Substituting for Q, we obtain

$$\tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\Sigma}} = -\tfrac{1}{2} \pm (\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}}$$

or

$$(\tfrac{1}{2} + \tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\Sigma}}) = \pm(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}}. \tag{A6}$$

Again,

$$\begin{aligned}(\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}})(\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}}) &= (\Sigma_1^2 + \Sigma_2^2 - \Lambda_3^2) - \tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\Sigma}} \\ &= (-\tfrac{3}{4} - \mathcal{C}) - (Q - \mathcal{C} - \tfrac{3}{4}),\end{aligned} \tag{A7}$$

since

$$\begin{aligned}C_0 = -\tfrac{3}{4} &= \boldsymbol{\Sigma}^2 - \boldsymbol{\Lambda}^2 \\ &= (\Sigma_3^2 - \Lambda_1^2 - \Lambda_2^2) - (\Lambda_3^2 - \Sigma_1^2 - \Sigma_2^2).\end{aligned}$$

Equation (A7) may be written as

$$(\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}})(\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}}) = -Q,$$

since

$$\begin{aligned}(-\tfrac{1}{2} + \tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}})(-\tfrac{1}{2} - \tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}}) &= \tfrac{1}{4} - (\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}})(\tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}}) \\ &= \tfrac{1}{4} + Q \\ &= [(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} \pm \tfrac{1}{2}]^2.\end{aligned} \tag{A8}$$

Note further that $\frac{1}{2} + \tilde{\boldsymbol{\sigma}} \cdot \tilde{\boldsymbol{\Sigma}}$ contributes to the diagonal elements of the mass matrix, whereas $-\frac{1}{2} + \tilde{\boldsymbol{\tau}} \cdot \tilde{\boldsymbol{\Lambda}}$ contributes to the off-diagonal ones. Thus the matrix $\tilde{m}$ can be written as

$$\tilde{m} = \begin{pmatrix} i(m_0 - m_1) + im_1(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} & im_1[(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} - \tfrac{1}{2}] \\ -im_1[(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} + \tfrac{1}{2}] & -i(m_0 - m_1) + im_1(\mathcal{C} + \tfrac{1}{4})^{\frac{1}{2}} \end{pmatrix}.$$

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† Present address: Department of Physics and Astrophysics. University of Delhi, Delhi, India.

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Convolution Approximation for the n-Particle Distribution Function

F. Y. Wu*
Department of Physics, Northeastern University, Boston, Massachusetts 02115

AND

M. K. Chien
Department of Physics, University of Maryland, College Park, Maryland 20740

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The convolution approximation introduced by Jackson and Feenberg for the 3-particle distribution function is extended to the n-particle distribution function g_n. It is shown that the generalized convolution form satisfies the limiting and the recursion relations connecting g_n and g_{n+1}.

I. INTRODUCTION

An important problem in the quantum mechanical and statistical consideration of many-particle systems is the approximation of the n-particle correlation function g_n by lower-order ones, usually the pair distribution function g_2. Many years ago, Kirkwood[1] introduced in the theory of classical fluid the superposition approximation for the 3-particle distribution function. The idea of superposition has been widely accepted and its extension to the n-particle distribution function has also been used.[2] An alternate approximation for the 3-particle distribution function, the convolution form, was proposed by Jackson and Feenberg[3] in the correlated basis function (CBF) approach to the theory of quantum fluids. The convolution form has proven to be more convenient to use in the evaluation of matrix elements occurring in the CBF formalism. In the evaluation of the excitation spectrum of He II, for example, the convolution form largely reduces the amount of numerical works while yielding results comparable to those obtained using the superposition approximation.[3] Similar simplifications have also been observed in its application to the theory of fermion liquids.[4,5] In the further perturbative treatments in the CBF formalism, convolution forms of higher-distribution functions are also needed. Thus Lee[6] has obtained and used the convolution form of g_4 to compute the second-order correction to the excitation spectrum of He II. More recently, calculations have been carried out for liquid ^{3}He and ^{3}He–^{4}He mixtures with partial contributions from g_5 and g_6 included.[7] It would then be of practical as well as theoretical interests to extend the previous results on the convolution approximation. Lee[6] used intuitive reasonings to generate the convolution form of g_4. However, we find it very difficult to go further beyond in the absence of precise statement of generalization. It is the purpose of the present paper to make the rule precise and generalize the convolution approximation to the n-particle distribution function.

