Journal of Statistical Physics, Vol. 27, No. 4, 1982

Estimates of General Mayer Graphs III: Upper Bounds Obtained by Means of Spanning n-Trees

Michel Lavaud[1]

Received October 23, 1978; final revision April 14, 1981

We obtain computable upper bounds for any given Mayer graph with n root-points (or n-graph). These are products of integrals of the type $(\int |f_L|^{z_{iL} y_i^{-1}} d\mathbf{x})^{y_i}$, where the z_{iL} and y_i are nonnegative real numbers whose sum over i is equal to 1. As a particular case, we obtain the canonical bounds (see their definition in Section 2.2):

$$\left| \int \prod_L f_L(\mathbf{x}_i, \mathbf{x}_j)\, d\mathbf{x}_{n+1} \cdots d\mathbf{x}_{n+k} \right| \leqslant \prod_L \left(\int |f_L|^{\alpha_L} d\mathbf{x} \right)^{\alpha_L^{-1}}$$

where the α_L's satisfy the condition $\alpha_L \geqslant 1$ for any L, and $\sum_L \alpha_L^{-1} = k$ (k is the number of variables that are integrated over). These bounds are finite for all n-graphs of neutral systems. We obtain also finite bounds for all irreducible n-graphs of polar systems, and for certain n-graphs occurring in the theory of ionized systems. Finally, we give a sufficient condition for an arbitrary n-graph to be finite.

KEY WORDS: Upper bound; covering; spanning n-trees; linear programming.

1. INTRODUCTION

In preceding articles,[1-3] we have developed a new estimation method for n-graphs. An n-graph is a multiple integral whose integrand is a product of 2-body functions, as given by Eq. (2.1) below. n-graphs arise when one studies, by perturbation or variation theoretic techniques, thermodynamic and transport properties of classical and quantum systems,[4,5] amplitudes of scattering processes,[6] energy levels of atoms and molecules,[7] interatomic and intermolecular potentials,[7] etc. For example, the equation of

[1] Centre de Recherches sur la Physique des Hautes Températures, CNRS, 1D, Avenue de la Recherche Scientifique, 45045 Orleans-Cédex, France.

0022-4715/82/0400-0745$03.00/0

state of a gas of classical particles interacting via a two-body interaction potential is[4]

$$P = \rho kT\left(1 - \sum_{k=1}^{\infty} \frac{k}{k+1}\, \beta_k \rho^k\right) \tag{1.1}$$

where ρ and T denote, respectively, the density and the temperature of the system, and $k!\,\beta_k$ is the sum over all irreducible 1-graphs with k field-points.

Our estimation method enables us to obtain upper bounds, for any given n-graph $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n)$, by means of the values of certain suitably chosen subgraphs of Γ. In this article, we make use of spanning n-trees as subgraphs. A spanning n-tree of Γ is an n-graph which contains all the field-points of Γ and which is made of n disjoint trees, each tree having one and only one root-point. (See for example Fig. 4b, where some 2-trees are drawn.) The use of spanning n-trees as subgraphs enables us to obtain very simple explicitly computable upper bounds. These bounds are independent of the coordinates $\mathbf{x}_1, \ldots, \mathbf{x}_n$.

In this article, we investigate the possibility of obtaining *finite* bounds for n-graphs that occur in *statistical mechanics*. We concentrate particularly on n-graphs of polar and ionized systems, because the bounds that are obtained by applying the theorem of the means (i.e., $|\int fg\,dx| \leqslant \sup|f| \int |g|\,dx$), according to the procedure of Riddell and Uhlenbeck[8] and Groeneveld,[9] are infinite for these systems. Bounds of this type will be called mean-value bounds, in the sequel. The possibility of obtaining finite bounds for n-graphs that occur in *quantum field theory* and in *quantum chemistry* will be investigated elsewhere. Some possible uses for our bounds have been proposed and described briefly in Refs. 1–3. A more detailed study of this point will be done in subsequent articles, when we investigate the relative accuracy of our bounds.

In Section 2, we recall briefly the definition and the graphical representation of an n-graph, and the results of our estimation method which are needed in this article. In Section 3, we first show that it is possible to cover any n-rooted graph by means of spanning n-trees. (A set of subgraphs γ_i of Γ covers Γ if $\bigcup_i \gamma_i = \Gamma$; cf. Ref. 2.) From this result, we deduce a procedure for constructing upper bounds of the type $\prod_L \|f_L\|_{\alpha_L}$ for any given n-graph, with $\|f\|_\alpha = (\int |f|^\alpha\, d\mathbf{x})^{\alpha^{-1}}$ for α finite, and $\|f\|_\infty = \sup|f|$. Then, we illustrate this procedure with an example, and apply it also to estimate the complete 1-graphs with m points, for any m. This is useful to have an idea about the accuracy of our estimation method, for arbitrary n-graphs. Finally, we show that a sufficient condition for an n-graph to be finite is that a certain linear programming problem (i.e., a system of linear equations with linear constraints) associated to the n-graph has a feasible

solution. This program incorporates the topological structure of the graph through the set of linear equations, and the shape of the functions f_L through the linear constraints. It is possible to express the sufficient condition in this very simple form because the functions encountered in statistical thermodynamics are of a very special type, which allows us to characterize their shape by a single number p.

2. GENERALITIES

2.1. Definition and Graphical Representation of n-Graphs

An n-graph is a multiple integral of the following type:

$$\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda) = \int_{\Lambda^k} \prod_{L \in \mathfrak{L}\Gamma} f_L(\mathbf{x}_i, \mathbf{x}_j)\, d\mathbf{x}_{n+1} \cdots d\mathbf{x}_{n+k} \tag{2.1}$$

where the symbols have been defined precisely in Refs. 2 and 3. We recall briefly their definitions. Γ is a graph with n root-points, or an n-rooted graph,[2] k field-points, and l lines L joining the pair i, j of points. The set of lines of Γ is denoted by $\mathfrak{L}\Gamma$. In (2.1), the product runs over all lines of $\mathfrak{L}\Gamma$, and the integration runs over the k field-points varying in the domain Λ. When the domain is infinite, Λ is very often omitted in (2.1). $\mathbf{x}_i$ represents the coordinates required to fix the spatial location $\mathbf{r}_i$ and, eventually, the orientation ω_i of particle i. The functions $f_L(\mathbf{x}_i, \mathbf{x}_j)$ are pairwise invariant (i.e., they are invariant by any translation and rotation of the system composed of the two particles as a whole), and can be all different. The various possible forms they can take in equilibrium statistical mechanical problems are described in detail in Ref. 3, Section 2.4, and in Section 3.5 below.

We restrict ourselves to *connected* n-graphs (i.e., every two points are joined by a chain), since it is known that any n-graph can be factorized into a product of connected m-graphs with $m \leqslant n$ (see, e.g., Ref. 3, paragraph 3.1.1). Note, however, that we do not assume that Γ is irreducible (i.e., no field-point is an articulation point) since Λ may be finite. Indeed, an n-graph can be factorized into a product of irreducible m-graphs with $m \leqslant n$ only if Λ is infinite.

