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Geometric Expansion of the Boundary Free Energy of a Dilute Gas

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Abstract. We consider a dilute classical gas in a volume $\varepsilon^{-1}\Lambda$ which tends to $\mathbb{R}^d$ by dilation as $\varepsilon \to 0$. We prove that the pressure $p(\varepsilon^{-1}\Lambda)$ is C^q in ε at $\varepsilon = 0$ (thermodynamic limit), for any $q \in \mathbb{N}$, provided the boundary $\partial\Lambda$ is C^q and provided the Ursell functions $u_n(x_1, \ldots, x_n)$ admit moments of degree q and have "nice" derivatives.

1. Introduction

In a recent paper [1], Pogosian derives the asymptotic expansion of the pressure $p(\varepsilon^{-1}\Lambda)$ in the thermodynamic limit $\varepsilon \to 0$, up to order d in ε,

$$p(\varepsilon^{-1}\Lambda) = a_0(\Lambda) + a_1(\Lambda)\varepsilon + \cdots + a_{d-1}(\Lambda)\varepsilon^{d-1} + a_d(\Lambda)\varepsilon^d + r_d(\varepsilon, \Lambda)\varepsilon^d$$

for a dilute gas in $\Lambda \subset \mathbb{Z}^d$ or $\Lambda \subset \mathbb{R}^d$. The remainder satisfies

$$|r_d(\varepsilon, \Lambda)| \leq \begin{cases} 0(\log \varepsilon^{-1}) & \text{in general} \\ 0(1) & d = 2 \\ 0(\varepsilon) & \text{if } \Lambda \subset \mathbb{Z}^d \text{ or } \Lambda \text{ polyhedron in } \mathbb{R}^d. \end{cases}$$

The hypotheses on $\partial\Lambda$ are the natural ones, the hypotheses on the interaction potential are rather complicated and are not optimal. The proof is based on the Mayer expansion and extensive use of Taylor expansions.

The present paper extends the above results and simplifies the proofs, for volumes $\varepsilon^{-1}\Lambda \subset \mathbb{R}^d$ with $\partial\Lambda$ smooth. We prove the absence of logarithms (as conjectured by Pogosian), and extend the expansion to all orders. The order d (dimension of space) has nothing special to it when the interaction is smooth, which we assume, as Pogosian does in his proof if we understand it correctly. It is clear however that strong singularities in the interaction potential would show up in the expansion at some order in ε depending on the dimension. We do not know whether a jump discontinuity in the Ursell functions (e.g. square hard core potential) would spoil the expansion at all.

Our hypotheses on the long range behaviour of the potential are the minimal hypotheses for the absolute convergence of the sums and integrals which define the coefficients of the expansion in the limit $\varepsilon = 0$.

It is well known that $a_0(\Lambda)$ and $a_1(\Lambda)$ are proportional respectively to $|\Lambda|$ and $|\partial\Lambda|$. Pogosian has shown (for Λ smooth):

$$a_2(\Lambda) \approx \int_{\partial\Lambda} H(x)dx,$$

where $H(x)$ is the mean curvature at $x \in \partial\Lambda$. We remark that the two point Ursell function does not contribute to $a_2(\Lambda)$:

$$\varepsilon^d \int_{(\varepsilon^{-1}\Lambda)^2} dxdyU_2(x-y) = b_0|\Lambda| + \varepsilon b_1|\partial\Lambda| + \varepsilon^3 b_3\langle R^{-2}\rangle_{\partial\Lambda} + 0(\varepsilon^4),$$

where R^{-1} denotes the normal curvature in a plane normal to $\partial\Lambda$ at $x \in \partial\Lambda$, and the average is taken over the orientation of the normal plane and over $x \in \partial\Lambda$. This explicit formula assumes rotation invariance, and is valid only for the two point function. General results and formulae for the n-point integral are given in Theorem 2. In general $a_j(\Lambda)$ will be a finite sum (not just one term as above), where each term is factorized into a potential dependent factor times a volume dependent factor.

Corollary 1 combines Theorem 2 with the Mayer expansion for the pressure, at small enough activity. Corollary 2 extends the results to the whole analyticity region in the activity, assuming bounds on the truncated correlation functions; it also gives recursion formulae for the expansion in ε of the average number of particles in volume $\varepsilon^{-1}\Lambda$.

Theorem 1 is the hard core of the paper, which we now explain in words. (The reader interested in final results might now go to Theorem 2 and corollaries).

The idea of our derivation is to write a Taylor expansion around $\varepsilon = 0$ of $p(\varepsilon^{-1}\Lambda)$. This will involve of course computing derivatives of that quantity. These derivatives will be expressed in terms of various integrals containing derivatives of the Mayer functions. Explicit expressions for these integrals will be determined by recursion over the order of derivation in ε. Due to the presence of ε^{-1} in the function $p(\varepsilon^{-1}\Lambda)$, derivations in ε will produce terms which are apparently singular in $\varepsilon = 0$. It turns out that under our regularity hypothesis these singularities cancel. This compensation is performed explicitly by using integration by parts over the space variables. Therefore a typical term in the Taylor expansion of $p(\varepsilon^{-1}\Lambda)$ will be a sum of integrals with some variables being integrated over the domain Λ, and the remaining variables over the boundary $\partial\Lambda$ of Λ. One can observe that two scales are present in the problem: the fixed scale of Λ, and the varying (large) scale ε^{-1}. This implies that the integrands can be regarded as functions of the space variables x on the one hand and of $y = \varepsilon^{-1}x$ on the other hand.