II. PRELIMINARIES

Consider a system of N identical particles confined in a volume Ω. The thermodynamic limit $N \to \infty$, $\Omega \to \infty$ will be taken, if necessary, with the density $N/\Omega = \rho$ kept constant. We define as usual[8] the n-particle distribution function

$$g_n(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) = \frac{N!}{(N-n)!}\rho^{-n}\frac{\int W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)\, d\mathbf{r}_{n+1}\cdots d\mathbf{r}_N}{\int W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)\, d\mathbf{r}_1\cdots d\mathbf{r}_N}, \tag{1}$$

with $W(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n)$ a function symmetric in the coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$. Explicitly, we have

$$W = \exp\,[-V(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)/kT], \quad \text{for a classical system,}$$
$$= |\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2, \quad \text{for a quantal system.}$$

Here V is the total potential energy and ψ the wavefunction describing the system. Physically,

$$\Omega^{-n} g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)$$

is the probability density function for n ($\ll N$) particles to situate at $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$.

Some implications now follow as consequences of the definition. It is clear that $g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ is nonnegative, symmetric in its n coordinates, and vanishes for strongly interacting systems when two particle coordinates coincide. The definition (1) also implies the recursion relation

$$\rho\int g_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1})\, d\mathbf{r}_{n+1} = (N-n) g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \tag{2}$$

and hence the normalization condition

$$\rho^n\int g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n)\, d\mathbf{r}_1\cdots d\mathbf{r}_n = \frac{N!}{(N-n)!}. \tag{3}$$

Furthermore, taking a particle to infinity is equivalent to removing one particle from the system. As a consequence, we expect the limiting condition

$$\lim_{r_{n+1}\to\infty} g_{n+1}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) = g_n(\mathbf{r}_1, \cdots, \mathbf{r}_n) \tag{4}$$

to hold. Any approximate form for the n-particle distribution function should be tested against these necessary conditions.

For a uniform system, we expect g_1 to be a constant. Normalization then requires

$$g_1(\mathbf{r}) = 1. \tag{5}$$

We also expect the pair distribution function g_2 to depend on the distance $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ only. We define the f function as

$$f_{12} = f(r_{12}) = g_2(r_{12}) - 1. \tag{6}$$

The normalization condition (3) then implies the following conditions on f:

$$\rho\int f(r)\, d\mathbf{r} = -1, \tag{7}$$

$$f(\infty) = 0. \tag{8}$$

In the following discussions, f is assumed to satisfy both (7) and (8).

The Kirkwood superposition approximation[1] $g_3^{(s)}$ for the 3-particle distribution function is

$$g_3^{(s)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = g_2(r_{12})g_2(r_{23})g_2(r_{31}). \tag{9}$$

This approximate form satisfies most of the necessary conditions on g_3 except the recursion and the normalization relations (2) and (3). In fact, explicit evaluations using (7) yield the results

$$\rho\int g_3^{(s)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\, d\mathbf{r}_3 = g_2(r_{12})\left(N - 2 + \rho\int f_{13}f_{23}\, d\mathbf{r}_3\right) \tag{10}$$

and

$$\rho^3 \int g_3^{(s)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)\, d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3$$
$$= N(N-1)(N-2) - N + \rho^3 \int f_{12} f_{23} f_{31}\, d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3. \quad (11)$$

The remainder term in (10) is deceptively small and, as it turns out, proves to be of primary importance in applications.[3] The generalized superposition form for the n-particle distribution function,

$$g_n^{(s)}(\mathbf{r}_1, \cdots, \mathbf{r}_n) = \prod_{1 \le i < j \le n} g_2(r_{ij}), \quad (12)$$

also fails to meet the requirements (2) and (3).

