tions to the state function $H(\sigma)$, depending on the state of the preshock gas:

$$\beta_c^2=\tfrac{2}{3}, \quad \text{region I} \tag{3.18}$$

$$\beta_c^2=4/9, \quad \text{region II} \tag{3.19}$$

$$\beta_c^2=\tfrac{1}{3}, \quad \text{region III.} \tag{3.20}$$

Since the signal speed for a gas in region III is $\beta_s^2=\frac{1}{3}$, all shocks into a relativistic gas are above the critical speed.

This special case is also characterized by the fact that $\theta_0=\theta_1$. This is most readily seen from combination of Eqs. (2.7), (2.9), and (2.12) at the equilibrium points, which gives the jump equation

$$\gamma_0 H_0=\gamma_1 H_1. \tag{3.21}$$

The phase-plane plot for this case is shown in Fig. 4. It is clear that case B2 applies here, since $d\theta/dx$ must be 0 at some point in the shock.

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Calculation of the Yang-Lee Distribution of Zeros

EERO BYCKLING
Department of Technical Physics, Institute of Technology, Otaniemi, Finland

(Received 1 June 1965)

The connection between the zeros of the grand partition function Z and the function $\chi=\lim V^{-1}\ln Z$ at infinite volume is discussed. Assuming a functional equation for χ given, conditions for the lines containing zeros and an expression for the density of zeros are derived. Explicit results are given in a special case with an attractive interaction potential.

INTRODUCTION

It is known that Yang and Lee based their phase-transition theory[1] on the observation that, if the zeros of the grand partition function $Z(z)$ in the limit of infinite volume have an accumulation point at a positive real value z_0 of the fugacity, some thermodynamic functions are discontinuous at z_0. For all thermodynamic systems which so far have yielded to an explicit solution,[2] the zeros fall on definite lines C in the complex z plane and become dense on C at $V\to\infty$. If this turns out to be a general feature of thermodynamic systems, phase-transition points z_0 are determined as the points of intersection of C and the positive real z axis. The nature of a transition is governed by the density of zeros on C near z_0.

Only in trivial cases is it possible to find the roots of $Z(z)=0$ directly, because when the number of particles N becomes large, $Z(z)$ is an extremely complicated polynomial of degree of the order of N. In certain cases, however, it is possible to find a functional equation, the solution of which is the limit of $V^{-1}\ln Z$ for $V\to\infty$. In this paper we consider the relation between the distribution of zeros and the solutions of an equation of this type. It is found that under certain conditions the lines of zeros are uniquely determined. An expression is derived for the density of zeros in terms of the limit function.

[1] C. N. Yang and T. D. Lee, Phys. Rev. **87**, 404 (1952).
[2] T. D. Lee and C. N. Yang, Phys. Rev. **87**, 410 (1952); E. H. Hauge and P. C. Hemmer, Physica **29**, 1338 (1963); P. C. Hemmer and E. H. Hauge, Phys. Rev. **133**, A1010 (1964).

As an application of the method the distribution has been explicitly solved in the case of a linear model with potential consisting of hard core and square-well attraction. The main features of the results are shown graphically.

ANALYTIC CONTINUATION OF $\chi'(z)$

We assume that in the limit $V\to\infty$ all the zeros of $Z(z,V,T)$ fall on definite smooth lines C in the complex z plane, and are dense on C. Denoting the number of zeros on the line element ds at $z=z(s)$ by $Vg(s)ds$, s being a real parameter taken along C, we have

$$\chi(z)=\lim_{V\to\infty}\frac{1}{V}\ln Z(z,V)=\int_C ds g(s)\ln\left(1-\frac{z}{z(s)}\right). \tag{1}$$

The derivative of $\chi(z)$ is

$$\chi'(z)=\int_C ds\frac{g(s)}{z-z(s)}. \tag{2}$$

Along the curve C we have $dz=dse^{i\phi(s)}$, where $\phi(s)$ is the argument of the tangent of C at the point $z(s)$. Define

$$G(z(s))=g(s)e^{-i\phi(s)}.$$

The real variable s can now be replaced by the complex variable, and Eq. (2) becomes

$$\chi'(z)=\int_C dt\frac{-G(t)}{t-z}. \tag{3}$$

An integral of this type is called a Cauchy integral.[3]