For our upper bounds, the domain is taken to be infinite. This assumption has the drawback of not allowing us to study all the n-graphs of

[2] When no confusion is possible between an n-graph, i.e., a multiple integral of type (2.1), and its representative n-rooted graph, the latter will also be called an n-graph. If some confusion is possible, we speak of "the n-graph $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$" and "the n-graph Γ," to distinguish the two notions.

polar systems and of the primitive model of ionic solutions.[3] Indeed, for these systems, certain n-graphs may not be defined in an infinite domain, as their lines decay like r^{-3} and r^{-1}, respectively, at large distances. Therefore, upper bounds are not defined either. On the other hand, this assumption allows us to simplify any n-tree $T(\mathbf{x}_1, \ldots, \mathbf{x}_n)$, which occurs in the upper bounds, into a product of constant factors (Ref. 3, Corollary 3.11):

$$T(\mathbf{x}_1, \ldots, \mathbf{x}_n) = \prod_{L \in \mathfrak{L}T} \int_{\Lambda_\infty} f_L(\mathbf{x})\, d\mathbf{x} \tag{2.2}$$

where Λ_∞ means that the domain is infinite.

In our examples of application, we restrict ourselves to n-graphs whose functions (or lines) f_L are powers of a function $f(r)$, namely,

$$f_L(r) = \left[f(r) \right]^{\alpha_L}, \qquad \alpha_L \text{ real positive} \tag{2.3}$$

An n-graph $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ is represented by the graph Γ with the weight α_L written near the line L (however, α_L is omitted if it is equal to 1).

2.2. Description of our Upper Bounds

Our estimation method gives the following upper bounds[1-3]:

$$\left|\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)\right| \leqslant \prod_{i=1}^{c} \left[\int_{\Lambda^k} \prod_{L \in \mathfrak{L}\gamma_i} |f_L|^{z_{iL} y_i^{-1}} d\mathbf{x}_{n+1} \cdots d\mathbf{x}_{n+k} \right]^{y_i} \tag{2.4}$$

where the γ_i's are a set of c line-subgraphs of Γ, which are assumed to make a covering of Γ (i.e., their union is equal to Γ). c is the number of these line-subgraphs. Furthermore, the z_{iL} and y_i are nonnegative real numbers whose sum over i is unity:

$$\sum_{i=1}^{c} z_{iL} = 1 \qquad \forall L \in \mathfrak{L}\Gamma \tag{2.5a}$$

$$z_{iL} \geqslant 0 \qquad \text{if} \quad L \in \mathfrak{L}\gamma_i \tag{2.5b}$$

$$z_{iL} = 0 \qquad \text{if} \quad L \notin \mathfrak{L}\gamma_i \tag{2.5c}$$

$$\sum_{i=1}^{c} y_i = 1 \tag{2.6a}$$

$$y_i \geqslant 0 \tag{2.6b}$$

With the particular choice $y_i = c^{-1}$, we associate, to each covering of Γ a unique upper bound, which we call the *canonical bound* (associated with the

[3] For a precise definition of these systems, see, for example, Ref. 10.

covering). One then has

$$z_{iL} y_i^{-1} = \alpha_L \geqslant 1 \tag{2.7}$$

α_L is equal to cX_L^{-1}, where X_L denotes the number of subgraphs γ_i which contain the line L.

3. MAJORIZATION OF ARBITRARY n-GRAPHS BY MEANS OF SPANNING n-TREES

Throughout this chapter, $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ can be any connected n-graph. The subgraphs γ_i of Γ, which are used to obtain estimates of $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$, are considered as fixed parameters, unless stated otherwise.

3.1. Covering of the n-Graph Γ by Means of Spanning n-Trees

In Section 2.2, a set of upper bounds for $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ was associated by our estimation method to each covering of Γ by a set of c line-subgraphs γ_i. For these bounds to be useful, the γ_i must be chosen so that all the n-graphs in the right-hand side of (2.4) can be simplified into a product of easily computable factors. The simplest n-graphs in this respect are n-trees, because they can be simplified into a product of simple integrals [see Eq. (2.2)]. It is possible to bound any n-graph by means of n-trees because of the following:

Lemma 3.1. Any connected n-rooted graph can be covered by a set of spanning n-rooted trees.

Proof. We first cover the graph Γ by a set of spanning trees, and then cover each tree by a set of spanning n-rooted trees.

The first part of the proof is a straightforward consequence of the usual construction of a spanning tree in a connected graph[11,12]:

(i) Label all points.
(ii) Assign to each point i a weight w_i defined as the number of lines in the shortest path joining point i to point 1.
(iii) Delete all the lines joining two points of equal weight.
(iv) Delete all the lines joining points of weights w_i and $w_i - 1$, except the one for which the label on the point of weight $w_i - 1$ is least.

These steps are illustrated in Fig. 1.

The important point to notice here is that this construction gives a tree which contains *all lines* incident at point 1. Therefore if we perform the same construction by starting successively from point $2, 3, \ldots, n + k$ in-

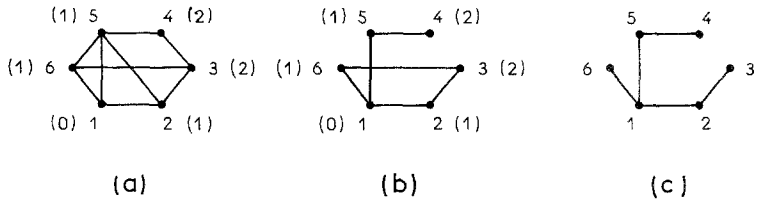


Fig. 1. Construction of a spanning tree out of a given graph. In (a), a label (number not in parentheses) and a weight (number in parentheses) are assigned to each point, according to steps (i) and (ii). (b) and (c) are obtained by applying steps (iii) and (iv).

stead of point 1, we obtain a set of spanning trees which contains all the lines of Γ, and thus form a covering of Γ.

Let us now show how to cover any spanning tree T of Γ by means of spanning n-trees of T (and thus of Γ). The first point is to find an algorithm which enables one to construct a spanning n-tree of T.

First of all, we must delete $(n-1)$ lines of T, because T has $n+k-1$ lines, whereas a spanning n-tree has k lines. But it is also clear (see Fig. 2c) that one cannot delete lines in any manner. Indeed, if we want to obtain finite upper bounds, each field-point of the reduced n-rooted graph must be linked to at least one root-point.

We are going to show that the following algorithm satisfies the preceding condition:

(i) Choose a root-point, say 1.
(ii) For each root-point i, delete from T the line L_i incident at i which belongs to the chain joining i to 1.

This construction is illustrated in Fig. 2. Our algorithm is well defined because, as T is a tree, there is a unique chain joining any pair of points.[13]

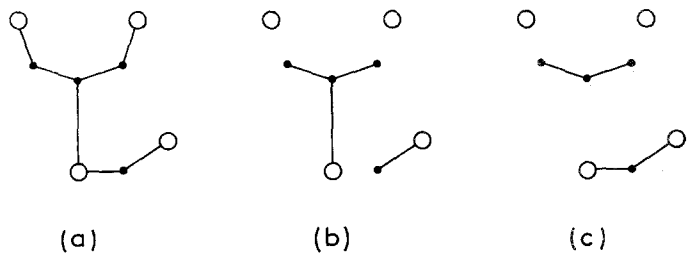


Fig. 2. Construction of a spanning n-tree out of a tree. (b) has been obtained from (a) by means of the algorithm of Lemma 3.1. (c) gives an incorrect way to delete lines, which would give rise to an infinite upper bound.