An alternate approximation of g_3 which exactly satisfies the recursion and the normalization relations is the convolution form[3]

$$g_3^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = 1 + f_{12} + f_{23} + f_{31} + f_{12}f_{23} + f_{23}f_{31} + f_{31}f_{12} + \rho \int f_{14}f_{24}f_{34}\, d\mathbf{r}_4. \quad (13)$$

It is easy to see that $g_3^{(c)}$ is symmetric in the particle coordinates and satisfies the recursion and the limiting conditions (2) and (4). However, it fails in the other tests. Namely, $g_3^{(c)}$ is not necessarily nonnegative and the approximation is poor for strongly interacting systems when the particle coordinates are close. But these are not critical objections in view of its convenience in applications. In fact, it is not known in actual calculations which approximation using $g_3^{(s)}$ or $g_3^{(c)}$ is more accurate.[3] With nothing better available, the convolution form remains a useful approximation in evaluating integrals involving nonsingular operators. Lee[6] has extended the convolution form to g_4 and obtained the explicit expression of $g_4^{(c)}$ which yields $g_3^{(c)}$ upon integrating over one particle coordinate. In the next section we shall generalize further to the n-particle distribution function. The resulting form is a generalization of the known expressions of $g_3^{(c)}$ and $g_4^{(c)}$ and satisfies both the recursion and the limiting relations (2) and (4).

III. CONVOLUTION APPROXIMATION FOR g_n

It is convenient to introduce a diagrammatic representation which will facilitate our discussions. We first give some definitions in the language of linear graphs.[9]

A linear graph is a collection of points with lines joining certain pairs of points. Examples of linear graphs are given in Fig. 1. A graph is said to be disconnected if it is possible to separate the points of the graph into two or more groups such that there is no line joining a point of one group with a point of the other. Otherwise the graph is said to be connected. Thus, Fig. 1(a) is disconnected and Figs. 1(b), 1(c) are connected. A line successively joining a set of points is called a path. If the final and the initial points of a path coincide, we speak of a cycle. For instance, points 2, 3, and 4 in Fig. 1(c) form a cycle. A Cayley tree is a connected linear graph containing no cycles. Figure 1(b) is an example of a Cayley tree. An isolated (unconnected) point is also a Cayley tree. The number of lines incident at each point is called the degree of the point. Therefore, the degree of the black point in Fig. 1(b) is three, and the degrees of all other points in the same graph are all one. If a point of the graph is given a numerical label, $1, 2, \cdots$, we call this point a root point and speak of a rooted graph. In the following, all root points will be denoted by open circles or open points, and all unlabeled points by black circles or black points, as shown in Fig. 1.

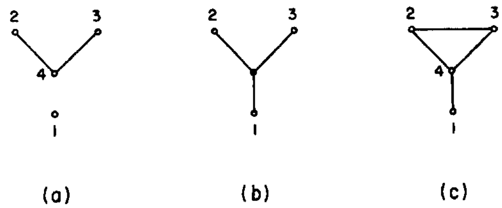


FIG. 1. Examples of linear graphs.

A diagrammatic representation for mathematical expressions is now in order. A factor f_{ij} is represented by a line joining two points with labels i and j. The point i is a black one if the coordinate $\mathbf{r}_i$ appears as the integration variable under an integral sign; otherwise it is an open point. In other words, a black point represents a factor $\rho \int d\mathbf{r}_k$ with the label k deleted from the graph. All isolated open points are taken to represent a numerical factor of 1. Thus, the graphs of Fig. 1 represent the following expressions:

$$f_{24}f_{34}, \qquad \text{for Fig. 1(a)},$$

$$\rho \int f_{14}f_{24}f_{34}\, d\mathbf{r}_4, \qquad \text{for Fig. 1(b)},$$

$$f_{14}f_{42}f_{23}f_{34}, \qquad \text{for Fig. 1(c)}.$$

As another example, the convolution approximation $g_3^{(c)}$ for the 3-particle distribution function given by (13) has the diagrammatic representation of Fig. 2.