If $g(s)$ and thus $G(z)$ is an analytic function on C except at a finite number of points ζ_j, and fulfills some obvious integrability conditions, the function $\chi'(z)$ exists and is a finite continuous function outside C. If the particles have a hard core, there is a maximum number of particles $M(V)$ that can be accommodated inside V. The quantity

$$\int_C ds\, g(s)=\lim_{V\to\infty}\frac{M(V)}{V}$$

is then finite and guarantees the integrability of $G(t)/(z-t)$. Finiteness of the integral of $g(s)$ is, however, not necessary for the existence of a finite $\chi'(z)$ everywhere outside C. The condition of a hard-core part in the potential can thus be relaxed as has been previously noted by Hauge and Hemmer.[2] Except at the singular points ζ_j, the derivative $\chi'(z)$ has finite limiting values as z approaches a point t on C from the left and from the right. If $G(t)$ does not vanish, these are unequal.

When z is real and positive, $\chi(z)$ and $\chi'(z)$ have a direct physical meaning given by

$$p/kT=\chi(z),$$

and

$$\rho=N/V=z(\chi'(z)). \tag{4}$$

Under our assumptions the transitions will be of the Yang-Lee type.[1] On the positive real z axis $\chi(z)$ is everywhere continuous and its derivatives are continuous except at a finite number of points.

Now let C_1 be a portion of C located between two points ζ_1 and ζ_2 and containing no other points ζ_j. One or both of the ends can lie at infinity. Call R_1 and R_2 two regions separated by C_1, and let $\chi_1'(z)$ and $\chi_2'(z)$ be the values of the function (3) in the two regions. Because of the analyticity of $G(z)$ the function $\chi_1'(z)$ can be analytically continued across C_1 into R_2 and similarly for $\chi_2'(z)$ into R_1. The discontinuity of the derivative $\chi_1'(z)-\chi_2'(z)$, is now found modifying the path of integration slightly as in Fig. 1. For a point z inside $C_1-\bar{C}_1$ we have

$$\chi_1'(z)-\chi_2'(z)=\int_{\bar{C}_1} dt\frac{-G(t)}{t-z}-\int_{C_1} dt\frac{-G(t)}{t-z}.$$

Applying the residue theorem into the integration over the closed path $C_1-\bar{C}_1$ we get after shrinking this path into a point

$$G(z)=-(2\pi i)^{-1}[\chi_1'(z)-\chi_2'(z)]. \tag{5}$$

The function of $G(z)$ was defined on C and thus Eq. (5) has a meaning only for a point z on the line C_1. It gives the difference between the values $\chi'(z)$ as z is approached from the two sides of C_1. After the analytic continuation of $\chi_1'(z)$ and $\chi_2'(z)$ has been performed, Eq. (5) defines a function $\hat{G}(z)$ in the region R_1+R_2. It is clearly an analytic continuation of $G(z)$ outside C_1.

Suppose now that the analytic continuation of all the contitutuents $\chi_k'(z)$ of the single-valued function $\chi'(z)$ have been effected. As a result there are one or several multiple-valued functions $\hat{\chi}_\nu'(z)$, which are continuous analytic functions in the whole z plane, except possibly at the points ζ_j which may be their branch points. Especially, if the z plane remains singly connected when cut along the lines C, the result of the analytic continuation is a single function $\hat{\chi}'(z)$. The integrals $\hat{\chi}_\nu(z)$ of $\hat{\chi}_\nu'(z)$ are the analytic continuations of the functions $\chi(z)$ in the different regions.