Lemma 2 deals with the derivation with respect to ε of such integrals. Lemma 3 is an identity from differential geometry which is used to exhibit cancellations of singular terms in the integration by parts (see for example [3] for the method of the moving frame). As explained above, our main result follows by recursive applications of Lemma 2.

2. Results

We first give a local result (Theorem 1, where the n-point function is anchored at $x_1=0$), then a global result with detailed formulae (Theorem 2), which we apply to the Mayer expansion for the pressure (Corollary 1); Corollary 2 deals with the number of particles, with hypotheses bearing on correlation functions rather than on Ursell functions.

Theorem 1. *Let* $\Lambda \subset \mathbb{R}^d$, $0\in\partial\Lambda$, $\partial\Lambda$ *a* C^r *hypersurface. Given integers* $n \geqq p_0 \geqq 1$, *let*

$$u(x_2,\dots,x_n;y_2,\dots,y_n)\in C^k((\partial\Lambda)^{p_0-1}\times\Lambda^{n-p_0}\times R^{(n-1)d}).$$

Let $0\leqq q\leqq \inf(k,r-1)$ *and suppose that all derivatives* $D^\alpha u$ *of total order* $0\leqq|\alpha|\leqq q$ *satisfy*

$$\int_{(\varepsilon^{-1}\partial\Lambda)^{p-1}\times(\varepsilon^{-1}\Lambda)^{n-p}} dy_2\cdots dy_n \prod_2^p |y_j|^{q_j}|D^\alpha u(\varepsilon y_2,\dots,\varepsilon y_n;y_2,\dots,y_n)|<c<\infty$$

for all $\varepsilon\in[0,\varepsilon_0]$, *for all* p *with* $p_0\leqq p\leqq n$, *and for all* $\{q_j\}$ *with*

$$q_j\geqq 0,\quad \sum_2^p q_j\leqq q+|\alpha|+p-p_0.$$

Suppose moreover that the above integrals are convergent as any $|y_j|\to+\infty$, *uniformly in the other variables (specially* ε*).*

Then the function

$$I_{n,p_0}(\varepsilon)=\int_{(\varepsilon^{-1}\partial\Lambda)^{p_0-1}\times(\varepsilon^{-1}\Lambda)^{n-p_0}} dy_2\dots dy_n u(\varepsilon y_2,\dots,\varepsilon y_n;y_2,\dots,y_n)$$

is C^q *at* $\varepsilon=0$.

Remark 1. If we assume $\partial\Lambda$ of class C^r only near the origin, we can conclude that $I_{n,p_0}(\varepsilon)$ is the sum of a C^q function and an $0(\varepsilon^q)$ function.

Remark 2. The function u is required to exist on a much wider domain than is necessary to define the integral I_{n,p_0}. The reason for this is that the domain of integration has a singularity at $\varepsilon=0$.

The next three lemmas will be the basis of the proof of Theorem 1 and also shed some light on its formulation.

Lemma 1. *Let* $\Lambda\subset\mathbb{R}^d$, $0\in\partial\Lambda$, $\partial\Lambda$ *a* C^r *hypersurface, let* $n(z)$ *be the inner normal to* $\partial\Lambda$ *at* z. *Then there is a function* $Q\colon\partial\Lambda\times\mathbb{R}^d\to\mathbb{R}$, *homogeneous of degree 2 in the second variable and* C^{r-2} *such that*

$$\varepsilon^{-2}z\cdot n(z)=Q(z,y)|_{y=\varepsilon^{-1}z}$$

Proof. There is an ε independent neighborhood V of 0 in $\mathbb{R}^d$ such that

1) If $z\in\partial\Lambda\cap V$, then $zt\in V\,\forall t\in[0,1]$.

2) If $x\in V$, the orthogonal projection $P(x)$ from x onto $\partial\Lambda$ is differentiable in V, and the vector $x-P(x)$ realizes the shortest distance between x and $\partial\Lambda$.

Let χ be a C^∞ function from $\mathbb{R}^d$ to $\mathbb{R}^+$ such that $\chi\equiv1$ on some neighborhood of 0 and $\chi\equiv0$ outside V.

We define a function $Q^{(2)}(z,y)$ by

$$Q^{(2)}(z,y)=\frac{z\cdot n(z)}{\|z\|^2}(1-\chi(z))\|y\|^2.$$

This function is C^{r-1} in z and quadratic in y. Moreover, if $z\notin V$,

$$z\cdot n(z)=Q^{(2)}(z,y)|_{y=\varepsilon^{-1}z}.$$

For $z\in\partial\Lambda$ and $t\in[0,1]$, let

$$g(t)=P(tz)\cdot n(P(tz))\chi(tz).$$

This function is well defined for any $z\in\partial\Lambda$, and any $t\in[0,1]$. From $g(0)=0$, we have

$$g(1)=\int_0^1\chi(tz)P(tz)\cdot Dn_{P(tz)}(DP_{tz}(z))dt+\int_0^1 P(tz)\cdot n(P(tz))D\chi_{tz}(z)dt$$

(the term DP-drops out).