In these notations, we now define the convolution approximation $g_n^{(c)}$ for the n-particle distribution

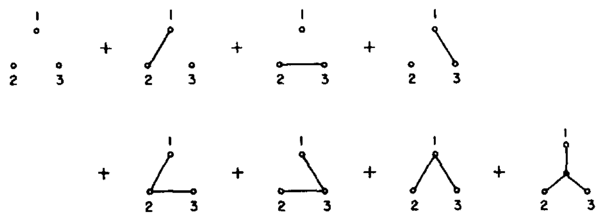


FIG. 2. Diagrammatic representation of the convolution approximation $g_3^{(c)}$ given by Eq. (13).

function as

$g_n^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) =$ the collection of all distinct graphs of rooted Cayley trees (connected and disconnected) with each graph consisting of n root points, labeled $1, \cdots, n$, and any number of unlabeled points provided that the degree of each unlabeled point is at least three. (14)

Clearly, $g_n^{(c)}$ is symmetric in the coordinates $\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n$. We now show that $g_n^{(c)}$ satisfies the limiting relation

$$\lim_{r_{n+1}\to\infty} g_{n+1}^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1}) = g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n) \quad (15)$$

and the recursion relation

$$\rho \int g_{n+1}^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_{n+1})\, d\mathbf{r}_{n+1} = (N - n) g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (16)$$

It is convenient to classify the graphs of $g_{n+1}^{(c)}$ according to the connectivity of the root point with the label $n + 1$ [the $(n + 1)$th root point]. We write

$$g_{n+1}^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_{n+1}) = G_1 + G_2 + G_3 + G_4, \quad (17)$$

where

$G_1 =$ the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is isolated,

$G_2 =$ the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is connected to precisely one open point,

$G_3 =$ the collection of graphs of $g_{n+1}^{(c)}$ in which the $(n + 1)$th root point is connected to precisely one black point,

$G_4 =$ the remaining graphs of $g_{n+1}^{(c)}$ in which the degree of the $(n + 1)$th root point is at least two.

First we note that G_1 contains precisely the graphs of $g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n)$ with the addition of isolated $(n + 1)$th root points. Since all isolated root points represent the same numerical factor 1, we then recognize the identity

$$G_1 = g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (18)$$

Now, G_2, G_3, and G_4 contain all graphs in which the $(n + 1)$th root point is connected. It follows then from (8) that all graphs of G_2, G_3, and G_4 vanish on taking the limit $r_{n+1} \to \infty$. Only G_1 survives on the left-hand side of (15) and this completes the proof of the limiting relation.

To prove the recursion relation (16), we note that the integration over an isolated point simply yields a numerical factor $\rho \int d\mathbf{r} = N$. Hence from (18) we have

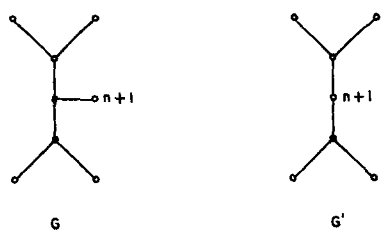
$$\rho \int G_1\, d\mathbf{r}_{n+1} = N g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (19)$$

Next, since G_2 contains all rooted Cayley trees in which the $(n + 1)$th root point is connected to precisely one root point, one may generate *all* graphs of G_2 by joining in graphs of G_1 the $(n + 1)$th root point to one of the n other root points. In fact, by joining to the n other root points in succession, n different graphs of G_2 are generated from a given graph of G_1. However, because of (7), these n graphs are all equivalent upon integrating over $d\mathbf{r}_{n+1}$. It follows then, using (7),

$$\rho \int G_2\, d\mathbf{r}_{n+1} = -nG_1 = -n g_n^{(c)}(\mathbf{r}_1, \cdots, \mathbf{r}_n). \quad (20)$$

We remark that we have, in the above, used the fact that G_1, or $g_n^{(c)}$, contains the collection of *all* rooted Cayley trees with n root points so that all graphs of G_2 are generated from G_1. Finally, we note that there exists a one-to-one correspondence between the graphs of G_3 and G_4. For each graph G of G_3, we may generate a graph G' of G_4 by first removing the $(n + 1)$th root point in G and then converting the black point originally connected to this $(n + 1)$th point into a root point with the label $n + 1$. Since the degree of the original black point is at least three, the degree of the new root point will be at least two and the resulting graph will certainly be contained in G_4. Conversely, for each graph of G_4, a unique graph of G_3 can be generated by the reversing process. An example of this correspondence is shown in Fig. 3. Now the integration over $\rho \int d\mathbf{r}_{n+1}$ simply changes the $(n + 1)$th root point into a black point in G' and

FIG. 3. An example of the one-to-one correspondence between graphs $G \in G_3$ and $G' \in G_4$. All labels of the root points have been deleted in G and G' except the label $n + 1$.