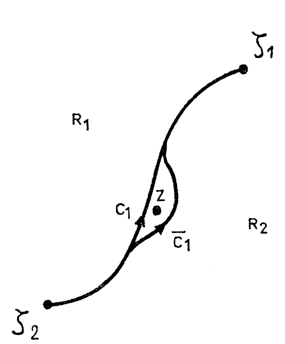

FIG. 1. Analytic continuation across the line C_1.

[3] N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff N. V., Groningen, 1953).

CONDITIONS FOR THE LINES OF ZEROS

Assume now that the limit function (1) fulfills a functional equation

$$F(\chi,z)=0. \tag{6}$$

Note, especially, that if the equation of state $p=p(\rho)$ of the system is given, substitution of Eqs. (4) yields an equation for χ, χ', and z. Integration then gives an equation of the form (6). Equation (6) is understood to be fulfilled by $\chi(z)$ at any complex value z in addition to the physically meaningful real and positive values. In the above case the equation of state $p=p(\rho)$ gives, through Eqs. (4) a unique equation (6) and thus a unique set of solutions once we assert its validity for complex z. In actual calculations the algebraic steps leading to the equation of state are usually automatically valid for complex values of z.

An equation of the type (6) has as solutions one or several functions, which are analytic functions in the whole z plane, except at isolated branch points given by $dz/d\chi=0$. As a simple example the equation

$$\chi^3-z\chi^2-z\chi+z^2=0$$

has the solutions $\chi_1=z$ and $\chi_2=z^{1/2}$, which have one- and two-sheeted Riemann surfaces, respectively, and the second has the origin as a branch point. Now in general because a solution of Eq. (6) is identical to the function (1) in a region of the z plane, the complete solutions of (6) are the analytic continuations $\hat{\chi}_\nu(z)$ which were discussed in the previous section.

One is then led to consider a procedure inverse to the one discussed in the previous section. A solution of Eq. (6) can be made to be single valued by cutting the z plane open along certain lines C and choosing a definite branch $\chi_k(z)$ of one of the $\hat{\chi}_\nu(z)$ for each of the ensuing connected regions. Because it is assumed that $\chi(z)$ fulfills Eq. (6), there is a set of boundaries C and a choice of branches $\chi_k(z)$ such that the previously defined single-valued function is identical with $\chi(z)$ in the whole z plane.

Assume that definite C and $\chi_k(z)$ have been chosen. Then the derivative $\chi'(z)$ is everywhere defined, and is analytic outside C. Take

$$G(z)=-(2\pi i)^{-1}[\chi_l'(z)-\chi_r'(z)] \tag{7}$$

to describe the discontinuity of $\chi'(z)$ from left to right at z on C. Further, let the expansion of $\chi'(z)$ for large $|z|$ be of the form

$$\chi'(z)=A_k z^k+A_{k-1}z^{k-1}+\cdots;$$

$\chi'(z)$ is said to be of the degree k at infinity.

It can be shown (see, e.g., Ref. 3, p. 229) that the analytic function with given discontinuities on the lines C and of degree $k(\geqq -1)$ at infinity is uniquely determined apart from a polynomial of degree k. We have then

$$\chi'(z)=\int_C dt\frac{-G(t)}{t-z}+P_k(z). \tag{8}$$

The polynomial $P_{-1}(z)$ is by definition identically zero. In order that a set of cuts C and a choice of branches $\chi_k'(z)$ will make $\chi'(z)$ single valued, it is required that all the branch points included in the chosen regions of the Riemann surfaces lie on the boundary lines C. The resulting function $\chi'(z)$ with described discontinuities is of the form (8). When C and the $\chi_k(z)$ have been chosen to give (3), the polynomial $P_k(z)$ vanishes identically. Further, the quantity

$$g(s)ds=G(z)dz, \tag{9}$$

where dz is along the tangent of C at $z=z(s)$, is the number of roots in the interval ds. It must then be real and positive.

The preceding discussion and the interpretation of $\chi(z)$ give the following set of conditions for the determination of the lines C. (1) The branch points must lie on C. (2) Near the origin the branch $\chi_k(z)$ must be chosen giving $\chi=0$ for $z=0$. (3) On the positive real axis $\chi(z)$ is continuous. (4) The quantity $G(z)dz$ along C must be real and positive.

