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Estimates of General Mayer Graphs. IV. On the Computation of Gaussian Integrals by the Star-Mesh Transformation

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We point out that, to compute by hand a Gaussian integral $\int \exp \cdot (-\sum_{L \in \mathcal{L}\Gamma} y_L r_{ij}^2)\, d\mathbf{r}_{n+1} \cdots d\mathbf{r}_{n+k}$, where the sum runs over all lines $L = (i, j)$ of a graph and $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$, the simplest way is to use the star-mesh transformation, well known in electrical network theory. We apply this to test, on a relatively complicated n-graph, the accuracy of an estimation method that we proposed elsewhere [*Phys. Lett.* **62A**:295 (1977)].

KEY WORDS: Gaussian integral; graph; star-mesh transformation.

1. INTRODUCTION

In preceding articles,[1-3] we have developed an estimation method that provides upper bounds for arbitrary n-graphs. An n-graph is a multiple integral of the following type:

$$\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_n; \Lambda) = \int_{\Lambda^k} \prod_{L \in \mathcal{L}\Gamma} f_L(\mathbf{r}_i, \mathbf{r}_j)\, d\mathbf{r}_{n+1} \cdots d\mathbf{r}_{n+k} \tag{1.1}$$

(For definition of the symbols, see Ref. 2.) In considering physical problems, it is important to know whether our estimation method can provide a correct order of magnitude for the n-graphs. To try to answer this question, it is instructive to test quantitatively the accuracy of our estimates on Gaussian n-graphs. Indeed, in this case, both the n-graph and any of its upper bounds can be computed analytically. A Gaussian n-graph is an n graph with Gaussian lines and $\Lambda = \mathbb{R}^d$. Gaussian lines are defined as

$$f_L(r) = \exp(-y_L r^2) \tag{1.2}$$

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y_L can be any real positive number and is called the weight (or the admittance) of line L.

In their fundamental review article on Mayer's theory of classical systems at equilibrium,[4] Uhlenbeck and Ford have recalled the formulas that give Gaussian n-graphs in terms of determinants of minors of the admittance matrix of Γ. These formulas are proved by diagonalizing the quadratic form $\sum_L y_L r_{ij}^2$. (See, for example, Ref. 5.) They are well adapted to electronic computers, and have been used to compute a certain number of Gaussian 1- and 2-graphs.[4,6] However, if one wants to compute n graphs by hand, the use of these formulas is laborious, and one may prefer topological methods. Uhlenbeck and Ford[4] have recalled Kirchhoff's method, which expresses these determinants as sums of admittance tree products, and the recurrence method of Brooks *et al.*,[7] which expresses these determinants as sums of determinants associated with simpler graphs, obtained by deleting and contracting lines.

These powerful methods are of constant use in electrical network theory. (See, for example, Ref. 8.) However, to compute n-graphs, it is much simpler to use the star-mesh transformation,[9,10] as we point out in this paper.

In Section 2, we compute by elementary means the n-graph $K_{1,n}(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ made of one field point linked to n root points. In Section 3, we show that computing a Gaussian n-graph by performing the partial integrations is equivalent to computing the above-mentioned determinants through the star-mesh transformation.[9,10] In Section 4, we compare the various ways of computing Gaussian n-graphs. In Section 5, we test the accuracy of our estimation method on an example.

2. EXPRESSION OF THE STAR $K_{1,m}(\mathbf{r}_1, \ldots, \mathbf{r}_m)$ AND OF THE CHAIN $C_m(\mathbf{r}_1, \mathbf{r}_2)$

We want to compute the following m graph:

$$K_{1,m}(\mathbf{r}_1, \ldots, \mathbf{r}_m) = \int \prod_{i=1}^{m} \exp\left(-y_i r_{ip}^2\right) d\mathbf{r}_p \tag{2.1}$$

This integral is represented graphically in Fig. 1a, and its representative graph $K_{1,m}$ is called a star.[2] We have

[2] This definition of a star should not be confused with the definition used in Ref. 4, where a star means any connected graph without articulation point.