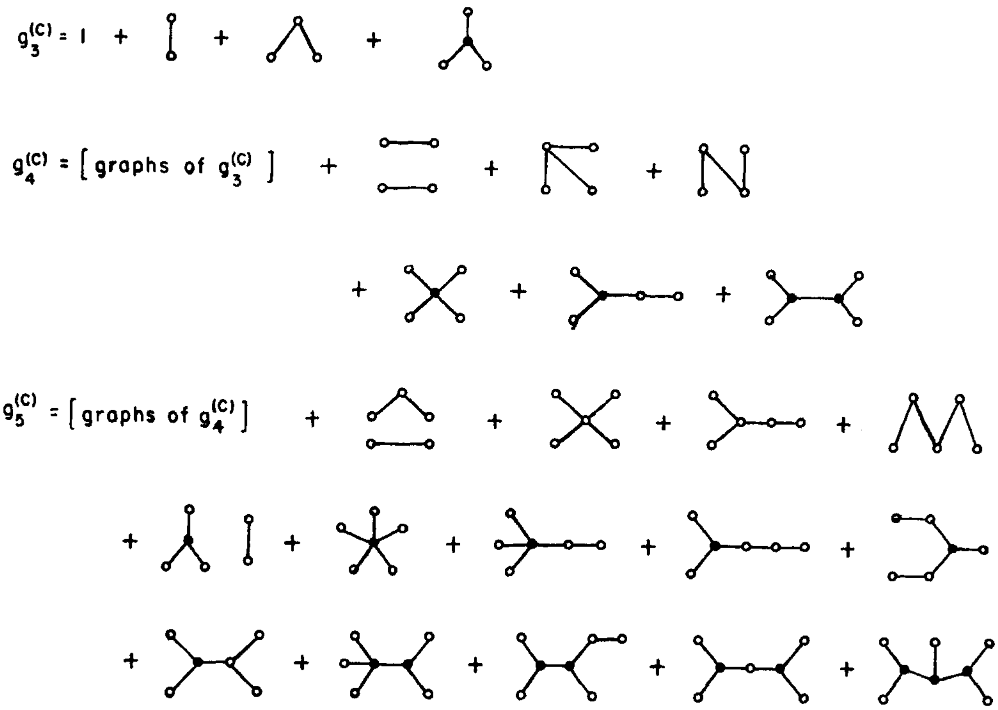


FIG. 4. A compact diagrammatic representation of $g_3^{(c)}$, $g_4^{(c)}$, and $g_5^{(c)}$. Only the topologically distinct graphs are included with all the labels and isolated points deleted.

removes the $(n+1)$th root point in G, the following relation between G and G' then follows from (7):

$$\rho \int G \, d\mathbf{r}_{n+1} = -\rho \int G' \, d\mathbf{r}_{n+1}$$

or

$$\rho \int (G + G') \, d\mathbf{r}_{n+1} = 0.$$

The one-to-one correspondence of the graphs of G_3 and G_4 then ensures

$$\rho \int (G_3 + G_4) \, d\mathbf{r}_{n+1} = 0. \tag{21}$$

The recursion relation (16) now follows as a result on combining (19)–(21).

IV. CONCLUSION

We have shown that the convolution approximation of the n-particle distribution function given by (14) satisfies the limiting relation (15) and the recursion relation (16). The explicit expressions of $g_3^{(c)}$, $g_4^{(c)}$, and $g_5^{(c)}$ are collected in Fig. 4 in a more compact graphical notation in which only the topologically distinct graphs are shown with all labels and isolated points deleted.[10] For example, all the $\binom{n}{2}$ terms of the form f_{ij} are represented by a single graph. Thus the 4 graphs of $g_3^{(c)}$ represent a total of 8 terms, the 10 graphs of $g_4^{(c)}$ represent 58 terms and the 24 graphs of $g_5^{(c)}$ represent a total of 617 terms. In this simplified notation, the expression (14) for $g_n^{(c)}$ can be rewritten as

$g_n^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_n) =$ the collection of all distinct graphs of connected and disconnected Cayley trees excluding isolated points and consisting of n or less open points and any number of black points, provided that the degree of each black point is at least three.

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