From $P(0)=0$, we have if $tz\in V$,

$$P(tz)=\int_0^t DP_{\tau z}(z)d\tau$$

We now define a function $Q^{(1)}(z,y)$ by

$$Q^{(1)}(z,y)=\int_0^1 dt\chi(tz)\int_0^t d\tau DP_{\tau z}(y)\cdot Dn_{P(tz)}(DP_{tz}(y))$$
$$+\int_0^1 dtD\chi_{tz}(y)\int_0^t d\tau DP_{\tau z}(y)\cdot n(P(tz)).$$

Notice that by the star-shape of $V, Q^{(1)}$ is well defined for any z in $\partial\Lambda$, since $tz\in V$ implies $\tau z\in V$ for any $\tau\in[0,t]$. $Q^{(1)}$ is obviously C^{r-2} in z and quadratic in y. Moreover

$$g(1)=P(z)\cdot n(P(z))=z.n(z)=Q^{(1)}(z,z).$$

The result follows if we set $Q(z,y)=Q^{(1)}(z,y)+Q^{(2)}(z,y)$.

Q.E.D.

Lemma 2. *Formulae for $I_{n,p}(\varepsilon)$ and its first derivative:*

$$I_{n,p}(\varepsilon)=\varepsilon^{-(n-1)d+p-1}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\dots dx_n u(x_2,\dots,x_n;\varepsilon^{-1}x_2,\dots,\varepsilon^{-1}x_n)$$

$$\frac{d}{d\varepsilon}I_{n,p}(\varepsilon)=\varepsilon^{-(n-1)d+p-1}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n v(x_2\cdots;\varepsilon^{-1}x_2\cdots)$$
$$+\sum_{j=p+1}^{n}\varepsilon^{-(n-1)d+p}\int_{(\partial\Lambda)^p}dx_2\cdots dx_p dx_j\int_{\Lambda^{n-p-1}}dx_{p+1}\cdots d\check{x}_j\cdots dx_n w_j(x_2\cdots;\varepsilon^{-1}x_2\cdots),$$

where

$$v(x_2,\dots,x_n;y_2,\dots,y_n)=-\sum_{j=2}^{p}Q(x_j,y_j)\left(n_j\cdot\frac{\partial}{\partial y_j}u\right)$$
$$+\sum_{j=2}^{p}(d-1)H(x_j)(y_j\cdot n_j)u+\sum_{j=2}^{n}y_j\cdot\frac{\partial u}{\partial x_j}$$

and

$$w_j(x_2,\dots,x_n;y_2,\dots,y_n)=Q(x_j,y_j)u.$$

where $Q(x,y)$ *is defined in Lemma 1 and* $H(x_j)$ *is the mean curvature as defined in Lemma 3.*

Proof. The formula for $I_{n,p}(\varepsilon)$ is obvious from the definition. We now compute

$$\frac{d}{d\varepsilon}I_{n,p}(\varepsilon)=[-(n-1)d+p-1]\varepsilon^{-(n-1)d+p-2}\int\cdots u\cdots$$
$$-\sum_{j=2}^{n}\varepsilon^{-(n-1)d+p-3}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n\,x_j\cdot\frac{\partial}{\partial y_j}u(x_2,\dots,x_n;\varepsilon^{-1}x_2,\dots,\varepsilon^{-1}x_n).$$

In the last term, notice that for $2\leqq j\leqq p$, $\varepsilon^{-1}x_j$ belongs to $\varepsilon^{-1}\partial\Lambda$. However the function u is defined and differentiable in a much larger domain, this is why the above formula is true.

Let us first consider $j\geqq p+1$ in the last term. Integration by parts on Λ gives

$$-\sum_{j=p+1}^{n}\varepsilon^{-(n-1)d+p-3}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n x_j\cdot\left(\frac{\partial}{\partial y_j}u\right)(x_2\cdots x_n;\varepsilon^{-1}x_2\cdots\varepsilon^{-1}x_n)$$
$$=(n-p)d\varepsilon^{-(n-1)d+p-2}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n u$$
$$+\sum_{j=p+1}^{n}\varepsilon^{-(n-1)d+p-2}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n x_j\cdot\frac{\partial}{\partial x_j}u$$
$$+\sum_{j=p+1}^{n}\varepsilon^{-(n-1)d+p}\int_{(\partial\Lambda)^{p}}dx_2\cdots dx_p dx_j\int_{\Lambda^{n-p-1}}dx_{p+1}\cdots d\check{x}_j\cdots dx_n(\varepsilon^{-2}x_j\cdot n_j)u.$$