In particular, there is a unique chain C_i joining the root-point i to 1, and thus the line L_i is uniquely defined, too.

Now, to prove that we obtain an n-rooted tree by our procedure, we have to check that each field-point is linked by a chain of field-points to one and only one root-point. Let us first note that the graph τ obtained by deleting the $(n-1)$ lines L_i has no cycle, because T is a tree.[13] Therefore the number of components of τ is equal to its number of points minus its number of lines,[14] i.e., $(n+k)-k=n$. On the other hand, the n root-points of τ belong necessarily to different components. For, as we already noticed, any two root-points i and j are linked in T by a unique chain C_{ij}. As i and j are known to be linked already to the point 1, by means of chains C_i and C_j, C_{ij} is necessarily contained in $C_i \cup C_j$. Therefore, after having deleted the lines L_i and L_j, the root-points i and j cannot be linked any more by a chain.

Indeed, either one of the root-points i or j lies on the chain linking the other root-point to 1, or it does not. If it does, let us assume that j lies on C_i. Then, the deletion of L_i disconnects root-point i from all other points of C_i, and in particular from root-point j. If it does not, then L_j does not belong to C_i (otherwise, both end points of L_j would lie on C_i, and in particular root-point j) and thus L_j belongs to $C_{ij} = C_i \cup C_j - C_i \cap C_j$. This is illustrated in Fig. 3. Finally, the deletion of both lines L_i and L_j ensures that, in both cases, the root-points i and j become disconnected.

In short, we have seen that τ has exactly n components, and that none of these components contains more than one root-point. But, as there are n

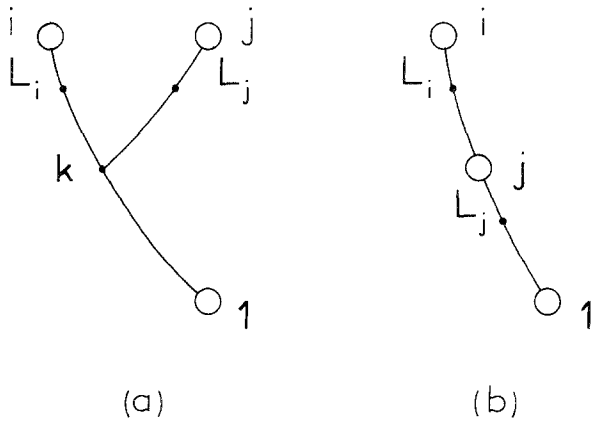


Fig. 3. The only two possible configurations for a given pair of root-points, in a tree (k can be identical to point 1). When applying the algorithm of Lemma 3.1, we delete both lines L_i and L_j, so that in both cases, i and j become disconnected.

root-points, this implies that each component of τ contains exactly one root-point. Therefore, τ is an n-tree.

Now, the important property of the n-tree that we have constructed is that it contains *all lines* incident at root-point 1. This implies that, if we perform the same construction by choosing successively each of the root-points of T, instead of point 1, we obtain a set of n-trees which contain all the lines of T, and thus form a covering of T.

In the case where we want to estimate a 1-graph, the preceding construction reduces to its first step because spanning trees are also spanning 2-trees.

It is useful, for the following, to reformulate Lemma 3.1 in the language of linear programming theory.[15] In this language, Lemma 3.1 says that there exists at least one set of real positive numbers z_{iL} which satisfy the linear constraints (2.5), if the γ_i's are chosen to be *all* the possible spanning n-trees of Γ. Note that, in Section 2.2, the situation was completely different, because the constraints (2.5) were *assumed* to be satisfied, insofar as the γ_i's were *assumed* to make a covering of Γ.

3.2. Upper Bounds for $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$

Now that we have proved that *any* n-graph Γ can be covered by a set of spanning n-trees of Γ, upper bounds are immediately deduced by combining this result with Eqs. (2.2) and (2.4) above. This gives the following theorem:

Theorem 3.2. Let $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ be any n-graph, and $T_1, \ldots, T_c$ be a covering of Γ made of c spanning n-rooted trees. One has the infinite set of upper bounds

$$|\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)| \leqslant \prod_{i=1}^{c} \prod_{L \in \mathfrak{L} T_i} \left(\int |f_L|^{z_{iL} y_i^{-1}} d\mathbf{x} \right)^{y_i} \tag{3.1}$$

where the z_{iL}'s and y_i's are nonnegative real numbers constrained only to satisfy conditions (2.5) and (2.6).

Corollary 3.3. The canonical upper bound associated to the covering $T_1, \ldots, T_c$ is written as

$$|\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)| \leqslant \prod_{L \in \mathfrak{L}\Gamma} \left(\int |f_L|^{\alpha_L} d\mathbf{x} \right)^{\alpha_L^{-1}} \tag{3.2}$$

where α_L is equal to c divided by the number of n-trees T_i which contain the line L. Moreover, one has

$$\alpha_L \geqslant 1 \qquad \text{for any } L \tag{3.3}$$

with at least one α_L strictly larger than 1 if Γ is not reduced to an n-rooted tree.

Proof. This is an immediate consequence of (3.1) and of Corollary 4.3 given in Ref. 3 [see also (2.7)]. Note that one has the relation

$$\sum_{L \in \mathfrak{L}\Gamma} \alpha_L^{-1} = k \tag{3.4}$$

where k denotes the number of field-points of Γ. This is a consequence of the definition of the α_L's, combined with the fact that the total number of lines, in the covering, is equal to ck. Equation (3.4) gives a useful way to check results, in practical calculations.

For the upper bounds (3.2) to be finite, it is necessary that all the f_L's decay to zero at large distances (at least, if pathological forms are excluded), because the α_L's are finite numbers. Therefore, if some f_L's do not decay to zero, we have first to get rid of these by making use of the mean value estimation method[8,9,3] before applying (3.2). Equivalently, we can get rid of these f_L's directly from (3.2), provided the corresponding α_L's are taken to be infinite (see Ref. 3, Section 4.4). Note that the assumption $\alpha_L = +\infty$ is compatible with the constraints (3.3) and (3.4).

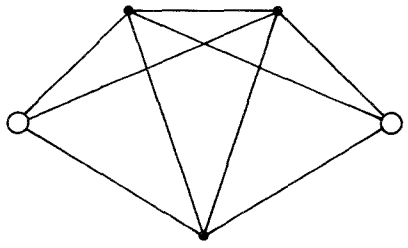
3.3. An Example of Application

In Section 3.1, we have given a method to construct a covering for any given n-graph by means of spanning n-trees. We illustrate this method of construction by an example, and compute the corresponding canonical bound, and make some comments on our estimation method.

