

where  $\Gamma_5(pqk)$  is the renormalized full vertex function. From Eqs. (4.1) to (4.3) follows that

$$\Gamma_5(pqk) \sim Z_1 \gamma_5 \tau_i = 0, \quad k^2 \rightarrow \infty. \quad (4.4)$$

For  $p^2$  or  $q^2 \rightarrow \infty$ , the corresponding relation involves the other constants too, so that a clear-cut statement is not possible without the knowledge of the magnitude of these constants.

The results obtained in this paper need not necessarily be restricted to the specific model we have chosen, in view of the general character of the approach. It is conceivable, however, that not exactly the same conclusions may be obtained for other theories. In quantum electrodynamics, for example, the Ward identity  $Z_1 Z_2^{-1} = 1$  would be an additional relation which must be taken into account.

## New Approach to the Many-Body Problem\*

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The dynamical behavior of  $N$  interacting particles may be simplified by the introduction of  $3N$  collective coordinates. A geometric interpretation of collective coordinates is described which is analogous to a type of random walk problem. Considerations on the validity of the transformation from ordinary spatial coordinates to symmetrical collective coordinates are discussed. The difficult problem of the boundary of collective coordinate space is touched upon.

In the second half of the paper, the Lagrangian formulation for the dynamical problem is carried out by means of collective coordinates. Conditions for the equivalence of the physical Lagrangian and the collective coordinate Lagrangian are established. This leads to the problem of the Fourier representation of a potential by a finite number of terms. Finally, preliminary remarks on a modified Dirac  $\delta$  function are presented.

### INTRODUCTION<sup>1</sup>

IN this and the next few papers, we shall be concerned primarily with describing the collective aspects of the many-body problem and how they arise out of the individual particles. Little or no emphasis will be placed on the actual evaluation of immediate, concrete, physical phenomena. Our aim is to furnish a sequence of analyses, each more refined and deeper than the preceding. Applications will be considered at the conclusion of each major stage of development. We hope to discuss at some future time the interaction of the individual with the collective and the description of deeper collectives such as the nucleus.

Our approach to the many-body problem is by means of a transformation from the individual to the collective. The possibility of focusing one's attention on a particular particle and following its behavior in detail appears to be destroyed. The collective coordinate places all particles of the same nature on an equal footing. Lengthy probing will be necessary to obtain familiarity with the dynamical behavior of the collective coordinates. In the zeroth order of the collective

approach to the many-body problem (which is the primary concern of our first set of papers), only the collective manifests itself; higher order approximations lead successively to the individual manifestations of the collective in the same way that the usual individual approach leads in higher order approximations to the collective.

### PART A. CONCEPT OF COLLECTIVE COORDINATES

#### I. Many-Body Problem

We desire to replace the  $N$ -body problem of interacting particles by an equivalent problem which is more amenable to analytical treatment. This apparently can be achieved by the use of  $3N$ ,  $2N$ , or  $N$  (depending upon the dimensionality of physical space) one-dimensional, bounded harmonic oscillators, which we shall label as  $q_k$ . This will be done in Part B.

Let us consider the following Lagrangian [Eq. (1)] which describes  $N$  particles in one dimension. These particles are considered to lie within a box of length  $L$  with periodic boundary conditions.

$$L_x = \frac{1}{2} \sum_i m \dot{x}_i^2 - \sum_i \sum_{j>i} V(x_i - x_j). \quad (1)$$

Equation (1) is much too difficult to treat analytically in any detail because of its nonlinear character. Instead, if one seeks its solution, one must attempt to transform the nonlinear equations into some sort of linear problem. This apparently can be done by the use of col-

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<sup>1</sup> This paper is a condensation of a lengthy and detailed analysis available at cost from the Department of Physics, Stevens Institute of Technology, Hoboken, New Jersey.

lective coordinates first explicitly introduced by Bohm and Pines<sup>2</sup> in the treatment of the many-body problem for long-range Coulomb forces. In all of their methods,<sup>3</sup> no attempt was made to place the total emphasis upon collective coordinates as *bona fide* dynamical coordinates of the system. For example, Bohm and Pines in their work found it necessary, in order to describe the thermal motion of particles, to introduce individual-particle variables as well as collective coordinates.

The collective coordinates which we propose to use are the simplest possible in form although it is conceivable that, for a particular problem, better collective coordinates may be devised. We indicate, at a later stage of the analysis, a general method of procedure for obtaining a suitable description of a dynamical system with arbitrary collective coordinates.