Let us now consider $j\leqq p$. From Lemma 3 below we have for $x_j\in\partial\Lambda$ and $y_j=\varepsilon^{-1}x_j$,

$$\operatorname{div}^{\mathrm{cov}}_{x_j}(T_{x_j}(x_j)u)=T_{x_j}(x_j)\cdot\frac{\partial u}{\partial x_j}+\varepsilon^{-1}T_{x_j}(x_j)\cdot\frac{\partial u}{\partial y_j}+(d-1)u+(d-1)H(x_j)(x_j\cdot n_j)u.$$

Integration by parts on $\partial\Lambda$ then gives

$$-\sum_{j=2}^{p}\varepsilon^{-(n-1)d+p-3}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n x_j\cdot\frac{\partial u}{\partial y_j}$$
$$=-\sum_{j=2}^{p}\varepsilon^{-(n-1)d+p-3}\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}}dx_2\cdots dx_n\left[T_{x_j}(x_j)\cdot\frac{\partial u}{\partial y_j}+(x_j\cdot n_j)n_j\cdot\frac{\partial u}{\partial y_j}\right]$$

$$= -\sum_{j=2}^{p} \varepsilon^{-(n-1)d+p-1} \int_{(\partial\Lambda)^{p-1}\times\Lambda^{p-1}} dx_2 \cdots dx_n \Big[(\varepsilon^{-2} x_j \cdot n_j) n_j \cdot \frac{\partial u}{\partial y_j} -$$

$$- (d-1) H(x_j) u \varepsilon^{-1} (x_j \cdot n_j) - \varepsilon^{-1} T_{x_j}(x_j) \cdot \frac{\partial u}{\partial x_j} \Big]$$

$$+ (p-1)(d-1) \varepsilon^{-(n-1)d+p-2} \int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}} dx_2 \cdots dx_n u.$$

For later purposes, note that if $x_j \in \partial\Lambda$, then $\partial u/\partial x_j$ is tangent to $\partial\Lambda$ at x_j. Therefore

$$\varepsilon^{-1} T_{x_j}(x_j) \cdot \frac{\partial u}{\partial x_j} = \varepsilon^{-1} x_j \cdot \frac{\partial u}{\partial x_j}.$$

Collecting all terms gives Lemma 2. Notice the cancellation of the singular terms (as $\varepsilon \to 0$) proportional to

$$\varepsilon^{-(n-1)d+p-2} \int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}} dx_2 \ldots dx_n u(x_2, \ldots, x_n; \varepsilon^{-1} x_2, \ldots, \varepsilon^{-1} x_n). \quad \text{Q.E.D.}$$

Lemma 3. *Let $T_x(x)$ be the orthogonal projection of the vector $x \in \mathbb{R}^d$, defining a point $x \in \partial\Lambda$, onto the tangent plane at $x \in \partial\Lambda$. Then*

$$\operatorname{div}^{\text{cov}} T(x) = d - 1 + (d-1) H(x) x \cdot n(x),$$

where $H(x)$ is the mean curvature of $\partial\Lambda$ at x, *defined with the inner normal $n(x)$ as follows: if $e_1, \ldots, e_{d-1}, n(x)$ is a moving frame at $x \in \partial\Lambda$* [3], *then*

$$((d-1) H(x)) = n(x) \cdot \sum_{l=1}^{d-1} de_l(e_l).$$

Proof. Let the 1-forms σ_k be defined by

$$\sigma_k(e_l) = \delta_{k,l} \qquad k = 1, \ldots, d-1; l = 1, \ldots, d-1$$

so that

$$dx = \sum_{1}^{d-1} e_k \sigma_k,$$

$$de_k = \sum_{l=1}^{d-1} de_k(e_l) \sigma_l,$$

$$d\sigma_k = \sum_{l=1}^{d-1} \sum_{l'=1}^{d-1} (de_l(e_{l'}) \cdot e_k) \sigma_l \Lambda \sigma'_l.$$

The covariant divergence on $\partial\Lambda$ is defined, appropriately for integration by parts on $\partial\Lambda$, as

$$\operatorname{div}^{\text{cov}} T(x) = \sum_{k=1}^{d-1} (-)^{k-1} d\{(e_k \cdot T(x)) \sigma_1 \wedge \cdots \wedge \check{\sigma}_k \wedge \cdots \wedge \sigma_{d-1}\} / \sigma_1 \wedge \cdots \wedge \sigma_d,$$

where $T(x)$ could be replaced by any vector field in the tangent plane.

The proof of Lemma 3 is a straightforward computation, following the rules of exterior differentiation and using

$$de_k(e_l)\cdot e_l + de_l(e_l)\cdot e_k = d(e_k\cdot e_l)(e_l) = 0.$$

Proof of Theorem 1. By induction over q, consider first

$$q=0, \quad k=0, \quad r=1.$$

In a neighborhood of the origin, the equation for $\partial\Lambda$ may be written

$$x = (z_\Lambda(\mathbf{x}), \mathbf{x}),$$

where $z_\Lambda(\mathbf{x})$ is a C^1 function of $\mathbf{x}\in\mathbb{R}^{d-1}$ and

$$z_\Lambda(0)=0, \quad \frac{\partial}{\partial\mathbf{x}} z_\Lambda(0) = 0.$$

The equation for $y\in\varepsilon^{-1}\partial\Lambda$ will then be

$$y(\varepsilon, \mathbf{y}) = (\varepsilon^{-1} z_\Lambda(\varepsilon\mathbf{y}), \mathbf{y}).$$