Let us then study the following 2-graph, called $\epsilon 9(\mathbf{x}_{12})$ by Kim et al.,[16] and which is defined by the equality

$$\epsilon 9(\mathbf{x}_{12}) = \int_{\Lambda_\infty^3} f_{13} f_{14} f_{15} f_{23} f_{24} f_{25} f_{34} f_{35} f_{45} \, d\mathbf{x}_3 \, d\mathbf{x}_4 \, d\mathbf{x}_5 \tag{3.5}$$

Graphically, this is denoted as

$\epsilon 9(\mathbf{x}_{12}) =$  (3.6)

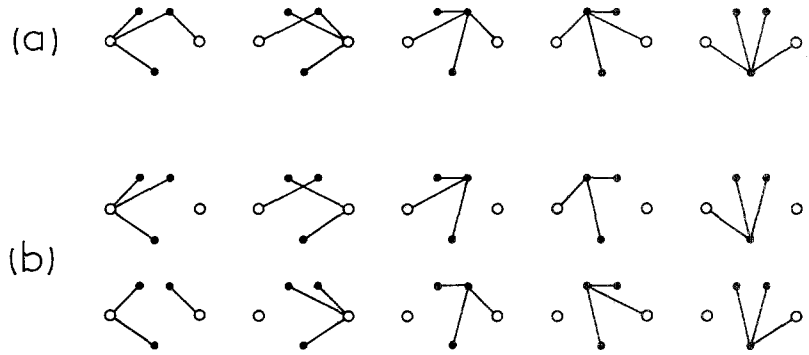


Fig. 4. Illustration of the algorithm of Lemma 3.1, which enables one to construct a covering, for any n-graph, by means of spanning n-trees. The 2-graph $\epsilon 9$ [defined by Eq. (3.6)] is first covered by means of the five spanning trees given in (a). Then, each tree of (a) is covered by means of the two spanning 2-trees of (b) which belong to the same column.

This is the most complicated 2-graph which has been computed, up to now, for realistic radially symmetric interaction potentials.[16] The covering of $\epsilon 9$ obtained by the method of the preceding paragraph is shown in Fig. 4. It yields the following canonical upper bound:

$$|\epsilon 9(\mathbf{x}_{12})| \leqslant \left(\int |f(\mathbf{x})|^{10/3}\, d\mathbf{x}\right)^{9/5} \left(\int |f(\mathbf{x})|^{5/2}\, d\mathbf{x}\right)^{6/5} \tag{3.7}$$

For the Gaussian gas, we have $\epsilon 9(r) = 50^{-3/2} \exp(-3r^2/2) = 2.83 \times 10^{-3} \exp(-3r^2/2)$, with $r = |\mathbf{r}_1 - \mathbf{r}_2|$, whereas our upper bound (3.7) is equal to 7.45×10^{-3}. Therefore, the latter overestimates the maximum of $\epsilon 9(r)$ by a factor 2.63. This shows that (3.7), although extremely simple, is nevertheless relatively accurate for small values of r. [Note that the mean value bound, which is equal[9,3] to $M^{l-k}B^k$, with $M = \sup|f(\mathbf{x})|$ and $B = \int|f(\mathbf{x})|\, d\mathbf{x}$, overestimates $\epsilon 9(r)$ by a factor of 353.]

The situation may not be so favorable for realistic interparticle potentials. Nevertheless, it seems reasonable to hope that the upper bound (3.7) also has a correct order of magnitude for realistic systems, provided the temperature is not too low.[3,17,18]

The method of Section 3.1 provides a simple algorithm which, for any given n-graph with k field-points, produces a covering made of $n(n+k)$ spanning n-trees. However, for a given n-graph, there is a large number of different coverings made of n-trees, and the former is usually not the simplest one [i.e., there are usually coverings which have a number of n-trees smaller than $n(n+k)$]. This can be checked easily in the case of the preceding 2-graph $\epsilon 9(x_{12})$. Indeed, we see from Fig. 4 that $\epsilon 9$ can be

covered with only four 2-trees (the first, the second, the eighth, and the tenth of Fig. 4b) instead of ten. In fact, one can even find a simpler covering, made only of three 2-trees, as indicated in Fig. 5 below. The corresponding canonical bound is equal to

$$|\epsilon 9(\mathbf{x}_{12})| \leqslant \left[\int |f(\mathbf{x})|^3 \, d\mathbf{x}\right]^2 \tag{3.8}$$

Note that one cannot find a covering simpler than the one of Fig. 5, because $\epsilon 9$ has nine lines, while a spanning 2-tree of $\epsilon 9$ has three lines.

It will be shown elsewhere[1,19] that the upper bound (3.8) is the best one which can be obtained by our estimation method, if one makes use only of spanning 2-trees to cover $\epsilon 9$. In the case of the Gaussian gas, (3.8) is equal to 7.13×10^{-3}. This shows that (3.7) is already a good bound.

The bounds (3.7) and (3.8) are finite for polar systems, because $|f|^{10/3}$, $|f|^{5/2}$, and $|f|^3$ decay at large distances like r^{-10}, $r^{-7.5}$, and r^{-9}, respectively. This is not a surprise, because we had already proven in Refs. 2 and 3 that all irreducible n-graphs of polar systems are finite. Equations (3.7) and (3.8) are nevertheless interesting, because they are improvements over the bound obtained in Ref. 3, paragraph 4.5.3.

On the contrary, in the case of the one-component three-dimensional plasma (i.e., when the lines are equal to e^{-r}/r), the bounds (3.7) and (3.8) are infinite, due to the divergence at small r of the integrals. This is not because our estimation method fails to be valid, but because $\epsilon 9(r)$ diverges logarithmically at the origin. As these bounds are constants independent of the coordinates, they must be larger than the maximum of $\epsilon 9(r)$, and thus be infinite. More generally, any bound which would be expressed by means of 1-graphs[1,22] is necessarily infinite, for the same reason.

For a bound to be useful, it therefore should not be constant. Such a bound can be obtained for example by making use of the covering of $\epsilon 9$ made of the spanning trees of Fig. 4a. One obtains in this way

$$|\epsilon 9(\mathbf{x}_{12})| \leqslant \left(\int f^{5/2} \, d\mathbf{x}\right)^2 \cdot \left(\int f_{13}^{5/2} f_{32}^{5/2} \, d\mathbf{x}_3\right)^{2/5} \cdot \left(\int f_{13}^{5/3} f_{32}^{5/3} \, d\mathbf{x}_3\right)^{3/5} \tag{3.9}$$

It can be checked by direct computation of the convolution products that (3.9) is finite everywhere except at the origin, and decays to zero at large distances.

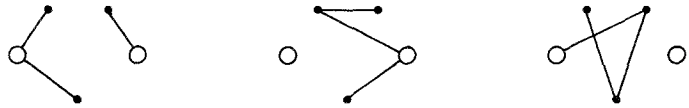


Fig. 5. Covering of the 2-graph $\epsilon 9$ [defined by Eq. (3.6)], by means of three 2-trees.

Upper bounds that decay to zero at large distances will be discussed systematically elsewhere (see also Ref. 1).

3.4. The Complete 1-Graphs $K_m(\mathbf{x}_1)$

In the preceding section, we have seen on a particular example, how the algorithm of Lemma 3.1 enables us to obtain computable upper bounds. Let us now apply this algorithm to the complete 1-graphs $K_m(\mathbf{x}_1)$. The study of these 1-graphs is useful to evaluate the relative accuracy of our estimates for arbitrary n-graphs. Indeed, as has been suggested in Ref. 3, one can consider that a given n-graph with k field-points is estimated with a relative accuracy lying between the accuracy of the estimates for the cycle C_{n+k} with $n+k$ lines and for the complete 1-graph K_{n+k}.