However, we shall here restrict ourselves to the following collective coordinates:

$$q_k = \sum_i e^{ikx_i}, \quad (2)$$

where  $x_i$  denotes the position of the  $i$ th particle in the periodic cell of length  $L$  and  $k$  is an integral (positive or negative) multiple of  $k_0$ , defined by

$$k_0 \equiv 2\pi/L. \quad (3)$$

Since the above  $q_k$  are complex rather than real quantities, one may also use real coordinates which are defined in terms of the real and imaginary parts of the  $q_k$ 's, namely

$$\begin{aligned} c_k &\equiv \sum_i \cos kx_i, \\ s_k &\equiv \sum_i \sin kx_i. \end{aligned} \quad (4)$$

## II. Some Elementary Remarks on Collective Coordinates

Before employing collective coordinates to transform the physical problem, we shall devote some space to elucidation of both the properties of these rather novel coordinates and of the legitimacy of the transformation.

Let us briefly discuss at this point some properties of the  $q_k$ . We observe that if the  $x_i$  are randomly distributed, the mean values of the  $q_k$ 's are clearly zero. This should not be interpreted as meaning that the  $q_k$ 's spend their time about zero. One observes, in fact, that the  $c_k$ 's and  $s_k$ 's have root mean square values equal to  $\sqrt{N}$ , if the  $x_i$  are randomly distributed. One immediately notices that when  $k$  is exceedingly large, the phases of the  $kx_i$ 's will in general have a random appearance (*mod*  $2\pi$ ) so that the  $\sqrt{N}$  criterion will prevail. For low  $k$ 's where the concept of periodicity enters more importantly, the  $q_k$ 's may have a value extending to  $N$ , which is the maximum value possible for any  $q_k$ . For example, suppose there is a periodic effect of wave number  $k$  extending over a distance  $d$ ; then  $q_k$  will have an absolute value of the order of  $(Nd)/L$  instead of zero.  $q_k$ 's whose indices are multiples

of  $k$  will also center about this value. This is clearly important for the solid state. Since exact periodicity cannot exist in reality, we shall expect that this effect will be distributed over a narrow band of  $k$ 's.

A geometrical way of looking at the above is the following:  $q_k$  may be regarded as the terminus of a chain of  $N$  unit vectors in the complex plane, the  $i$ th vector being at angle  $kx_i$ . It is seen that near randomness of the  $x_i$ 's cause the  $q_k$  to cluster around the origin, more so for the higher  $k$ 's since a small motion in coordinate space tends to alter violently the direction of the links. The relation of this effect to the random walk problem is evident. Secondly, although each  $q_k$  has a maximum possible value of  $N$ , its attainment of this value fixes the other  $q_k$ 's; thus the boundary in  $q_k$ -space is one in which the  $q_k$ 's are intimately connected.

The complicated boundary of the  $q_k$ 's is an unfortunate concomitant of the collective coordinate approach. However, before considering this boundary in more detail, it is certainly incumbent upon us to verify that the  $q_k$ 's constitute a valid coordinate system. To this problem we now turn our attention.

## III. Discussion of the Validity of $q_k$ 's as a Coordinate System

We are now prepared to investigate the sense in which the  $q_k$ 's (or  $c_k$ 's,  $s_k$ 's) constitute a valid coordinate system. The transformation

$$q_k = \sum_i e^{ikx_i} \quad (2)$$

is implicitly multivalued in the sense that the interchange of two or more particles clearly does not affect the value of the  $q_k$ 's. In fact, for a given set of values of the  $q_k$ 's, there are certainly  $N!$  points in the  $N$ -dimensional  $x$  space to which this corresponds. Due to indistinguishability of particles, this is no drawback, for we shall show below (see Appendix) that the region in the  $N$ -dimensional  $x$ -space,

$$x_1 > x_2 > x_3 > \cdots > x_N \quad (5)$$

(or any of the equivalent  $N!$  regions obtained by interchange of particles), maps in a one-to-one manner onto all of  $q_k$  space. Thus the behavior of the particles in this region is completely determined by the corresponding behavior in  $q_k$  space.