The uniform convergence of the integral defining $I_{n,p_0}(\varepsilon)$ means that for any $\eta > 0$, there exists a ball $B\subset\mathbb{R}^d$ such that for all $\varepsilon\in[0,\varepsilon_1]$,

$$\left| I_{n,p_0}(\varepsilon) - \int_{B^{n-1}\cap\{(\mathbb{R}^{d-1})^{p_0-1}\times(\varepsilon^{-1}\Lambda)^{n-p_0}\}} d\mathbf{y}_2\cdots d\mathbf{y}_{p_0} dy_{p_0+1}\cdots dy_n \prod_2^{p_0}\left|\frac{dy_j(\varepsilon\mathbf{y}_j)}{d\mathbf{y}_j}\right| \right.$$
$$\left. \cdot u(y_2(\varepsilon,\mathbf{y}_2),\ldots,y_{p_0}(\varepsilon,\mathbf{y}_{p_0}), y_{p_0+1},\ldots,y_n) \right| < \eta/2,$$

where ε_1 is such that $\varepsilon_1 B$ is contained in the neighborhood of the origin as above.

The integrand is continuous in $\varepsilon\in[0,\varepsilon_1]$, $\mathbf{y}_2,\ldots,\mathbf{y}_{p_0}\in\mathbb{R}^{d-1}\cap B$, $y_{p_0+1},\ldots,y_n\in B$ and is therefore bounded by a constant. The characteristic function of $(\varepsilon^{-1}\Lambda)^{n-p_0}$ is also bounded. The dominated convergence theorem then implies that $I_{n,p_0}(\varepsilon)$ is continuous at $\varepsilon=0$.

We now proceed by induction over q. If Theorem 1 is valid up to $\mathbf{q}-1$, it will be valid up to q if we can apply it to $(d/d\varepsilon)I_{n,p_0}(\varepsilon)$. We only have to check the hypothesis for v and w_j in Lemma 2.

The hypothesis

$$\sum_2^p q_j \leqq q + |\alpha| + p - p_0,$$

enters as follows. Each derivative in ε requires one moment (hence q), except when a derivative of u with respect to y_j is taken (hence $|\alpha|$), or when the dimension of the integration domain decreases by one (hence $p-p_0$). This concludes the proof of Theorem 1.

Theorem 2. *Let* $\Lambda\subset\mathbb{R}^d$, Λ *compact connected, and* $\partial\Lambda$ *of class* C^r. *Let* $u_n(x_1,x_2,\ldots,x_n)$ *be a* C^k *function of* $x_1,x_2,\ldots,x_n\in\mathbb{R}^d$, *symmetric under permutations of* $x_1,\ldots,x_n$, *invariant under simultaneous translations of* $x_1,\ldots,x_n$ *Let* $1\leqq q\leqq$

Min$(k+2, r)$ *and suppose that all derivatives* $D^\alpha u_n$ *with respect to* $x_1, x_2, \ldots, x_n$ *of total order* $0 \leqq |\alpha| \leqq \mathrm{Max}(0, q-2)$ *satisfy* $u_n(0, y_2, \ldots, y_n) \in L^1(\mathbb{R}^{(n-1)d})$, *and*

$$\int_{\partial\Lambda} dx_1 \int_{(\varepsilon^{-1}(\partial\Lambda - x_1))^{p-1} \times (\varepsilon^{-1}(\Lambda - x_1))^{n-p}} dy_2 \cdots dy_n \cdot \prod_2^n |y_j|^{q_j} |D^\alpha u_n(0, y_2, \ldots, y_n)| < c < \infty$$

for all $\varepsilon \in [0, \varepsilon_0]$, *for all* p *with* $1 \leqq p \leqq q$, *for all* $\{q_2, \ldots, q_n\}$ *with*

$$q_j \geqq 0 \qquad \forall j,$$
$$q_j \leqq 1 \qquad \text{if } j > p,$$
$$\sum_2^n q_j \leqq q + |\alpha| + p - 1.$$

Suppose moreover that the above integrals are convergent, as any $|y_j| \to \infty$, *uniformly in the other variables (particularly* ε *and* x_1). *Then the function*

$$I_n(\varepsilon, \Lambda) = \varepsilon^d \int_{(\varepsilon^{-1}\Lambda)^n} dx_1 \cdots dx_n u_n(x_1, \ldots, x_n)$$

is C^q *in* ε *at* $\varepsilon = 0$. *Moreover*

$$I_n(0, \Lambda) = |\Lambda| \int_{(\mathbb{R}^d)^{n-1}} dy_2 \cdots dy_n u_n(0, y_2, \ldots, y_n) \equiv |\Lambda| C_0(u_n),$$

$$\frac{d}{d\varepsilon} I_n(0, \Lambda) = -\int_{\partial\Lambda} dx_1 \int_{(\mathbb{R}^d_{x_1+})^{n-1}} dy_2 \cdots dy_n \left(\sum_2^n (y_j - x_1) \cdot n_1 \right) u_n(x_1, y_2, \ldots, y_n)$$