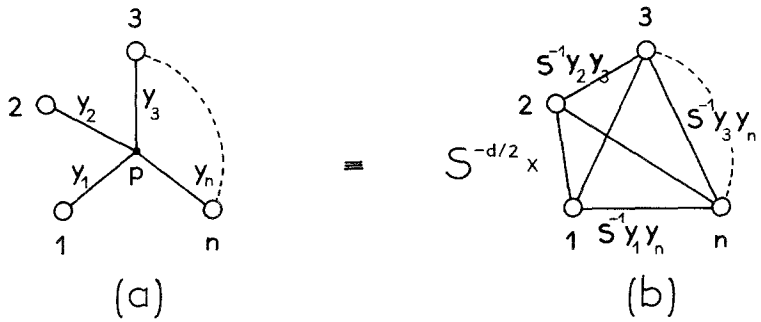

Fig. 1. The m-graph $K_{1,m}(\mathbf{r}_1, \ldots, \mathbf{r}_m)$ defined by Eq. (2.1) is represented in (a) by the star $K_{1,m}$. It is equal, by Eq. (2.2), to the Gaussian function $S^{-d/2}K_m(\mathbf{r}_1, \ldots, \mathbf{r}_m)$, represented in (b) by the complete graph K_m (also called a mesh) with modified weights $S^{-1}y_i y_j$.

$$K_{1,m}(\mathbf{r}_1, \ldots, \mathbf{r}_m) = S^{-d/2} \exp\left(- \sum_{1 \leqslant i < j}^{m} S^{-1} y_i y_j r_{ij}^2 \right) \tag{2.2a}$$

with

$$S = \sum_{i=1}^{m} y_i \tag{2.2b}$$

(2.2) can of course be proved easily as a consequence of Kirchhoff's theorem[4,11] but it is instructive to obtain it by elementary means.

To this end, let us set $\mathbf{r}_{ip} = \mathbf{r}_{i1} + \mathbf{r}_{1p}$ and take point 1 as the origin of the coordinate system.

(2.1) is then reexpressed as

$$\begin{aligned} K_{1,m} &= \exp\left(- \sum_{i=2}^{m} y_i r_{i1}^2 \right) \int \exp\left[- \left(S r_{1p}^2 + 2\mathbf{r}_{1p} \cdot \sum_{i=2}^{m} y_i \mathbf{r}_{i1} \right) \right] d\mathbf{r}_{1p} \\ &= S^{-d/2} \exp\left(- \sum_{i=2}^{m} y_i r_{i1}^2 + \frac{1}{S} \sum_{i,j=2}^{m} y_i y_j \mathbf{r}_{i1} \cdot \mathbf{r}_{j1} \right) \end{aligned} \tag{2.3}$$

By making use of the identity $-2\mathbf{r}_{i1} \cdot \mathbf{r}_{j1} = r_{ij}^2 - r_{i1}^2 - r_{j1}^2$, (2.3) transforms into (2.2).

3. THE STAR-MESH TRANSFORMATION[9,10] FOR GAUSSIAN n-GRAPHS

To compute a given Gaussian n-graph, we can perform the integrations in any order. Let us assume we integrate first over $\mathbf{r}_{n+k}$:

$$\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_n) = \int d\mathbf{r}_{n+1} \cdots d\mathbf{r}_{n+k-1} \prod' f_L(r_{ij}) \int \prod'' f_L(r_{i,n+k})\, d\mathbf{r}_{n+k} \quad (3.1)$$

where the first product $\prod'$ runs over all lines of Γ not incident on point $n+k$, and the second product $\prod''$ runs over all lines that are incident on $n+k$. The last integral in (3.1) is of type (2.1), and thus we have the following lemma.