The complete 1-graph $K_m(\mathbf{x}_1)$ has m points and $\frac{1}{2}m(m-1)$ identical lines, and is defined by

$$K_m(\mathbf{x}_1) = \int_{\Lambda_\infty^k} \prod_{i<j} f_{ij}\, d\mathbf{x}_2 \cdots d\mathbf{x}_m \tag{3.10}$$

As the domain is infinite, $K_m(\mathbf{x}_1)$ is a constant (see Ref. 3, Corollary 3.6). So, when no confusion is possible between the graph and the 1-graph, $K_m(\mathbf{x}_1)$ will be also written simply K_m.

As $K_m(\mathbf{x}_1)$ is a 1-graph, we have just to look for a set of spanning trees of K_m which cover the latter. The construction of Lemma 3.1 gives, as a covering of K_m, a set of m spanning trees, each one being made out of the $(m-1)$ lines joining one given point to all the others. In the case of K_4, we find the covering given in Fig. 6.

By this covering of K_m, we obtain the following canonical upper bound for $K_m(\mathbf{x}_1)$:

$$K_m(\mathbf{x}_1) \leqslant \left[\int |f(x)|^{m/2}\, d\mathbf{x}\right]^{m-1} = \overline{T_m} \tag{3.11}$$

This is an immediate consequence of the fact that each line appears exactly in two spanning trees.

For the Gaussian gas, we find $\overline{T_m} = (m/2)^{-3(m-1)/2}$. The exact value is equal to $K_m = m^{-3(m-2)/2}$, because the complexity of K_m (i.e., its total

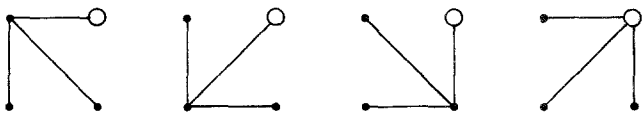


Fig. 6. Covering of the 1-graph K_4 by means of spanning 1-trees.

Table I. Relative Accuracy of our Bound $\overline{T_m}$ and of the Mean Value Bound T_m for the Complete 1-Graph K_m with m Points, in the Case of the Gaussian Gas. We Give the Value of the Ratios $\overline{T_m}/K_m$ and T_m/K_m for Different Values of m

m	3	4	5	6	7
$\overline{T_m}/K_m$	1.54	2.83	5.72	12.3	27.6
T_m/K_m	5.20	64	1.40×10^3	4.67×10^4	2.18×10^6

number of spanning trees[4]), is equal[4,11] to $m^{-(m-2)}$. Therefore, the ratio $\overline{T_m}/K_m$ of our bound to the exact value is asymptotically equal to

$$\overline{T_m}/K_m \sim m^{-3/2} 2^{3(m-1)/2} \tag{3.12}$$

for large values of m.

It is interesting to compare our bound (3.11) to the mean value bound. The latter is written as

$$|K_m(\mathbf{x}_1)| \leqslant M^{(m-1)(m-2)/2} \left[\int |f(\mathbf{x})|\, d\mathbf{x} \right]^{m-1} = T_m \tag{3.13}$$

For the Gaussian gas, the right-hand side of (3.13) is equal to $T_m = 1$. In Table I above, we have compared T_m and $\overline{T_m}$ to the exact value of K_m. This table shows that our bounds are much more accurate than the mean value bounds for the Gaussian gas.

On the contrary, for the hard-sphere gas, both types of bounds are identical, as we have $|f(x)|^m = |f(x)|$ for any x, in this case. Note, however that the mean value bounds are much more accurate for the hard-sphere gas than for the Gaussian gas. This can be seen by comparing the results of Table I to those of Table II.

Remarks. Equation (3.11) is the best upper bound which can be obtained by means of spanning trees.[1,19]

For the particular 1-graphs K_m, our estimation method, using Lemma 3.1, amounts to writing the identity

$$\prod_{i<j} f_{ij} = \prod_{i=1}^{m} \left(\prod_{j=1}^{m} f_{ij}^{1/2} \right) \tag{3.14}$$

Table II. Common Value of the Ratios $\overline{T_m}/K_m$ and T_m/K_m for the Hard-Sphere Gas, and for Different Values of m

m	3	4	5	6	7
$\overline{T_m}/K_m = (T_m/K_m)$	2.13	6.31	22.6	90.6	393

and then applying Hölder's inequality with $y_i = 1/m$ to the product of the m factors in the right-hand side of (3.14).

In Ref. 3, paragraph 4.3.1, we have obtained for K_4 the same bound (3.11) which is equal in this case to $(\int |f(\mathbf{x})|^2 d\mathbf{x})^3$, by making use of a simpler covering. This shows that different coverings do not necessarily give different canonical upper bounds.

3.5. Definition of the Classes of Functions to be Used

We have seen that our estimation method provides, for any n-graph, upper bounds which are extremely simple. Indeed, they involve just the computation of integrals of the type $\int |f_L|^\alpha dx$. However, to be useful, these bounds have to be finite. Therefore, we are naturally led to look for certain classes of functions, which are sufficiently large to include all the functions which are encountered in practice, and at the same time sufficiently small to ensure that the bounds are finite, provided the f_L's are chosen inside these classes.

3.5.1. Analysis of the various functions encountered in equilibrium statistical mechanics. The various functions which can be encountered in most articles dealing with realistic systems have been described in detail in Ref. 3, Section 2.4. For our present purposes, it is convenient to classify these functions into three classes, according to their behavior at short and at long distances.

(i) Functions which are bounded everywhere and go to a nonnull constant at large distances. To this class belong the Boltzmann factors $\exp[-\beta\varphi(r)]$, where $\varphi(r)$ is the interparticle potential, and the distribution functions $g(r)$.

(ii) Functions which are asymptotically proportional to r^{-m} *at small distances* (m being a fixed number), are bounded everywhere else, and decay exponentially at large distances. To this class belong the Debye–Hückel function $b(r) = -\epsilon e^{-r}/r$ and the Abe–Meeron function $B(r) = \exp[b(r)] - 1 - b(r)$, as also the generalized Debye–Hückel functions $[b(r)]^{\alpha_L}$, for α_L real positive.[3]

(iii) Functions which are bounded everywhere and decay to zero *at large distances as a certain power* r^{-m} of the interparticle distance or faster (for example exponentially). To this class, belong the Mayer functions of all the usual interparticle potentials, for example the hard-sphere and square-well potentials (which are identical to zero from a certain distance), the soft-sphere and the Lennard–Jones potentials (which decay like r^{-m}, $m > 3$), as also the interaction potentials of polar systems and of the

primitive model of ionic solutions (which decay, respectively, like r^{-3} and r^{-1}). To this class belong also some other functions, which may occur in integrands of n-graphs, for example finite sums of chains of Mayer functions, as used for example by Salpeter,[23] and two-body correlation functions that occur in integral equations for the distribution function $g(r)$ (see, for example, Ref. 24).