Whether these conditions give a unique solution in the general case cannot be answered without specifying Eq. (6) more closely. It is to be noted that a cut in a single Riemann surface between two branch points is uniquely determined, requiring that the quantity (9) be real. Once the cuts have been found, the density of zeros on C is given directly by Eqs. (7) and (9).

EXPLICIT RESULTS WITH ATTRACTIVE POTENTIAL

As an illustration we consider the linear system with only nearest-neighbor interaction. The relation between pressure and fugacity is given by[4]

$$z\int_0^\infty dr\frac{\partial}{\partial r}[e^{-u(r)/kT}]e^{-\chi r}=\chi. \tag{10}$$

This gives immediately the inverse function $z=z(\chi)$. This equation can be derived by the matrix method,[5] i.e., by dividing the system into segments of length a, and setting up a matrix, the nth power of which accounts for all possible configurations in a system of length na. Let the range of the potential be ha. The eigenvalues λ of the matrix are found to be given by

$$\lambda^h-\lambda^{h-1}-za\sum_{\nu=0}^{h}[e^{-u(\nu a+a)/kT}-e^{-u(\nu a)/kT}]\lambda^{h-\nu}=0.$$

In the limit $a\to 0$ this gives Eq. (10), when one notices that the largest eigenvalue is $\lambda=e^{a\chi}$. This serves as an example of the fact that the reality of z is usually nowhere required in calculations of $\chi(z)$.

To be able to carry out explicit computations we choose a definite form for $u(r)$, the square-well potential with infinite repulsion for $r<d$, and square well of depth $-\epsilon$ for $d<r<2d$. Measuring χ and z in units $1/d$, we find

$$z=\chi/[Ee^{-\chi}-(E-1)e^{-2\chi}], \tag{11}$$

where $E=e^{-\epsilon/kT}$. The case $\epsilon=0$ has been studied by Hauge and Hemmer.[2]

The function $\chi=\chi(z)$ defined by Eq. (11) is an analytic function in the whole z plane except at the points where $d\chi/dz$ is infinite. Differentiating Eq. (11) we find for the value of $\chi(z)$ at the branch points ζ_j the equation

$$(E/E-1)e^{\chi}=2-(1+\chi)^{-1}. \tag{12}$$

$\chi(z)$ is an infinitely many-valued function.

When E is in the interval $1<E<E_0$, with $E_0=(1-e^{-3/2}/4)^{-1}\cong 1.059$, Eq. (12) has two real roots χ_1 and χ_2, and an infinite number of complex roots. The points ζ_1 and $\zeta_2(>\zeta_1)$ are on the negative real z axis. $\chi(z)$ can be made single-valued by making a cut C along the real axis from ζ_1 to $-\infty$. Choosing the Riemann surface which maps $z=0$ to $\chi=0$, the image of C is of the form $\bar{C}$ shown in Fig. 2, and the z plane

[4] H. Takahasi, Proc. Math. Phys. Soc. (Japan) **24**, 60 (1942).
[5] G. F. Newell and E. W. Montroll, Rev. Mod. Phys. **25**, 353 (1953).

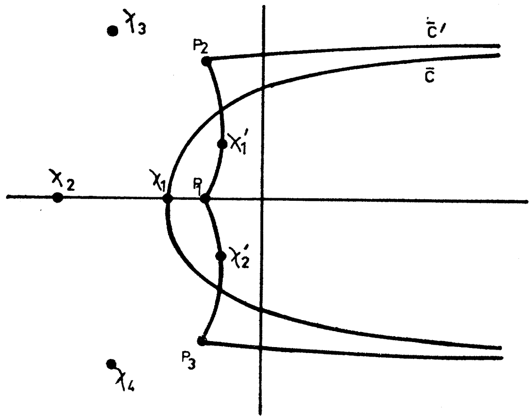

FIG. 2. The χ plane. Images of the branch points and the cut.

is mapped on the region of χ plane inside $\bar{C}$. All the points χ_2, χ_3, $\cdots$, are on the outside of $\bar{C}$. Thus ζ_2, ζ_3, $\cdots$, are on the discarded Riemann surfaces, and the function $\chi(z)$ is single-valued in the cut z plane. The density $g(s)$ is real and positive. It becomes infinite at ζ_1 and vanishes at infinity as in the case $E=1$.