Restating the problem: Is the transformation from  $q$ -space to  $x$ -space one-to-one except for order? First, let us restrict the term  $q$ -space to that region of infinite  $q$ -space which is the image of  $x$ -space. (The precise location of this bounded region in  $q$ -space, especially the boundary, is an important matter to be dealt with in detail later.) To each point in  $q$ -space there is at least one sequence of  $x_i$ 's for which  $x_1 > x_2 > x_3 > \cdots > x_N$ , but is there more than one? We treat this problem, first, essentially by means of the implicit function theorem which, for our purposes, will be used in the following form: If a set of simultaneous algebraic

<sup>2</sup> D. Pines and D. Bohm, Phys. Rev. **85**, 338 (1951).

<sup>3</sup> D. Bohm and D. Pines, Phys. Rev. **92**, 609 (1953).

equations is solvable uniquely at a point, then it is solvable uniquely in the vicinity of the point providing that the Jacobian is not equal to zero.

The Jacobian  $J = |\partial q_k / \partial x_j| = |ik \exp(ikx_j)|$  is zero whenever  $x_i = x_j$ ; but in addition  $J$  possesses factors other than  $x_i - x_j$  which can vanish. These can be spurious as in the vanishing of the Jacobian of  $y = x^3$  when  $x = 0$ , or they may correspond to natural boundaries in  $q$ -space. Our task is to show that except for the obvious natural boundary corresponding to  $x_i = x_j$ , the singular surfaces on which  $J$  vanishes do not destroy the univalence of the collective coordinate transformation.

In the Appendix, the uniqueness proof is presented for an arbitrary sequence of wave numbers. To accomplish this, we first show that there exists a point in  $q$ -space at which the inverse transformation is single valued. Next, a lengthy but straightforward analysis proves that the property of uniqueness of the inverse at a point may be extended to a neighborhood of the point, irrespective of the proximity of singular surfaces. Thus the adequacy of the collective coordinates  $q_k$  for the representation of the state of a physical system containing identical particles is firmly established.

#### IV. Boundary in $q$ -Space

We have seen, from the definition  $q_k = \sum_{j=1}^N \exp(ikx_j)$  that not only is each  $q_k$  bounded and less than  $N$  in amplitude, but also that  $q_k$  does not wander much past  $\sqrt{N}$ ; this suggests a boundary of some complexity, and we would like to know the nature of the true boundary surface in order to determine, e.g., to what extent it can be approximated by an  $N$ -dimensional sphere or cube. For the present, however, we limit ourselves to some general considerations; in particular, we verify explicitly a property which has already appeared indirectly in several places: the relation of the boundary to the transformation Jacobian.

Consider then the expression  $c_p = \sum_j \cos p x_j$ ; the boundary surface is determined by the condition that  $c_p$  is stationary under variation of the  $x_j$ 's for a fixed set of values of the remaining  $c_k$ 's and  $s_k$ 's. Using the Lagrange method of multipliers, we can express this in such a form that the following quantity must be stationary:

$$c_p + \sum_{k \neq p} \lambda_k c_k + \sum_k \lambda'_k s_k, \quad (6)$$

where  $\lambda_k$  and  $\lambda'_k$  are Lagrange multipliers. Thus,

$$\frac{\partial c_p}{\partial x_j} + \sum_{k \neq p} \lambda_k \frac{\partial c_k}{\partial x_j} + \sum_k \lambda'_k \frac{\partial s_k}{\partial x_j} = 0 \quad (7)$$

for all  $j$ ; these  $N$  equations in the  $N-1$  unknown  $\{\lambda_k, \lambda'_k\}$  are solvable providing that the full determinant is zero. Since a nonsingular linear transformation does not affect the singularity of a determinant, this may equally well be written as  $|\partial q_k / \partial x_j| = 0$ : at the boundary surface, the Jacobian must be zero. If we can now

show that the additional surfaces on which the Jacobian is zero are physically extraneous, the boundary will be given by the equations  $x_i = x_j$  alone. This is, of course, a condition in  $x$ -space, but, in principle, there is no difficulty in converting to  $q$ -space. Since the order of  $x$ 's is immaterial, the bounding surface may be specified simply by setting  $x_{N-1} = x_N$ . We then have  $q_k = \sum_{j=1}^{N-2} e^{ikx_j} + 2e^{ikx_N}$  for each  $k$ , and eliminating the  $(N-1)$   $x_j$ 's between these, a surface of dimension  $N-1$  thereby results. The case  $N=2$  yields a simple circular domain, but unfortunately, it is very difficult to carry out such a calculation for large  $N$ . In a succeeding paper, several indirect methods will be presented for estimating the major physical characteristics of the  $q$ -space boundary.