Indeed, the former decay to zero like the potential itself, for any density and temperature,[20] and the latter decay at least as fast as the potential at small activities.[25] Finally, to this class belong also the functions which occur in the theory of liquids,[4] provided the interparticle potential is split into the sum of two terms φ_0 and φ_1 in a suitable way, as explained in Ref. 3, Section 2.4.3. In that case, the long-range part φ_1 is bounded everywhere and decays to zero at large distances like r^{-m}, so that the lines $(-\beta\varphi_1)^p$, which arise when expanding the function $\exp(-\beta\varphi_1)$ in powers of φ_1, can be considered (i.e., have the same overall shape) as Mayer functions of neutral systems, and belong to class (ii). In particular, the splitting of the Lennard–Jones potential introduced by Weeks et al.,[27] and which has proved very important for the applications, is of the preceding type.

3.5.2. The Classes of Functions D_p and D^p. To ensure that all functions are integrable, we require them to be continuous (except perhaps at a finite number of points). This reasonable hypothesis is satisfied by most of the functions of the preceding section (except perhaps by correlation or distribution functions, since this has not been proven rigorously).

In the preceding section, we have classified in three disjoint sets the functions which can be encountered in practice, in statistical mechanics, so that the functions in each set share a common property, when one takes their norm[28] $\|f\|_\alpha = (\int |f|^\alpha dx)^{1/\alpha}$. With this we can make the following three statements:

Each function f of class (i) satisfies the property

(P1): $\|f\|_\alpha$ is finite if and only if $\alpha = +\infty$. (We recall that $\|f\|_\infty = \sup|f|$).

Each function f of class (ii) satisfies the property

(P2): There exists a real positive number $p = d/m$ uniquely defined by f such that $\|f\|_\alpha$ is finite provided $\alpha < p$, and infinite otherwise.

[4] See, for example, Ref. 26 and references therein.

Each function f of class (iii) satisfies the property

(P3): There exists a real positive number $p = d/m$ uniquely defined by f such that $\|f\|_\alpha$ is finite provided $\alpha > p$, and infinite otherwise.

Let us prove the last statement. (The other two can be proven in a quite analogous way).

If $f(r)$ is a function class (iii) that decays as r^{-m} at large distances, it satisfies, by definition, the inequalities

$$|f(r)| < B \qquad \forall r \tag{3.15a}$$

$$|f(r)| < Ar^{-m} \qquad \forall r > R \tag{3.15b}$$

for some positive constants A, B, and R. Therefore, $\|f\|_\alpha$ is clearly finite for any α larger than $p = d/m$, where d is the space dimensionality. Also, $\|f\|_\alpha = \infty$ for $\alpha = d/m$ [since $f(r) \cdot r^m \to$ nonzero constant, as $r \to \infty$]. Furthermore, by applying the Cauchy–Schwarz inequality to the identity $|f|^p = |f|^{(p/2)-k}|f|^{(p/2)+k}$ for any k real positive, we find $\|f\|_p^2 \leqslant \|f\|_{p-2k}\|f\|_{p+2k}$. This shows that $\|f\|_{p-2k}$ is infinite for any $k > 0$, because $\|f\|_p$ is, whereas $\|f\|_{p+2k}$ is finite.

The classes of functions which have properties (P2) or (P3) will be called, respectively, D_p and D^p. The class of functions which have property (P1) will be called D^∞. (This notation is coherent with the definition of D^p, for p finite.)

With these definitions, we see that the Debye–Hückel function $b(r)$ and the Abe–Meeron function $B(r)$ both belong to D_3, while the Coulomb function $C(r) = \exp(-L/r) - 1$ belongs to D^3. The Mayer functions belong to D^1 for a polar system, and to $D^{1/2}$ for a Lennard–Jones system. More generally, the Mayer functions of neutral systems[3] (i.e., systems whose interparticle potential is bounded below and decay at large distances at least as fast as r^{-m}, $m > d$, for a d-dimensional system) belong to D^p with $p = d/m < 1$.

3.6. Sufficient Condition for an n-Graph to be Finite

For the upper bound (3.1) to be finite, it is necessary and sufficient that each factor $\int |f_L|^{z_{iL}y_i^{-1}} d\mathbf{x}$ be finite. With the preceding definitions this can be stated in the following form:

Theorem 3.5. Let us assume that, for each L, the line f_L of the n-graph $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ belongs to the class D^{p_L} (or D_{p_L}). A necessary and sufficient condition for the upper bound (3.1) to be finite is that the z_{iL} and

y_i satisfy the inequalities

$$z_{iL} - p_L y_i > 0 \quad \text{if} \quad f_L \in D^{p_L} \text{ and } L \in T_i \tag{3.16a}$$

$$z_{iL} - p_L y_i < 0 \quad \text{if} \quad f_L \in D_{p_L} \text{ and } L \in T_i \tag{3.16b}$$

As a consequence, a sufficient condition for $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ to be finite is that there exists a set of real nonnegative numbers z_{iL} and y_i which satisfy simultaneously the system of inequalities (2.5), (2.6), and (3.16).

The main point about these inequalities is that they are *linear* in the variables z_{iL} and y_i. Therefore, to know whether there exists a finite bound, we have to solve a linear programming problem.[15] Such a problem is known to be solvable in a finite number of steps by means of the simplex algorithm.[15]

It is important to note that the preceding linear program enables us to realize explicitly the objective of our estimation method, as described in Ref. 3, which is to obtain information on the numerical value of an arbitrary n-graph $\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)$ simply by making use of some global information on the topological structure of Γ and on the shape of the functions f_L. Indeed, the topological structure of Γ is incorporated into the linear program through the linear system $\sum z_{iL} = 1$, since it is determined by the incidence matrix of Γ with all its spanning n-trees, and the shape of the f_L's is incorporated through the constraints (3.16).

As there are known algorithms to construct all the spanning trees of Γ (and thus all the spanning n-trees of Γ, by Lemma 3.1), we have now at our disposal an algorithm that *solves formally* the problem of finding *finite* bounds of type (3.1), for *any* n-graph (in particular, the f_L's can be all different). But, if we want to construct *practically* a finite bound for a *given* n-graph, there are usually other ways much simpler than using the general algorithm. Indeed, the preceding linear program involves $C(l+1)$ variables, where C is the total number of spanning n-trees of Γ, and this number may be very large. For example, for the 2-graph $\epsilon 9(\mathbf{x}_{12})$, we would have 500 variables. Of course, if the f_L's (or, more precisely, the p_L's) are all different, as can occur in quantum chemistry, it may happen that we have no other choice than trying to solve the complete linear programming problem. But if the n-graph is not too complicated, for example if the f_L's are all identical or equal to a few simple powers of the same function, as occurs in statistical mechanics, it is usually much simpler, in practice, to try to satisfy conditions (3.16) with some suitably chosen z_{iL} and y_i associated to some simple coverings, rather than solving the complete linear programming problem. Furthermore, if we restrict ourselves to making use of canonical bounds, we then only have to find a covering which satisfies the

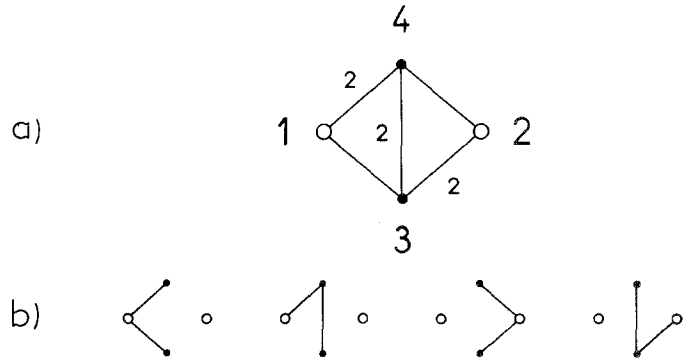


Fig. 7. (a) Graphical representation of the 2-graph defined by Eq. (3.18). (b) Covering of this 2-graph by means of spanning 2-trees.

very simple conditions

$$X_L < cp_L^{-1} \qquad \forall L \tag{3.17}$$

where X_L denotes, as usual, the number of spanning n-trees of the covering which contain the line L.