When E approaches E_0, χ_1 and χ_2 approach $-\frac{3}{2}$ and coincide. At $E>E_0$, they are complex and complex conjugate of each other. The numbers ζ_1 and ζ_2 are then also complex and complex conjugate. To preserve continuity with respect to E, the cut C must be of the form shown in Fig. 3, consisting of the parts $(P,-\infty)$, (P,ζ_1), and (P,ζ_2). The point P on the real z axis maps into three points P_1, P_2, P_3 on the image curve $\bar{C}'$.

The arcs C can now be computed numerically using the reality condition for $G(z)dz$. The density $g(s)$ is simultaneously obtained. In Fig. 4 the density of zeros on the line (P,ζ_1) is shown as a function of the distance s along C from P. The density $g(s)$ on the line $(P,-\infty)$ is of the order 0.1 at P in all the given cases, and vanishes for large $|z|$ as for hard rods.[2] Because a one-dimensional system with finite range potential does not show a phase transition, the lines of zeros do not cross the positive real z axis. The contour described by the branch points is given in Fig. 5.

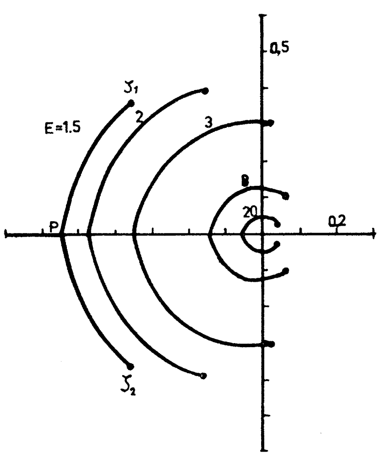

FIG. 3. The lines of zeros for different values of E.

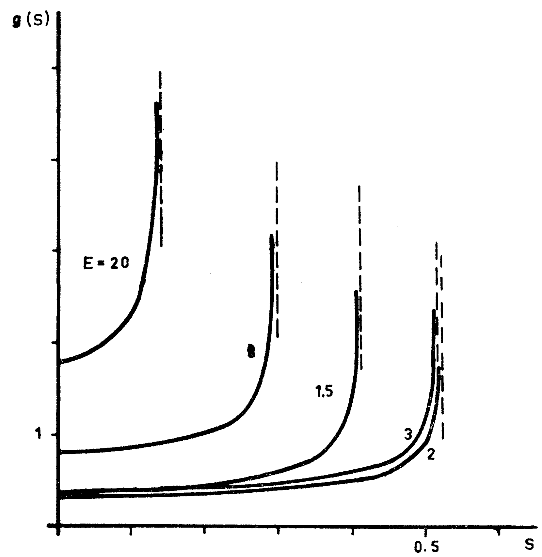

FIG. 4. The density on arcs (P,ζ_1).

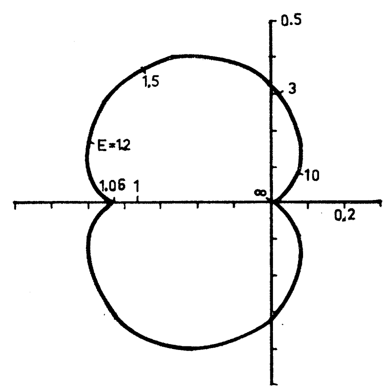

FIG. 5. The contour described by the branch points.

ACKNOWLEDGMENTS

The author is indebted to K. Suominen for valuable discussions and to J. Arponen for numerical calculations. This work has been supported by the Finnish State Committee for Technical Research.