### PART B. LAGRANGIAN FORMULATION OF THE MANY-BODY PROBLEM

#### I. Introduction

The physical basis for our problem lies in the Lagrangian given by Eq. (1). The resulting equations defy conventional techniques of solution because of their intricate nonlinearity. We seek to replace this Lagrangian by an equivalent Lagrangian leading to linear equations which approximate the real problem. This is done by using the collective coordinates  $q_k$ . We assume that the  $q_k$ 's may be regarded as representing a set of one-dimensional elementary harmonic oscillators and we shall now verify the extent to which this assumption is valid. Expressed otherwise, we maintain that the real motion of  $N$  particles is intimately related to the motion of  $N$  bounded harmonic oscillators,  $q_k$ . For nonequilibrium processes, the first-order theory, not given in this paper, reveals that coupling between oscillators exists which contributes to irreversibility. It should be clearly stated that the exact theory contains coupling between all the oscillators irrespective of the type of physical process encountered.

#### II. Equivalence of Lagrangians

Since we maintain that the motion of  $N$  bodies having a Lagrangian given by Eq. (1) can be represented approximately by the motion of  $q_k$ 's regarded as  $N$  independent harmonic oscillators, then the most general form which the Lagrangian in  $q$ -space can take is

$$L_q = \sum_{k \neq 0} \frac{1}{2} f_k (|\dot{q}_k|^2 - \omega_k^2 |q_k|^2) + B \\ = \sum_{k > 0} [f_k (\dot{c}_k^2 - \omega_k^2 c_k^2) + f_k (\dot{s}_k^2 - \omega_k^2 s_k^2)] + B, \quad (8)$$

where the constant

$$B = N \sum_{k \neq 0} \frac{1}{2} \omega_k^2 f_k - \frac{1}{2} N(N-1)A \quad (9)$$

has been inserted for convenience and  $A$  is another constant to be determined later. Since  $|q_k|^2 = |q_{-k}|^2$ , we may choose  $f_k = f_{-k}$  and  $\omega_k = \omega_{-k}$  in Eq. (8). This is not unrelated to the invariance of the exact Lagrangian under spatial reflection. The  $f_k$  can be looked upon as the fictitious masses and the  $\omega_k$  as the fictitious fre-

quency of the oscillators. These frequencies can possibly be imaginary.

To what extent does this Lagrangian represent the true Lagrangian given by Eq. (1)? If we substitute  $q_k = \sum_i \exp(ikx_i)$ , we get

$$L_q = \sum_i \frac{1}{2} (\sum_{k \neq 0} f_k k^2) \dot{x}_i^2 - \sum_i \sum_{j \neq i} (\sum_{k \neq 0} \frac{1}{2} \omega_k^2 f_k e^{ik(x_i - x_j)}) + \sum_i \sum_{j \neq i} \sum_{k \neq 0} \frac{1}{2} f_k k^2 e^{ik(x_i - x_j)} \dot{x}_i \dot{x}_j - \frac{1}{2} N(N-1)A. \quad (10)$$

This is to be compared with Eq. (1) which we rewrite

$$L_x = \sum_i \frac{1}{2} m \dot{x}_i^2 - \sum_i \sum_{j \neq i} \frac{1}{2} V(x_i - x_j). \quad (1')$$

For the kinetic energy terms to coincide, we must have

$$\sum_{k \neq 0} f_k k^2 = m, \quad (I)$$

whereas the "velocity-dependent potential" terms must be close to zero:

$$\sum_i \sum_{j \neq i} \sum_{k \neq 0} \frac{1}{2} f_k k^2 e^{ik(x_i - x_j)} \dot{x}_i \dot{x}_j \approx 0. \quad (II)$$

Finally, for the potential energy terms to coincide,

$$V(x_i - x_j) = \sum_{k \neq 0} \omega_k^2 f_k e^{ik(x_i - x_j)} + A. \quad (III)$$

Condition I can obviously be satisfied exactly. Our problem now is to select  $N$  parameters  $f_k$  at our disposal,  $N$  other parameters  $\omega_k^2$  also at our arbitrary disposal, and  $A$ , in such a fashion that conditions II and III are satisfied in the best possible way. If we have enough degrees of freedom (i.e., enough  $q_k$ 's), then in principle we could satisfy condition III exactly, whereas we can never satisfy totally condition II. Because condition II cannot be satisfied exactly, its neglect would be expected to play a role in certain physical processes, which, we will demonstrate in a future paper, are connected with nonequilibrium and nonuniform states. The fact that the number of particles is so large (for one dimension,  $> 10^7$  per cm) allows the possibility of satisfying quite closely conditions I, II, and III. The succeeding paper will be devoted to verification of this; we shall content ourselves for the present with an analysis of some of the problems involved in optimization of the correspondence between the true Lagrangian and its harmonic oscillator counterpart.