$$\equiv -|\partial\Lambda| C_1(u_n) \text{ if } u_n \text{ is rotation invariant, where}$$

$$\mathbb{R}^d_{x_1+} = \{x \in \mathbb{R}^d : (x - x_1) \cdot n_1 \geqq 0\},$$

$$\frac{d^2}{d\varepsilon^2} I_n(0, \Lambda) = \begin{cases} 0 \quad \text{if } n = 2 \\ -\frac{1}{2}(n-1) \int_{\partial\Lambda} dx_1 \int_{\mathbb{R}^{d-1}_{x_1}} dy_2 \int_{(\mathbb{R}^d_{x_1+})^{n-2}} dy_3 \cdots dy_n \end{cases}$$

$$((y_2 - x_1) \cdot Dn_1(y_2 - x_1)) \left(\sum_3^n (y_j - x_1) \cdot n_1 \right) u_n(x_1, y_2, \ldots, y_n)$$

$$\equiv +\tfrac{1}{2}(n-1) \left(\int_{\partial\Lambda} dx H(x) \right) C_2(u_n) \text{ if } u_n \text{ is rotation invariant,}$$

where

$$\mathbb{R}^{d-1}_{x_1} = \{x \in \mathbb{R}^d : (x - x_1) \cdot n_1 = 0\},$$

and

$$C_2(u_n) = \int_{\mathbb{R}^{d-1}_{x_1}} dy_2 (y_2 - x_1)^2 \int_{(\mathbb{R}^d_{x_1+})^{n-2}} dy_3 \cdots dy_n \left(\sum_3^n (y_j - x_1) \cdot n_1 \right) u_n(x_1, y_2 \cdots y_n),$$

$$\frac{d^3}{d\varepsilon^3} I_n(0, \Lambda) = \frac{n-1}{4} \int_{\partial\Lambda} dx_1 \int_{\mathbb{R}^{d-1}_{x_1}} dy_2 \int_{(\mathbb{R}^d_{x_1+})^{n-2}} dy_3 \cdots dy_n ((y_2 - x_1) \cdot Dn_1(y_2 - x_1))^2.$$

$$\cdot\left\{\left(1+\left(\sum_3^n (y_j-x_1)\cdot n_1\right)\left(n_1\cdot\frac{\partial}{\partial y_2}\right)\right\} u_n(x_1,y_2,\ldots,y_n)$$

$$-\frac{(n-1)(n-2)}{4}\int_{\partial\Lambda} dx_1 \int_{(\mathbb{R}^{d-1}_{x_1})^2} dy_2 dy_3 \int_{(\mathbb{R}^d_{x_1+})^{n-3}} dy_4\cdots dy_n((y_2-x_1)\cdot Dn_1(y_2-x_1)).$$

$$\cdot((y_3-x_1)\cdot Dn_1(y_3-x_1))\left(\sum_4^n (y_j-x_1)\cdot n_1\right) u_n(x_1,y_2,\ldots,y_n)$$

$$\equiv \frac{(n-1)}{4}\left(\int_{\partial\Lambda} dx\left(H^2-\frac{2}{3}\frac{d-2}{d-1}K\right)\right) C_3(u_n) \text{ if } n=2 \text{ or } 3 \text{ and } u_n \text{ is rotation invariant,}$$

where K is the gaussian curvature.

Proof. $I_n(\varepsilon,\Lambda)$ can be put in the form

$$I_n(\varepsilon,\Lambda)=\varepsilon^{-(n-1)d}\int_{\Lambda^n} dx_1\ldots dx_n u_n(0,\varepsilon^{-1}(x_2-x_1),\ldots,\varepsilon^{-1}(x_n-x_1)).$$

We then compute, using integration by parts as in the proof of Lemma 2:

$$\frac{d}{d\varepsilon}I_n(\varepsilon,\Lambda)=-\varepsilon^{-(n-1)d}\int_{\partial\Lambda\times\Lambda^{n-1}} dx_1\cdots dx_n\sum_2^n(\varepsilon^{-1}(x_j-x_1)\cdot n_1)$$

$$\cdot u_n(0,\varepsilon^{-1}(x_2-x_1),\ldots,\varepsilon^{-1}(x_n-x_1)),$$

where n_1 is the inner normal to $\partial\Lambda$ at x_1. Lemma 2 can now be applied to give

$$\frac{d^2}{d\varepsilon^2}I_n(\varepsilon,\Lambda)=-(n-1)\varepsilon^{-(n-1)d+1}\int_{(\partial\Lambda)^2\times\Lambda^{n-2}} dx_1,\ldots,dx_n(\varepsilon^{-2}(x_2-x_1)\cdot n_2)$$

$$\cdot\left(\sum_2^n \varepsilon^{-1}(x_j-x_1)\cdot n_1\right)u_n(0,\varepsilon^{-1}(x_2-x_1),\ldots,\varepsilon^{-1}(x_n-x_1)).$$

So far, it has not been necessary to compute any gradients with respect to variables on the boundary. This explains why the hypotheses in Theorem 2 are slightly milder than in Theorem 1.