Lemma 3.1. (Star-mesh transformation for Gaussian n-graphs.) Let Γ be an arbitrary weighted graph with weight y_L attached to any line L and $\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_n)$ the Gaussian n-graph with lines $f_L(r) = \exp(-y_L r^2)$, represented by Γ. We have

$$\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_n) = S^{-d/2} \gamma(\mathbf{r}_1, \ldots, \mathbf{r}_n) \quad (3.2)$$

where γ is the weighted graph obtained from Γ by replacing a star $K_{1,m}$ of Γ (i.e., a subgraph of Γ made of one given point p, together with all its adjacent points and all its incident lines) by the complete graph K_m (also called a mesh) obtained by joining each pair (i, j) of points adjacent to p by a line L and assigning to L the weight

$$w_L = S^{-1} y_i y_j \quad (3.3)$$

In (3.2) and (3.3), y_i and y_j are the weights of lines (p, i) and (p, j) in Γ, and $S = \sum y_i$ is the sum of the weights of all the lines incident to p.

We see that γ is exactly the graph obtained from Γ by applying the star-mesh transformation at point p,[9,10] i.e., by replacing in Γ the star $K_{1,m}$ by the mesh K_m. Since γ has one field point less than Γ, after k successive applications of Lemma 3.1, we obtain an n-graph with no field point, i.e., a Gaussian function.

4. COMPARISON OF THE VARIOUS METHODS OF COMPUTATION OF GAUSSIAN n-GRAPHS

For the sake of simplicity, we restrict our discussion to the case of 1-graphs. We have[4]

$$\Gamma(\mathbf{r}_1) = \pi^{(1/2)dk} \left[\Delta(\Gamma)\right]^{-d/2} \quad (4.1)$$

where $\Delta(\Gamma)$ is the determinant of a first-order minor of the admittance matrix of Γ, and the graph Γ has k field points and l lines.

$\Delta(\Gamma)$ can be computed by generating the set of all spanning trees T_i of Γ (see, for example, Ref. 12) and making use of Kirchhoff's theorem[4,11]:

$$\Delta(\Gamma) = \sum_i \prod_{L \in \mathcal{L} T_i} y_L \tag{4.2}$$

where the product in (4.2) runs over all lines of T_i.

Another method to compute $\Delta(\Gamma)$ is to make use of the recurrence relation of Brooks *et al.*[7,4]:

$$\Delta(\Gamma) = \Delta(\Gamma^{(L)}) + y_L \Delta(\Gamma_{(L)}) \tag{4.3}$$

where $\Gamma^{(L)}$ is the graph with $(k + 1)$ points and $(l - 1)$ lines obtained from Γ by deleting line L, *and* $\Gamma_{(L)}$ is the graph with k points and $(l-1)$ lines obtained by contracting line L (i.e., by identifying its two end points).

The number of graphs that must be generated, when using formulas (4.2) or (4.3), rapidly becomes very large as the number of points and lines are increased. For example, if we use (4.2), we must generate $(k + 1)^{k-1}$ trees for the complete graph K_{k+1}, and more than $(l/k)^k$ trees for a uniformly coverable graph.[3b] If we use (4.3), the total number of graphs generated in the process can be estimated to be of order a^k, where a is the average number $k^{-1}\Sigma_i l_i'$ (this is exact if all the l_i' are equal) $l_i' = l_i - (k-i)$, where l_i is the number of lines of the graph obtained from Γ after contracting i lines.

On the other hand, the star-mesh transformation given in Lemma 3.1 generates only k 1-graphs and, more generally, k n-graphs. Therefore, it is much more convenient than (4.2) and (4.3) to compute Gaussian n-graphs by hand, as can be seen in Fig. 2. It must be noted that the star-mesh

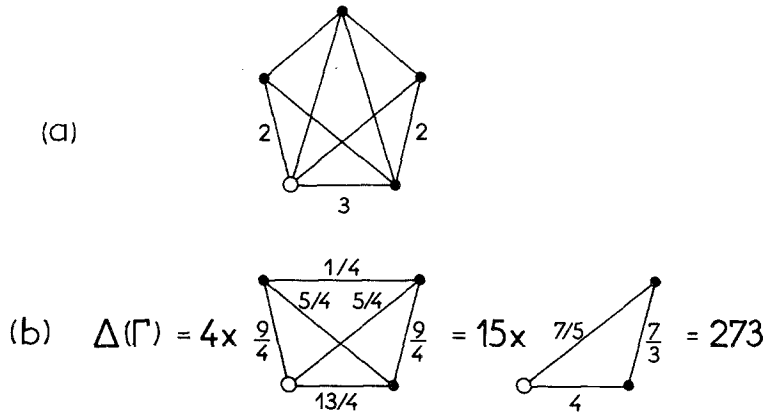

Fig. 2. The determinant $\Delta(\Gamma)$ associated to the 1-graph (a) is computed in (b) by means of the star-mesh transformation. To compute it by the recurrence method of Brooks *et al.*, we would have to draw about 20 graphs, and by Kirchhoff's method, 75 spanning trees.