### III. Nature of Potential

The first problem which we shall consider briefly is the following: To what extent are we able to represent the potential  $V(x)$  with  $N$   $q_k$ 's? Or how can we satisfy condition III?

Clearly

$$V(x) = \sum_{\text{all } k} V_k e^{ikx}, \quad (11)$$

with

$$V_k = (1/L) \int_{-L/2}^{L/2} e^{-ikx} V(x) dx, \quad (12)$$

where all  $k$  refer to integral multiples of  $k_0 = 2\pi/L$ , and this is valid for  $-L \leq x \leq L$  because  $V(x)$  was constructed as having period  $L$ . But the number of  $q_k$ 's available is only  $N$ , so that the number of positive  $k$ 's is  $N/2$ . If we take  $\Delta k = k_0$  (the most obvious choice, corresponding to taking every point but the origin of the  $k$ -lattice), then the  $k$ 's can run only between  $-Nk_0/2$  and  $+Nk_0/2$ .

A simple example will easily convince one that this choice fails to satisfy condition III for many physical problems. Since we have  $N$  particles per length  $L$ , the average interparticle spacing is  $d = L/N$ . For a gas, liquid, and solid, the major portion of the potential lies inside  $d$ . If the potential, for example, is constructed from terms of the form  $1/(x^2 + a^2)$ , then terms must be included for which  $a$  is smaller than  $d$ . Now if we attempt to represent such a potential by choosing only  $k$ 's between  $-Nk_0/2$  and  $+Nk_0/2$ , an explicit computation using the criterion of minimum mean square deviation shows that the portion of the potential for  $x < d$  is "washed out" by the approximation.

It would seem to be possible to dispense with the minimum mean square criterion and to attribute more general validity to the effects appearing in the above example by making use of the results of the Heisenberg uncertainty principle. However, one can show that it is not legitimate to use the Heisenberg uncertainty principle as a proof of one's inability to construct a narrow wave packet, because the restriction  $\Delta k \Delta x \geq 1$  comes about by weighting too heavily small fluctuations at large distances from the origin. There is no reason to believe that the physics of the problem is sensitive to such small fluctuations. Nevertheless, we have been unable to exhibit with  $\Delta k = k_0$  a suitable Fourier expansion for the class of potentials in which we are interested.

### IV. Preliminary Remarks on the $d$ -Function

Since we are restricted only by the number  $N$  of the coordinates  $q_k$  and not by the particular  $k$ 's, we are at liberty to choose  $k$ 's other than those with  $\Delta k = k_0$ . This allows a wide choice of possibilities, some of which may be unexpectedly effective in satisfying condition III. It will simplify matters greatly if we observe that the problem reduces itself to that of finding a representation of a Dirac  $\delta$  function by means of  $N$  Fourier components. To show this, we can write

$$V(y) = \int_{-L/2}^{L/2} V(x) \delta(y-x) dx. \quad (13)$$

Now for our problem, it is not necessary to employ the exact  $\delta(y-x)$ ; rather, any function  $d(y-x)$  which is sufficiently sharp compared with  $V(x)$  will suffice as an averaging function.

Now if  $d(x)$  can be expanded in the form

$$d(x) = (1/L) \sum d_k e^{ikx}, \quad (14)$$

where  $N$  different  $k$ 's in addition to  $k=0$  have been utilized, it then follows that

$$\begin{aligned} V^*(y) &\equiv \int_{-L/2}^{L/2} V(x) d(y-x) dx \\ &= \sum d_k (1/L) \left( \int_{-L/2}^{L/2} V(x) e^{-ikx} dx \right) e^{iky}, \quad (15) \end{aligned}$$

which has the desired form. We note that this also can be written as

$$V^*(y) = \sum d_k V_k e^{iky}. \quad (16)$$

Another important consequence of a satisfactory  $d$ -function is that, when buttressed by physical arguments, it provides for the treatment of condition II. Again, because of the lengthy analysis, we present our arguments in the succeeding paper.