We now give a general recursion formula:

Lemma 4. *For $q\geqq 3$ we have*

$$\frac{d^q}{d\varepsilon^q}I_n(\varepsilon,\Lambda)=-\int_{\partial\Lambda} dx_1\sum_{p=2}^{\mathrm{Min}(q,n)}\frac{(n-1)!}{(n-p)!}\varepsilon^{-(n-1)d+p-1}$$

$$\int_{(\partial\Lambda)^{p-1}\times\Lambda^{n-p}} dx_2\cdots dx_n F^q_{p,n}(x_1\cdots x_p;\varepsilon^{-1}(x_2-x_1)\cdots\varepsilon^{-1}(x_n-x_1))$$

with

$$F^q_{p,n}(x_1\cdots x_p;y_2\cdots y_n)$$

$$=G^q_p\left(x_1;x_2\cdots x_p;y_2\cdots y_p;\frac{\partial}{\partial y_2}\cdots\frac{\partial}{\partial y_p}\right)\left(\sum_2^n y_j\cdot n_1\right)u_n(0,y_2\cdots y_n).$$

The operators G^q_p are defined recursively by

$$G^2_2\left(x_1;x_2;y_2;\frac{\partial}{\partial y_2}\right)=Q_{x_1}(x_2,y_2),\qquad G^2_1\equiv 0,$$

where $Q_{x_1}(z,y)$ is defined as in Lemma 1 (where $x_1=0$) and

$$G_p^{q+1}\left(x_1;x_2\cdots x_p;y_2\cdots y_p;\frac{\partial}{\partial y_2}\cdots\frac{\partial}{\partial y_p}\right)$$
$$=\sum_{j=2}^{p}\left\{-Q(x_j,y_j)n_j\cdot\frac{\partial}{\partial y_j}+(d-1)H(x_j)n_j\cdot y_j+\frac{\partial}{\partial x_j}\cdot y_j\right\}$$
$$\cdot G_p^q(\cdot;\cdots;\cdots;\cdots)+Q_{x_1}(x_p,y_p)G_{p-1}^q(\cdot;\cdots;\cdots;\cdots),$$

so that $G_p^q(x_1\cdots x_p;y_2\cdots y_p;(\partial/\partial y_2)\cdots(\partial/\partial y_p))$ is a polynomial in $\{y_j\}_j$ and $\{n_j\cdot(\partial/\partial y_j)\}_j$ with coefficients continuous functions of $x_1\cdots x_p\in\partial\Lambda$. The order of G_p^q (i.e. the degree in $\{\partial/\partial y_j\}_j$) is at most $q-2$. The total degree of G_p^q in $\{y_j\}_j$ (counted positively) and $\{\partial/\partial y_j\}_j$ (counted negatively) is at most $q+p-1$.

Proof of Lemma 4 and Theorem 2. The proof is now straightforward, using Lemma 2 and Theorem 1.

Corollary 1. *Let $\Lambda\subset\mathbb{R}^d$, Λ compact connected and $\partial\Lambda$ of class C^r. Let*

$$u_n(x_1,x_2,\ldots,x_n)=\sum_{G\in g(x_1,\ldots,x_n)}\prod_{(x,x')\in G}(e^{-\beta\Phi(x,x')}-1),\tag{1}$$

where $g(x_1,\ldots,x_n)$ is the set of graphs connecting $x_1,\ldots,x_n$ by two body unrepeated links (x,x'), and where the potential $\Phi(x,x')$ depends only on the distance $|x-x'|$ and is stable and regular for moments up to $2q-2$:

$$\forall n\in\mathbb{N},\forall(x_1,\ldots,x_n)\in(\mathbb{R}^d)^n,\prod_{i<j}(1+|x_i-x_j|)^{2q-2}|e^{-\beta\Phi(x_i,x_j)}-1|<e^{n\beta B_q}$$

and

$$\int_{\mathbb{R}^d}dx(1+|x|)^{2q-2}|e^{-\beta\Phi(0,x)}-1|<C_q(\beta).$$

Suppose moreover that $e^{-\beta\Phi(0,x)}$ is C^k in x with $k=\mathrm{Max}(0,q-2)$ and

$$\int_{\mathbb{R}^d}dx|x|^{q+\alpha}\left|\frac{d^\alpha}{d|x|^\alpha}e^{-\beta\Phi(0,x)}\right|<\infty$$

for $1\leqq\alpha\leqq q-2$.

Let the pressure $p(\varepsilon^{-1}\Lambda)$ in the volume $\varepsilon^{-1}\Lambda$ be defined by

$$\beta|\varepsilon^{-1}\Lambda|p(\varepsilon^{-1}\Lambda)=\sum_{n=1}^{\infty}\frac{z^n}{n!}\int_{(\varepsilon^{-1}\Lambda)^n}dx_1\cdots dx_n u_n(x_1,\ldots,x_n)$$

and the activity z be such that

$$z<e^{-\beta B_q}(C_q(\beta))^{-1}.$$

Then the pressure $p(\varepsilon^{-1}\Lambda)$ is C^q in ε at $\varepsilon=0$.

