, \frac{6}{2s-\kappa}\,\frac{1}{r^3 s^2}<1-\varepsilon,\ s>\kappa\right\} \cup \left\{k \,\middle|\, \frac{6}{r^3}\,\frac{1}{|t| s^2}<1-\varepsilon,\ s>0\right\} \tag{5.3}$$

in the upper half-plane and with

$$\lim_{\operatorname{Re} k\to -\infty} (\operatorname{Im} k)=0.$$

We take the part of the contour in the lower half-plane to be the reflection. Then if we assume for simplicity that negative energy states are absent [1]

$$\frac{1}{2\pi \mathrm{i}}\int_C \mathrm{d}z\, \mathrm{e}^{-\beta z}\langle \operatorname{Tr}(G-G_0)\rangle = -\operatorname{Im}\frac{1}{\pi}\int_C \mathrm{d}z\, \mathrm{e}^{-\beta z}\langle \operatorname{Tr}(G-G_0)\rangle \tag{5.4}$$

where $z=k^2$.

By the results of section 3 the entire contour C is in the region where our expansion converges. To leading order in ρ (5.4) equals

$$\operatorname{Im}\frac{1}{\pi}\int_C \mathrm{d}z\, \mathrm{e}^{-\beta z}\sum_{m=1}^{N}\left(\alpha_m-\frac{\mathrm{i}\sqrt{z}}{4p}\right)^{-1}\left(-\frac{1}{8\pi \mathrm{i}\sqrt{z}}\right) \tag{5.5}$$

where we have used the computations leading to (4.3).

Before performing the integral we take the thermodynamic limit. By (4.27)

$$\lim_{N\to\infty}\frac{1}{V(N)}\mathscr{L}^{-1}\langle \operatorname{Tr}(G-G_0)\rangle$$

$$=\operatorname{Im}\frac{1}{\pi}\int_C \mathrm{d}z\, \mathrm{e}^{-\beta z}\frac{1}{8\pi \mathrm{i}\sqrt{z}}\rho 2\sqrt{2\pi}\,\frac{\gamma}{\sigma}\left[1-\phi\left(\sqrt{\frac{-\gamma^2}{2\sigma^2}}\right)\right]\frac{\pi}{\sqrt{-\gamma^2}}\,\mathrm{e}^{-\gamma^2/2\sigma^2} \tag{5.6}$$

with $\gamma(k)=\gamma(\sqrt{z})=\kappa-M+ik$. From (4.18) and (4.19) we see that the argument of the error function ϕ is large for low density. Hence [9]

$$2\sqrt{2\pi}\,\frac{\gamma}{\sigma}\left[1-\phi\left(\sqrt{\frac{-\gamma^2}{2\sigma^2}}\right)\right]\frac{\pi}{\sqrt{-\gamma^2}}\,\mathrm{e}^{-\gamma^2/2\sigma^2}=-\frac{4\pi}{\gamma} \tag{5.7}$$

and (5.6) becomes

$$\operatorname{Im}\frac{\rho}{\pi}\frac{\gamma}{\sigma}\int_C \mathrm{d}z\, \mathrm{e}^{-\beta z}\left(-\frac{\mathrm{i}}{2\sqrt{z}}\right)\left(\frac{1}{-\kappa+M-\mathrm{i}\sqrt{z}}\right). \tag{5.8}$$

At this point there are no obstacles to deforming the contour so that runs arbitrarily close to the real axis. Then (5.8) becomes

$$\int_0^{+\infty}\mathrm{d}z\, \mathrm{e}^{-\beta z}\left(\frac{1}{2\sqrt{z}}\right)\left[-\kappa+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right]\left\{\left[-\kappa+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right]^2+z\right\}^{-1}$$

$$=\tfrac{1}{2}\operatorname{sgn}\left[-\kappa+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right]\exp\beta\left[-\kappa+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right]^2$$

$$\times\left[1-\phi\left(\sqrt{\beta\left[-\kappa+4\pi\rho\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right]}\right)\right] \tag{5.9}$$

with

$$\operatorname{sgn}(x) = \begin{cases} 1 & x \geqslant 0 \\ -1 & x < 0 \end{cases}$$

$$\phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{d}t\, \mathrm{e}^{-t^2}.$$

To express this result more transparently we make a Taylor expansion in the density ρ and we obtain for the continuum contribution

$$\rho 4\pi^{3/2}\beta^{3/2}\left\{[1-\phi(\sqrt{\beta\kappa^2})]\,\mathrm{e}^{\beta\kappa^2}+\rho\left[8(\beta\pi)^{1/8}\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}-8\pi\beta\kappa\right.\right.$$
$$\left.\left.\times\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\,\mathrm{e}^{\kappa^2\beta}\right][1-\phi(\sqrt{\beta\kappa^2})]\right\}. \tag{5.10}$$