The problem of actually obtaining the  $d$ -function is a serious one and considerable analysis is required. This is developed at some length in the succeeding paper. There we shall indicate that a narrow  $d$ -function can be constructed by the use of gaps in  $\Delta k$ , and that its form is improved by allowing  $L, N \rightarrow \infty$  such that  $n = N/L$  remains constant.

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#### APPENDIX. ANALYSIS OF JACOBIAN WHEN $\Delta k \neq 1$

In this Appendix, we indicate a method, of necessity indirect, for analyzing the Jacobian and establishing the uniqueness of the collective coordinate transformation for a wave number spectrum in which gaps may appear.

The evaluation of the Jacobian is readily reduced to that of the determinant  $|y_j^k|$ , where

$$y_j = \exp(ik_0 x_j); \quad (1)$$

by multiplying various rows by appropriate powers, this may be converted into a determinant in which only non-negative powers exist. Computation of determinants of this type has been carried out by mathematicians<sup>4</sup>; we merely state the final result. If  $C_j$  now denotes the elementary symmetric function of the  $y_i$ 's

<sup>4</sup> A. C. Aitken, *Determinants and Matrices* (Interscience Publishers, Inc., New York, 1946), fourth edition, p. 116.

taken  $n'-j$  at a time, where  $n'$  is the largest power of the  $y$ 's present, then

$$|y_j^k| = \prod_{i > j} (y_i - y_j) \begin{vmatrix} C_{\nu_1} & C_{\nu_2} & \cdots & C_{\nu_n} \\ C_{\nu_1-1} & \cdot & & C_{\nu_n-1} \\ C_{\nu_1-2} & \cdot & & C_{\nu_n-2} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \end{vmatrix}, \quad (2)$$

where the  $\nu_i$  are the positions of the missing powers. (It is to be noted that the expression for the determinant in (1) is independent of any preliminary multiplication—negative powers of  $y_i$  affect only the factor outside the determinant.) The determinant tells us the location of the singular surfaces. It must then be established that they play no physical role.

We now present an infinitesimal analysis, which it would be pointless to carry out in complete rigor, for showing the uniqueness of the  $q$ -space transformation and thus the physical unimportance of the interior singular surfaces. No increase in complexity is occasioned if we consider generalized collective coordinates:

$$q_k = \sum_i g_k(x_i). \quad (3)$$

To initiate the proof, let us show that, given the  $q_k$  of (3), a unique solution for the  $x_i$  (to within order) exists in the vicinity of some point. We shall restrict our attention to those sets of  $g_k(x)$  whose real maxima  $m_k$  occur at a common point  $x=a$ , and for which only  $x=a$  has this property; further we assume that the Wronskian of the  $dg_k/dx$  does not vanish at  $x=a$ . As long as the totality of  $k$ 's does not have a common factor greater than  $k_0$ , the set  $\{e^{ikx}\}$  is included in the category. Consider then the point

$$q_k = Nm_k \quad (\text{all } k); \quad (4)$$

under the conditions just delineated, this highly singular point clearly has the unique inverse  $x_1 = x_2 = \cdots = x_N = a$ . Nearby, we have

$$Nm_k + dq_k = \sum_j \sum_{p=0}^{\infty} g_k^{(p)}(a) (dx_j)^p / p!,$$

or if  $\sigma_p$  is the sum of  $p$ th powers of the  $dx$ 's, then restricting to  $N$ th-order infinitesimals,

$$dq_k = \sum_{p=1}^N g_k^{(p)}(a) \sigma_p / p!. \quad (5)$$

Since the determinant of (5) is just the Wronskian at  $a$ , (5) may indeed be solved uniquely for the  $\sigma_p$  and hence for the  $x_i$  to within order. It is also useful to observe that the Jacobian at  $(a+dx_i)$  is not identically zero; to see this, we need only note that

$$|g_k'(a+dx_j)| = |g_k^{(p)}(a)| \prod_{i < j} (dx_i - dx_j) / \prod (i-j)!,$$

to lowest order infinitesimals, and this expression vanishes only on the natural boundary  $x_i = x_j$ .