Proof. It is sufficient to prove

$$\int_{(\varepsilon^{-1}\partial\Lambda)^{p-1}\times(\varepsilon^{-1}\Lambda)^{n-p}}dy_2\cdots dy_n\prod_2^p|y_j|^{q_j}|D^\alpha u_n(0,y_2\cdots y_n)|<n!e^{n\beta B_q}C_q(\beta)^n(1+n)^{d_q}\tag{2}$$

for some d_q and all n, for all $\{q_2,\ldots,q_p\}$ and α and ε as in Theorem 2.

We replace u_n by the Mayer expansion (1) and apply the derivatives. Leibniz's rule leads to $O(n^{|\alpha|})$ choices of differentiated links. We now consider one such choice, so that at most $(q+1)$ links are differentiated.

We then note that every y_j is connected to y_1 by a succession of links y_k, y_l and replace $|y_j|$ in (2) by the bound

$$|y_j| \leqq \prod (1+|y_k-y_l|),$$

where the product runs along the path from y_j to y_1.

We are now in a position to apply the Kirkwood Salsburg equation with the kernel

$$(1+|y_k-y_l|)^{2q-2}(e^{-\beta\Phi(y_k,y_l)}-1)$$

for all links except the $q+1$ prescribed differentiated links. The bound (2) is then a standard result [2].

In Corollary 1, it was assumed that the activity z was small enough, but the result should be valid in the whole domain where the pressure is analytic in z, assuming bounds for the truncated correlation functions rather than for the Ursell functions. This requires a resummation of the expansion in z^n, and will be easier to formulate in terms of the average number of particles $\bar{N}(z,\varepsilon^{-1}\Lambda)$ or in terms of the average density

$$\begin{aligned}\bar{n}(z,\varepsilon^{-1}\Lambda) &= |\varepsilon^{-1}\Lambda|^{-1}\bar{N}(z,\varepsilon^{-1}\Lambda) = \beta z\frac{\partial}{\partial z}p(z,\varepsilon^{-1}\Lambda)\\ &= \sum_{n=1}^{\infty}\frac{z^n}{(n-1)!}|\Lambda|^{-1}I_n(\varepsilon,\Lambda) \quad \text{if } z \text{ small.}\end{aligned}$$

Let $\rho_m^{\Lambda}(x_1\cdots x_m)$ be the m-point truncated function at activity z in volume Λ. For small z, we have

$$\rho_m^{\Lambda}(x_1\cdots x_m) = z^m\sum_{n=0}^{\infty}\frac{z^n}{n!}\int_{\Lambda^n} dy_1\cdots dy_n u_{m+n}(x_1\cdots x_m y_1\cdots y_n).$$

When $x_1\in\partial\Lambda$, let $\varepsilon^{-1}(\Lambda-x_1)$ and $\varepsilon^{-1}(\partial\Lambda-x_1)$ be the transforms of Λ and $\partial\Lambda$ under a scaling of amplitude ε^{-1} and center x_1. We can now formulate Corollary 2:

Corollary 2. *Under the hypotheses of Corollary 1, the average density $\bar{n}(z,\varepsilon^{-1}\Lambda)$ is C^q in ε at $\varepsilon=0$ and*

$$\begin{aligned}\frac{d^q}{d\varepsilon^q}\bar{n}(z,\varepsilon^{-1}\Lambda) = -|\Lambda|^{-1}\int_{\partial\Lambda} dx_1 \sum_{p=2}^{q}\ & \int_{(\varepsilon^{-1}(\partial\Lambda-x_1))^{p-1}} dy_2\cdots dy_p\\ &\cdot G_p^q\left(x_1;x_1+\varepsilon y_2,\ldots,x_p+\varepsilon y_p;y_2\cdots y_p;\frac{\partial}{\partial y_2}\cdots\frac{\partial}{\partial y_p}\right)\cdot\\ &\cdot\left\{\left(\sum_2^p y_j\cdot n_1\right)\rho_p^{\varepsilon^{-1}(\Lambda-x_1)}(x_1y_2\cdots y_p)\right.\\ &\left.+\int_{\varepsilon^{-1}(\Lambda-x_1)} dy_{p+1}(y_{p+1}\cdot n_1)\rho_{p+1}^{\varepsilon^{-1}(\Lambda-x_1)}(x_1y_2\cdots y_{p+1})\right\},\end{aligned}$$

where G_p^q is defined in Lemma 4.

Suppose now that for all $\varepsilon \in]0, \varepsilon_0[$, $\bar{n}(z, \varepsilon^{-1}\Lambda)$ *and its q first derivatives with respect to* ε *have an analytic continuation to a domain D containing the origin and are bounded uniformly in* $\varepsilon \in]0, \varepsilon_0[$.

Then $\bar{n}(z, \varepsilon^{-1}\Lambda)$ *and* $p(z, \varepsilon^{-1}\Lambda)$ *are* C^q *in* ε *at* $\varepsilon = 0$ *for all* $z \in D$.

Proof. The first part of the corollary is just a computation. The second part follows from Vitali's theorem. Note that the formula given in the first part is meant to be used for bounding the derivatives of $\bar{n}(z, \varepsilon^{-1}\Lambda)$ when using the second part of the corollary.

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