From (5.10) we see that the contribution coming from the first term of our expansion (3.3) after adding the bound state contribution is given by

$$\rho\{-4\pi^{3/2}\beta^{3/2}\,\mathrm{e}^{\beta\kappa^2}-8\pi\beta^2\kappa\}+\rho^2\left[32\pi^2\beta^2\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right.$$
$$\left.+32\pi^{5/2}\beta^{5/2}\kappa\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\,\mathrm{e}^{\kappa^2\beta}+64\pi^2\beta^3\kappa^2\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\right] \tag{5.11}$$

and

$$\rho\left(-4\pi^{3/2}\beta^{3/2}\,\mathrm{e}^{\beta\kappa^2}+\frac{4\pi\beta}{\kappa}\right)+\rho^2\left[64\pi^{5/2}\beta^{5/2}\kappa\left(\frac{r}{\kappa}+\frac{1}{\kappa^2}\right)\mathrm{e}^{-\kappa r}\,\mathrm{e}^{\kappa^2\beta}\right] \tag{5.12}$$

for high and low temperatures, respectively. The leading term in our expansion for the pressure contains terms proportional to ρ and higher powers of ρ, unlike, of course, the usual virial expansion. With little reflection one sees that the following terms of our expansion are at least proportional to ρ^2.

Therefore the second virial coefficient is

$$B \simeq -4\pi^{3/2}\beta^{3/2}\,\mathrm{e}^{\beta\kappa^2}-8\pi\beta^2\kappa \tag{5.13}$$

$$B \simeq -4\pi^{3/2}\beta^{3/2}\,\mathrm{e}^{\beta\kappa^2}+\frac{4\pi\beta}{\kappa} \tag{5.14}$$

for high and low temperatures, respectively.

6. Conclusions

We have proved that when $r > 0$ the series expansion (2.3) converges in a region large enough to apply the Watson transform. In any expansion, one needs to control the effects of multiple scattering. In the usual Born expansion, one uses a bound on the interaction to do this. With our singular interaction, we have no such bound. Rather, we will control multiple scattering using the diluteness of the scatterers in our model. The scatterers are increasingly dilute, of course, as the minimum radius r increases. The consistency of this method with previous analysis is shown by the fact that we recover the result of section 3 when we consider the contribution of just one scatterer when r goes to infinity.

The additional terms in (5.10) are of order of ρ^2, so their contribution to the third virial coefficient does not appear when r goes to infinity.

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Appendix A

Lemma A1. For α_m satisfying (1.10) we have

$$-\frac{\kappa}{4\pi} \leqslant \alpha_m < -\frac{\kappa}{4\pi} + \frac{3}{4\pi r^3 \kappa^2}. \tag{A1}$$

Proof. From section 2

$$\alpha_m = \frac{1}{4\pi}\left(-\kappa + \sum_{n \neq m} \frac{e^{-\kappa|R_m - R_n|}}{|R_m - R_n|}\right) \qquad \text{for } \kappa > 0. \tag{A2}$$

Intuitively when r is large, the scatterers are so far apart they act independently and α_m is very close to $-\kappa/4\pi$ as in the one-centre case. Of course $\alpha_m > -\kappa/4\pi$, so what we want is an upper bound for α_m in terms of κ and r which reduces to $-\kappa/4\pi$ as r goes to infinity.

To do this, we use a subharmonicity argument to bound the complicated sum in (A2) with an easily estimated integral.

Let

$$\rho_0(x) = \begin{cases} \dfrac{3}{4\pi r^3 \kappa^2} & |x| \leqslant r \\ 0 & |x| > r. \end{cases} \tag{A3}$$

Clearly ρ_0 is positive, spherically symmetric and

$$\int \rho_0(x)\, d^3x = 1.$$

Since

$$(\Delta - \kappa^2)\frac{e^{-\kappa|x|}}{|x|} = -\delta(x) \tag{A4}$$

we have

$$\Delta\left(\frac{e^{-\kappa|x|}}{|x|}\right) = \kappa^2 \frac{e^{-\kappa|x|}}{|x|} > 0 \qquad \text{for } x \neq 0. \tag{A5}$$

That is, the function

$$\frac{e^{-\kappa|x|}}{|x|}$$

is subharmonic away from $x=0$. Subharmonic functions have the property that their value at any point is less than their average value on any ball (in the region of subharmonicity) centred at that point [11]. Therefore if we define

$$\rho_m(x)=\rho_0(x-R_m) \tag{A6}$$

and

$$g(x)=\rho_m(x) \qquad f(x)=\sum_{n=1}^{N}\rho_n(x) \tag{A7}$$

we have (for m fixed)

$$\sum_{m\neq n}\frac{e^{-\kappa|R_m-R_n|}}{|R_m-R_n|}<\int\int g(x)\frac{e^{-\kappa|x-y|}}{|x-y|}f(y)\,d^3x\,d^3y. \tag{A8}$$

By condition (3.6) for all y

$$0\leqslant f(y)\leqslant\frac{3}{4\pi r^3}. \tag{A9}$$

Therefore

$$\int g(x)\frac{e^{-\kappa|x-y|}}{|x-y|}f(y)\,d^3x\,d^3y\leqslant\frac{3}{4\pi r^3}\int d^3x\,g(x)\int d^3y\frac{e^{-\kappa|x-y|}}{|x-y|} \tag{A10}$$

and since

$$\frac{3}{4\pi r^3}\int d^3x\,g(x)\int d^3y\frac{e^{-\kappa|x-y|}}{|x-y|}=\frac{3}{4\pi r^3}\left(\int d^3x\,g(x)\right)\frac{4\pi}{\kappa^2}=\frac{3}{r^3\kappa^2}. \tag{A11}$$

So

$$-\frac{\kappa}{4\pi}\leqslant\alpha_m<-\frac{\kappa}{4\pi}+\frac{3}{4\pi r^3\kappa^2}. \tag{A12}$$

Now we can estimate $\|A^{-1}\|$.