transformation is not always advantageous in electrical network theory, as compared to Kirchhoff's method, because the weights are *variable* (the graph being considered as *fixed*). On the other hand, in statistical mechanics the weights are *constant* (the graph describing the set of *all the graphs* of a certain type: connected, irreducible, etc.), and the star-mesh transformation is then very efficient.

5. USE OF GAUSSIAN n-GRAPHS TO TEST QUANTITATIVELY THE ACCURACY OF OUR ESTIMATION METHOD

Let us consider the 4-graph $\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_4)$ of Fig. 3a. It occurs in the development of the 4-body correlation function, in the coefficient of the fifth power of the density. It occurs also in other problems, for example in the scattering of particles associated with a self-interacting field with ϕ^4 interaction (see Fig. 3b).

The covering of Fig. 3c gives the canonical bound[2]:

$$\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_4) \leqslant \left[C_4(r_{12}) C_5(r_{12}) C_4(r_{13}) C_2(r_{14}) C_2(r_{23}) C_2(r_{24}) C_2(r_{34}) C_6(r_{34}) \right]^{1/4} \tag{5.1}$$

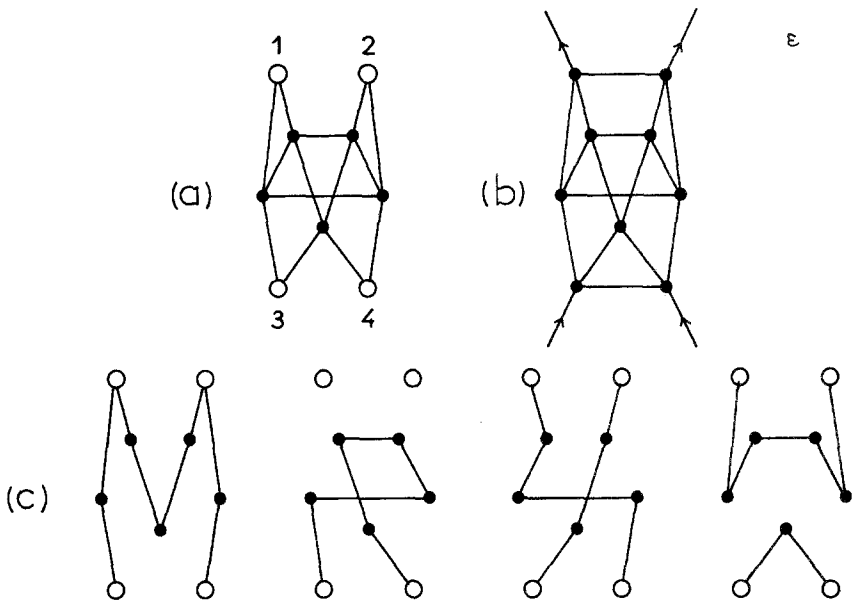

Fig. 3. The 4-graph (a) occurs in the development of the 4-body correlation function, and as a component of the diffusion graph (b). The subgraphs of (c) make a covering of (a).

where $C_m(r_{ij})$ denotes the chain with m lines $f^2(r)$ and end points i and j. $C_m(r)$ can be computed by Fourier transform[13]:

$$C_m(r) = \frac{1}{2\pi^2} \int_0^\infty \left[f^2(k) \right]^m \frac{k}{r} \sin kr \, dk \tag{5.2}$$

with

$$f^2(k) = 4\pi \int_0^\infty \frac{r}{k} f^2(r) \sin kr \, dr \tag{5.3}$$

$C_m(r)$, and thus the upper bound (5.1), can be computed easily for any line. For example, for the Debye–Hückel model of ionized gases (or when ϕ is a three-dimensional field of unit mass), we have $f(r) = e^{-r}/r$, and so

$$C_m(r) = \frac{(4\pi)^m}{2\pi^2 r} \int_0^\infty \left(\frac{1}{k} \arctan \frac{k}{2} \right)^m k \sin kr \, dk \tag{5.4}$$