Let us illustrate this with the following example:

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \Lambda) = \int_{\Lambda^2} C_{13} C_{14}^2 C_{34}^2 C_{32}^2 C_{42}\, d\mathbf{r}_3\, d\mathbf{r}_4 \tag{3.18}$$

where $C_{ij} = C(|\mathbf{r}_i - \mathbf{r}_j|)$, and $C(r) = \exp(-L/r) - 1$ is the Coulomb line. This 2-graph has been represented in Fig. 7a above. Note that each of its lines is nonintegrable in an infinite volume, because $C(r)$ decays like r^{-1} at large distances, and so it is not obvious whether $\Gamma(\mathbf{r}_1, \mathbf{r}_2; \Lambda)$ is finite or not. In particular, the mean value bounds are infinite. However, we are going to show that this 2-graph is actually finite. To this end, let us consider the covering given in Fig. 7b. We have $c = 4$, and $X_{14} = X_{34} = X_{42} = 2$, $X_{13} = X_{42} = 1$. Furthermore, as $C(r) \in D^3$ and $C^2(r) \in D^{3/2}$, we have also $p_{14} = p_{34} = p_{42} = \frac{3}{2}$ and $p_{13} = p_{42} = 3$. Therefore, we see that the condition $X_L < cp_L^{-1}$ is satisfied for any L, and so there exist finite upper bounds for $\Gamma(\mathbf{r}_{12}; \Lambda)$. The covering of Fig. 7b gives

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \Lambda) \leqslant \left[\int C^4(r)\, d\mathbf{r}\right]^2 \tag{3.19}$$

This upper bound can be computed analytically (see Appendix), and is equal to $[4\pi L^3 \cdot \frac{2}{3}(44 \ln 2 - 27 \ln 3)]^2$. We find

$$\Gamma(\mathbf{r}_1, \mathbf{r}_2; \Lambda) \leqslant 0.31058(4\pi L^3)^2$$

Finally, one can make the following remarks about canonical bounds of neutral, polar, and ionized systems:

For an n-graph of a *neutral* system (i.e., an n-graph whose lines are bounded and decay like r^{-m}, with $m > d$), all the canonical bounds [and in particular those of type (3.2)] are finite. Indeed, we have $p_L < 1$ for any L, in this case. Therefore, from inequality (2.7), the conditions (3.17) are automatically satisfied. This shows a posteriori the usefulness of canonical bounds. On the contrary, there are bounds of type (3.1) which are infinite, because it is always possible to choose a pair of numbers z_{iL} and y_i so that (3.16) is not satisfied.

For an n-graph of *polar* system (i.e., an n-graph whose lines are bounded and decay like r^{-d}), it is always possible to find a bound of type (3.2) which is *finite*, provided the n-graph is irreducible.[5] This can be seen by applying (3.2) to the right-hand side of the inequality [see Ref. 3, Eq. (4.44)]

$$|\Gamma(\mathbf{x}_1, \ldots, \mathbf{x}_n; \Lambda)| \leqslant \prod_{i=1}^{l} \left(\int \prod_{L \in \mathfrak{L}\gamma_i} |f_L|^{l/(l-1)} \, d\mathbf{x}_{n+1} \cdots d\mathbf{x}_{n+k} \right)^{1/l} \tag{3.20}$$

Here, the γ_i's are obtained from Γ by deleting one of its lines. Note that the bound obtained in this way is an improvement over the one given in Ref. 3, Eq. (4.48), because the latter was obtained by applying the mean value estimation method to the right-hand side of (3.20).

For an n-graph of *polar* system or of *ionic* solution (i.e., an n-graph whose lines decay like r^{-d} or less rapidly), canonical bounds may be *infinite* even if the n-graph itself is finite. To illustrate this point, let us consider once again the 2-graph $\Gamma(\mathbf{r}_1, \mathbf{r}_2; \Lambda)$ defined by Eq. (3.18). The first three 2-trees of Fig. 7b make a covering of this 2-graph. But, with this covering, condition (3.17) is not satisfied because we have $cX_{13} = 3$, while p_{13} is also equal to 3. This covering would give the canonical bound $[\int C^3(r)\, d\mathbf{r}]^{4/3} [\int C^6(r)\, d\mathbf{r}]^{2/3}$, which diverges logarithmically because of the first factor.

To be allowed to apply the theorems of simplification of n-graphs (see Ref. 3, Section 3.1) to a given n-graph, it is necessary to first prove that its integrand is absolutely integrable. For neutral systems the mean value estimation method[9,8,25] enables one to answer this question, but not for polar and ionized systems. The results of this section enable one to answer this question partly, for the latter systems. Note that, in practice, the theorems of simplification of n-graphs into products of irreducible compo-

[5] An n-graph is irreducible if any field-point lies on a chain of field-points linking two root-points. (If $n = 1$, the root-point is taken to be the initial and the final point of the chain.)

nents have always been assumed to be applicable[6] to these systems although this is questionable, especially for ionized systems in the framework of the Abe–Meeron theory,[30] where infinite n-graphs occur.[21,31]

ACKNOWLEDGMENTS

The author wishes to thank Professors J. Groeneveld and M. S. Wertheim for making very useful comments and suggesting many improvements on the manuscript, and Professor J. Chapelle for constant support and encouragements during this work.

APPENDIX A

In this Appendix, we compute the integrals $I_n = \int |C(r)|^n \, dr$, where $C(r) = 1 - \exp(-L/r)$ is the Coulomb line and n is an integer larger than 3. These integrals are useful to compute upper bounds for arbitrary n-graphs with Coulomb lines.

We have

$$I_n = \int |C(r)|^n \, d\mathbf{r} = 4\pi \int_0^\infty (1 - e^{-L/r})^n r^2 \, dr \tag{A.1}$$

With the change of variables $L/r = t$, we find

$$I_n = 4\pi L^3 \int_0^\infty (1 - e^{-t})^n \frac{dt}{t^4} \tag{A.2}$$

To compute this integral, it is convenient to reduce the negative power t^{-4}, by partial integration, to t^{-2}. We obtain

$$I_n = 4\pi L^3 \cdot \tfrac{1}{6} n \left[n J_n - (2n-1) J_{n-1} + (n-1) J_{n-2} \right] \tag{A.3}$$

where J_n is the known integral[7]

$$J_n = \int_0^\infty (1 - e^{-t})^n \, dt/t^2$$

$$= \sum_{k=2}^{n} (-1)^k k \binom{n}{k} \ln k \tag{A.4}$$

[6] See Ref. 29a; for polar systems the problem of the factorization of n-graphs into a product of irreducible components has been investigated in Ref. 29b. However, these authors do not solve this problem completely because they do not study the absolute convergence of the irreducible components. See also Ref. 30.