Lemma A2. With $k=t+is$, $s>0$

$$\|A^{-1}\|<\left|\frac{6}{4\pi r^3\kappa^2}-\frac{\kappa}{4\pi}\right|^{-1}$$

when

$$s\leqslant\frac{3}{r^3\kappa^2} \qquad \text{and} \qquad \kappa\geqslant\frac{6^{1/3}}{r}.$$

Also for all $k=t+is$

$$\|A^{-1}\|\leqslant\frac{4\pi}{|t|}.$$

Proof. By lemma A1 and the first condition above

$$\alpha_m + \frac{s}{4\pi} < -\frac{\kappa}{4\pi} + \frac{6}{4\pi r^3 \kappa^2}. \tag{A13}$$

Under the second condition above, the term on the RHS is negative and hence both terms are negative. So

$$\left|\alpha_m - \frac{\mathrm{i}k}{4\pi}\right| \geqslant \left|\alpha_m + \frac{s}{4\pi}\right| \geqslant \left|-\frac{\kappa}{4\pi} + \frac{6}{4\pi r^3 \kappa^2}\right|. \tag{A14}$$

Clearly

$$\|A^{-1}\| = \sup_m \left|\alpha_m - \frac{\mathrm{i}k}{4\pi}\right|^{-1} < \left|-\frac{\kappa}{4\pi} + \frac{6}{4\pi r^3 \kappa^2}\right|^{-1}. \tag{A15}$$

Appendix B

A straightforward argument based on separate consideration of the real and imaginary parts gives us

$$\|B\| \leqslant 2\|\tilde{B}\| \tag{B1}$$

where

$$\tilde{B}_{mn} = \frac{\mathrm{e}^{-s|R_m - R_n|}}{4\pi|R_m - R_n|}(1 - \delta_{mn}) \tag{B2}$$

and again $k = t + \mathrm{i}s$, $s > 0$.

Lemma B1. For $k = t + \mathrm{i}s$, $s > 0$ we have

$$\|B\| < \frac{3}{2\pi r^3 s^2}.$$

Proof. Since $\tilde{B}$ is self-adjoint

$$\|\tilde{B}\| = \sup_{\|v\|=1} |v_m B_{mn} v_n| \tag{B3}$$

where

$$\|v\| = \left|\sum_m |v_m|^2\right|^{1/2}. \tag{B4}$$

We can estimate

$$\sum_{m,n} v_m \tilde{B}_{mn} v_n \tag{B4}$$

using the subharmonicity argument of lemma A1.

Let

$$f(x) = \sum_{m=1}^{N} v_m \rho_m(x) \tag{B5}$$

with ρ_m as before. Then as in lemma A1

$$\sum_{m,n} v_m \frac{e^{-s|R_m-R_n|}}{|R_m-R_n|} v_n < \iint f(x) \frac{e^{-s|x-y|}}{|x-y|} f(y)\, d^3x\, d^3y. \tag{B6}$$

As [12]

$$\iint f(x) \frac{e^{-s|x-y|}}{|x-y|} f(y)\, d^3x\, d^3y = \langle f, (-\Delta+s^2)^{-1} f \rangle \tag{B7}$$

we have

$$\sum_{m,n} v_m \frac{e^{-s|R_m-R_n|}}{|R_m-R_n|} v_n < \frac{1}{s^2} \int f^2(x)\, d^3x \tag{B8}$$

and we obtain using the condition (3.6)

$$\sum_{m,n} v_m \frac{e^{-s|R_m-R_n|}}{|R_m-R_n|} v_n < \left(\frac{3}{4\pi r^3}\right)^2 \frac{4\pi r^3}{s^2} \left(\sum v_m^2\right). \tag{B9}$$

We have finally

$$\|B\| < \frac{3}{2\pi r^3 s^2}.$$

We summarise as follows.

Theorem B1. Under the condition (3.6) the series expansion (3.3) for $\Gamma_\alpha^{-1}(k)$ converges uniformly for $k = t + is$ in the region

$$\left\{k \,\middle|\, \frac{6}{2s-\kappa} \frac{1}{r^3 s^2} < 1, s > \kappa\right\} \cup \left\{k \,\middle|\, \frac{6}{r^3} \frac{1}{|t| s^2} < 1, s > 0\right\}.$$

Proof. Just combine the lemmas.

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