The remainder of the proof consists in showing that uniqueness of the solution of (3) at a point implies uniqueness along sufficiently short paths leading from the point, not excluding paths which cut across internal singular surfaces. To accomplish this, we shall base ourselves at a point  $\{x_i\}$ , assume uniqueness of solution at  $\{x_i - \frac{1}{2}dx_i\}$ , and try to prove uniqueness at  $\{x_i + \frac{1}{2}dx_i\}$ . Since

$$q_k(\dots, x_i + \frac{1}{2}dx_i, \dots) - q_k(\dots, x_i - \frac{1}{2}dx_i, \dots) = \sum_i [g'_k(x_i)dx_i + (1/24)g'''_k(x_i)(dx_i)^3 + \dots]; \quad (6)$$

we must then verify unique solvability of

$$dx = [g' + (1/24)g'''(\delta x)^2 + \dots]dx; \quad (7)$$

here  $dq$  and  $dx$  refer to the vectors  $dq_k$  and  $dx_i$ , the matrix of  $g_k^{(p)}(x_i)$  is denoted by  $(g_{ki}^{(p)})$ , and the diagonal matrix  $dx_i \delta_{ij}$  by  $(\delta x_{ij})$ . To analyze (7), we consider two cases.

*Case I.*—The Jacobian  $|g'| \neq 0$ ; then, dropping infinitesimals higher than first order, we have at once the unique solution

$$dx = (g')^{-1}dq. \quad (8)$$

This is the usual case.

*Case II.*—The Jacobian  $|g'| = 0$ . The rank of  $g'$  may be assumed as precisely  $N-1$ , for the cofactor

$$G_{ba}' \equiv |g'|_{ab} \quad (9)$$

does not contain  $x_b$ , so that no single relation can cause all cofactors to vanish; thus the rank is  $< N-1$  only on surfaces of dimension  $\leq N-2$ , and these are of no consequence in assessing the connectivity of  $q$ -space. We now write (7) in the form

$$\sum |g' + (1/24)g'''(\delta x)^2 + \dots|_{kj} dq_k = |g' + (1/24)g'''(\delta x)^2 + \dots| dx_j. \quad (10)$$

Since  $|g'| = 0$ , the lower order terms in  $|g' + (1/24)g''' \times (\delta x)^2 + \dots|$  are proportional to  $(dx)^2$ ; thus  $dq$  is a third-order infinitesimal with respect to  $dx$ . Dropping

fourth-order infinitesimals and higher in (10), we then have

$$\begin{aligned} \sum G_{jk}' dq_k &= |g' + (1/24)g'''(\delta x)^2| dx_j \\ &= \left\{ |g' + (1/24)g'''(\delta x)^2|_{dx=0} \right. \\ &\quad \left. + \sum (dx_i)^2 \frac{\partial |g' + (1/24)g'''(\delta x)^2|_{dx=0}}{\partial (dx_i)^2} \right\} dx_j \\ &= \left\{ \sum (dx_i)^2 |g' + (1/24)g'''(\delta x)^2|_{ab} \right. \\ &\quad \left. \times \frac{\partial (g_{ab}' + (1/24)g_{ab}'''(dx_b)^2)}{\partial (dx_i)^2} \right\}_{dx=0} dx_j, \end{aligned}$$

yielding

$$\sum G_{jk}' dq_k = (1/24) dx_j \sum (G' g''')_{bb} (dx_b)^2, \quad (11)$$

the basic equation for Case II.

Since  $|g'| = 0$  corresponds to a singular surface, we are interested in paths connecting points on opposite sides of the surface. A relation of the form  $\sum G_{jk}' dq_k = 0$  which we have seen is nontrivial, implies that the vector  $dq_k$  is along the singular surface ( $dq$  is linearly dependent on the vectors  $\partial g / \partial x_i$  which span the surface) and so merits no consideration. Hence  $\sum (G' g''')_{bb} \times (dx_b)^2$  in (11) does not vanish. But on squaring (11), we obtain

$$\begin{aligned} \sum_j [(\sum G_{jk}' dq_k)^2 (G' g''')_{jj}] \\ = (1/24) [\sum (G' g''')_{bb} (dx_b)^2]^2 \neq 0, \quad (12) \end{aligned}$$

so that (11) may be solved at once as

$$dx_j = 4 \times 3^{\frac{1}{2}} [\sum_b (\sum G_{bk}' dq_k)^2 \times (G' g''')_{bb}]^{\frac{1}{2}} \sum G_{jk}' dq_k. \quad (13)$$

From the reality of  $x$ , this solution is unique, and our proof of the diffusion of uniqueness throughout  $q$ -space is now complete.