With lines $f(r) = e^{-r}/r$ or other lines of realistic models, the 4-graph $\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_4)$ is far too complicated to be computable with present-day computers. Therefore, to test the accuracy of (5.1), we resort to the Gaussian model. $\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_4)$, computed by the star-mesh transformation, yields (see Fig. 4).

$$\Gamma(\mathbf{r}_1, \ldots, \mathbf{r}_4) = 6.415 \times 10^{-5} \exp\left[-(0.327 r_{12}^2 + 0.298 r_{13}^2 + 0.548 r_{14}^2 + 0.548 r_{23}^2 + 0.298 r_{24}^2 + 0.473 r_{34}^2) \right] \tag{5.5}$$

and the upper bound (5.1) is equal to

$$B(\mathbf{r}_1, \ldots, \mathbf{r}_4) = 16.57 \times 10^{-5} \exp\left[-(0.225 r_{12}^2 + 0.125 r_{13}^2 + 0.250 r_{14}^2 + 0.250 r_{23}^2 + 0.167 r_{24}^2 + 0.333 r_{34}^2) \right] \tag{5.6}$$

(5.6) overestimates the value of (5.5) at the origin by a factor 2.6, and the coefficients of r_{ij}^2 by factors lying between 1.4 and 2.4. This shows that the particular estimate (5.1) has a correct order of magnitude for small-to-intermediate distances.

Upper bounds obtained by means of chains will be studied systematically elsewhere. We note here that such bounds give indications on the rate of decay of n-graphs at large distances or, equivalently, on the location of poles of their Fourier transforms (i.e., Feynman graphs in momentum space), since the rate of decay of chains can usually be easily determined from (5.2).

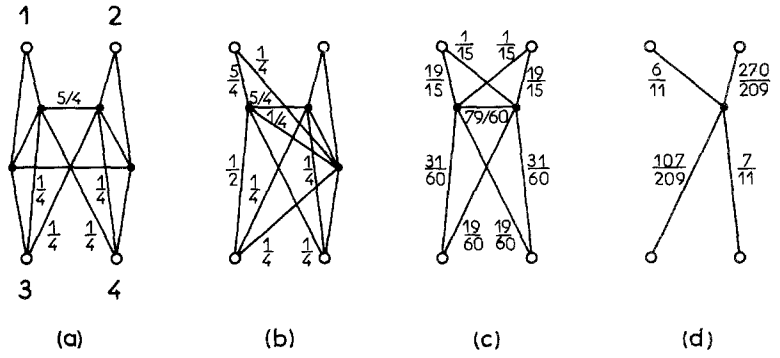

Fig. 4. Computation of the 4-graph of Fig. 4a by successive application of the star-mesh transformation. The additional factors are $4^{-d/2}\exp[-(1/4)r_{34}^2]$ for (a); $16^{-d/2}\exp-[(1/4)r_{13}^2+(1/4)r_{34}^2]$ for (b); $60^{-d/2}\exp-[(1/15)r_{12}^2+(4/15)r_{13}^2+(1/15)r_{14}^2+(1/15)r_{23}^2+(4/15)r_{24}^2+(19/60)r_{34}^2]$ for (c); $209^{-d/2}\exp-[(1/11)r_{12}^2+(5/11)r_{13}^2+(2/11)r_{14}^2+(16/209)r_{23}^2+(3/11)r_{24}^2+(4/11)r_{34}^2]$ for (d). The final result is $(624)^{-d/2}\exp-[(17/52)r_{12}^2+(57/104)r_{13}^2+(31/104)r_{14}^2+(31/104)r_{23}^2+(57/104)r_{24}^2+(295/624)r_{34}^2]$.

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