[7] See Ref. 32, Formula 3.411.20. In this formula and in the preceding one (3.411.19), the combinatorial factor $\binom{n}{k}$ is defined to be equal to $n(n-1)\cdots(n-k+1)$. We have checked these formulas, and it turns out that $\binom{n}{k}$ is in fact the usual combinatorial factor $(k!)^{-1} n \cdot (n-1)\cdots(n-k+1)$. Indeed it arises from the expansion of $(1 - e^{-t})^n$ by means of the binomial formula.

Table III. Value of the Integral $I_n = \int |C(r)|^n \, dr$, for Various Values of n. $C(r)$ Denotes the Coulomb Line, i.e., $C(r) = \exp(-L/r) - 1$. I_n Has Been Computed Numerically for n Noninteger

n	3	3.5	4	4.5	5	5.5
$I_n/4\pi L^3$	∞	1.40169	0.557296	0.316070	0.210152	0.153170
n		6	6.5	7	7.5	8
$I_n/4\pi L^3$		0.118537	0.0956848	0.0796831	0.0679633	0.0590715
n		8.5	9	9.5	10	∞
$I_n/4\pi L^3$		0.0521314	0.0465868	0.0420701	0.0383292	0

with $\binom{n}{k} = (k!)^{-1} n(n-1) \cdots (n-k+1)$. By combining (A.4) and (A.3), we obtain

$$
\begin{aligned}
I_4/4\pi L^3 &= \tfrac{2}{3}(\qquad\qquad\qquad\quad - 27\ln 3 + 44\ln 2) \\
I_5/4\pi L^3 &= \tfrac{5}{6}(\qquad\quad - 25\ln 5 - 54\ln 3 + 144\ln 2) \\
I_6/4\pi L^3 &= \qquad\quad - 125\ln 5 - 54\ln 3 + 376\ln 2 \\
I_7/4\pi L^3 &= \tfrac{7}{6}(- 49\ln 7 - 375\ln 5 + 81\ln 3 + 880\ln 2) \\
I_8/4\pi L^3 &= \tfrac{4}{3}(- 343\ln 7 - 875\ln 5 + 567\ln 3 + 2096\ln 2) \\
I_9/4\pi L^3 &= \tfrac{3}{2}(- 1372\ln 7 - 1750\ln 5 + 1602\ln 3 + 5376\ln 2) \\
I_{10}/4\pi L^3 &= \tfrac{5}{3}(- 4116\ln 7 - 3050\ln 5 + 2754\ln 3 + 14272\ln 2)
\end{aligned}
$$

REFERENCES

1. M. Lavaud, *Phys. Lett.* **62A**:295 (1977).
2. M. Lavaud, Estimates of general Mayer graphs. I: General theory, *J. Stat. Phys.* **27**:593 (1982).
3. M. Lavaud, Thesis, Part II, A and B (1978).
4. G. E. Uhlenbeck and G. W. Ford, in *Studies in Statistical Mechanics*, Vol. 1, J. de Boer and G. E. Uhlenbeck, eds. (North-Holland, Amsterdam, 1962).
5. A. Fetter and J. Walecka, *Quantum Theory of Many Particle Systems* (McGraw Hill, New York, 1972).
6. E. Speer, *Generalized Feynman Amplitudes* (Princeton University Press, Princeton, New Jersey, 1969).
7. R. Lefebvre and C. Moser, eds., *Advances in Chemical Physics*, Vol. 14, *Correlation Effects in Atoms and Molecules* (Interscience, New York, 1969).
8. R. J. Riddell and G. E. Uhlenbeck, *J. Chem. Phys.* **21**:2056 (1953).
9. J. Groeneveld, Thesis (1967). Published in *Proc. Koninkl. Nederl. Akad. Wetenschappen, Ser. B* **70**:454 (1967). See also Chap. 7 in *Graph Theory and Theoretical Physics*, F. Harary, ed. (Academic Press, New York, 1967), and Ref. 25.

10. A Münster, *Statistical Thermodynamics*, Vols. 1 and 2 (Springer Verlag, Berlin, 1969 and 1974).
11. C. Berge, *Graphes et hypergraphes* (Dunod, Paris, 1970).
12. O. Penrose, in *Statistical Mechanics* T. Bak, ed. (Benjamin, New York, 1967).
13. F. Harary, *Graph theory* (Addison Wesley, Reading, Massachusetts, 1969), Theorem 4.1.
14. F. Harary, Ref. 13, Corollary 4.5 (b).
15. M. Simonnard, *Programmation linéaire. Technique du calcul économique*, Vols. 1 and 2 (Dunod, Paris, 1972 and 1973); G. B. Dantzig, *Linear Programming and Extensions* (Princeton Univ. Press, Princeton, New Jersey, 1962).
16. S. Kim, D. Henderson, and L. Oden, *Trans. Faraday Soc.* **65**:2308 (1969).
17. M. Lavaud, Rapport d'activité au CNRS (1977).
18. M. Lavaud, Estimates of general Mayer graphs. VI: Discussion of the accuracy of the upper bounds obtained by means of spanning n-trees, for a Lennard–Jones system (in preparation).
19. M. Lavaud, Estimates of general Mayer graphs. V: The best upper bound obtained by means of spanning n-trees, for uniformly coverable n-graphs (in preparation).
20. M. Lavaud, *Phys. Lett.* **63A**:76 (1977).
21. M. Lavaud, Estimates of general Mayer graphs. II: Long-range behavior of 2-graphs occurring in the theory of ionized systems, *J. Stat. Phys.* **19**:429 (1978).
22. M. Lavaud, Communication at the 7th Conference on Thermophysical properties, Washington, D.C., 10–12 May 1977; communication at the 13th IUPAP Conference on Statistical Physics, Haifa, Israël, 24–30 August 1977.
23. E. E. Salpeter, *Ann. Phys. (N.Y.)* **5**:183 (1958).
24. E. Meeron, *J. Math. Phys.* **1**:192 (1960); J. M. J. Van Leeuwen, J. Groeneveld, and J. de Boer, *Physica* **25**:792 (1959).
25. J. Groeneveld, in *Statistical Mechanics*, T. Bak, ed. (Benjamin, New York, 1967).
26. H. C. Andersen, *Ann. Rev. Phys. Chem.* **26**:145 (1975).
27. J. D. Weeks, D. Chandler, and H. C. Andersen, *J. Chem. Phys.* **54**:5237 (1971).
28. N. Dunford and J. T. Schwartz, *Linear Operators* (Wiley, New York, 1957), Vol. 1, p. 119.
29. (a) J. O. Hirschfelder, C. F. Curtiss, and R. B. Byrd, Molecular theory of gases and liquids (Wiley, New York, 1964); (b) D. W. Jepsen and H. L. Friedman, *J. Chem. Phys.* **38**:846 (1963), Appendix A.
30. R. Abe, *Progr. Theor. Phys.* **22**:213 (1959).
31. M. Lavaud, Thesis, Part III B (1978), and Proceedings of the NATO Advanced Institute on Strongly Coupled Plasmas, Orléans-la-Source, France, 7–23 July 1977, G. Kalman, ed. (Plenum Press, New York, 1978).
32. I. S. Gradshteyn and I. N. Ryzhik, *Table of Integrals, Series and Products* (Academic Press, New York, 1965).