THE INVERSE PROBLEM OF PARTICLE MOTION †) AND ITS APPLICATION

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Summary

The theory of the inverse problem of charged particle motion is presented in this paper. A potential distribution required to guide a group of particles along a set of prescribed paraxial paths has been found. An application of the theory of the inverse problem to the design of an efficient ion source for the mass spectrometer is discussed. The potential distribution required to guide the ions along a set of exponentially converging and damped oscillatory paths has been found. An interesting situation is encountered, where a particle is turned back at certain points called mirror points.

The particles which do not satisfy the initial condition of uniform energy and direction may deviate considerably from their projected paths, leading to an unstable situation. A method for finding the perturbation function is developed. It was found that the system with exponentially converging paths is unstable, while the second system with damped oscillatory paths is stable.

§ 1. *Introduction.* In the usual problem of charged particle motion we are given an electrostatic potential distribution and we are required to find the particle trajectories. But in many of the applications we desire the particles to follow certain paths; for instance, the desired paths for maximum efficiency in the ion source of a mass spectrometer are shown in fig. 1. This gives rise to the inverse problem: that is, to find a potential distribution capable of guiding the particles along the prescribed paths. To the knowledge of the present writer, this problem has not been solved, although Pierce[1]) in 1954 has mentioned such a possibility.

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Starting from the basic trajectory equation and the Laplace equation we shall show in section 2 that for any prescribed path a unique potential distribution can be obtained. Next we shall generalize the problem: a unique potential distribution can be

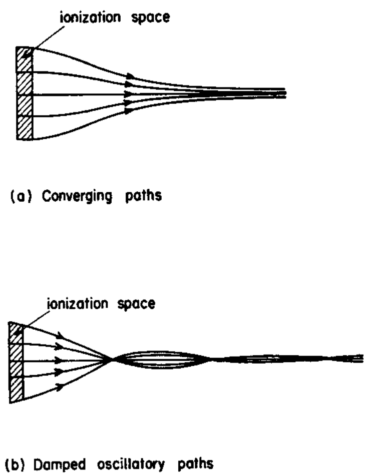

Fig. 1. Paths for maximum efficiency in the ion source of a mass spectrometer.
a. Converging paths.
b. Damped oscillatory paths.

found for a set of prescribed paths satisfying certain geometrical relations. Finally, an application to the design of an efficient ion source for a mass spectrometer will be illustrated in section 3 and the stability of trajectories will be discussed in section 4.

§ 2. *Theory.* Following are the two basic theorems in the theory of the inverse problem:

(i) there exists a potential distribution to guide a particle along any prescribed path;

(ii) a group of particles may be guided along a set of paraxial paths.

We shall now prove the above theorems for the two dimensional case. The equation of the trajectory of a charged particle in two dimensions is given by

$$y'\phi_x - \phi_y + \frac{2y''}{(1+y'^2)}\,\phi = 0, \tag{2.1}$$

where

$$y' = \frac{dy}{dx}, \qquad y'' = \frac{d^2y}{dx^2}$$

$$\phi_x = \frac{\partial\phi}{\partial x}, \qquad \phi_y = \frac{\partial\phi}{\partial y}$$

and

$$\phi = V_0 - V + \delta,$$

in which δ is the initial energy, V_0 the potential at the starting point and V the potential at any point $P(x, y)$. Furthermore ϕ must satisfy the Laplace equation

$$\phi_{xx} + \phi_{yy} = 0. \tag{2.2}$$

If we specify the path of a particle, y' and y'' in (2.1) will be known functions; therefore, to find the potential distribution ϕ we will have to solve the system of partial differential equations (2.1) and (2.2). The technique of solving the equations is as follows: To obtain ϕ, ϕ_x, and ϕ_y in the neighbourhood of the path we solve (2.1) given ϕ along the prescribed path. Now knowing ϕ_x and ϕ_y we may compute the normal derivative $\partial\phi/\partial n$. The potential ϕ and its normal derivative $\partial\phi/\partial n$ constitute the Cauchy boundary value problem for (2.2). The first order partial differential equation (2.1) is equivalent to a system of ordinary differential equations. If we introduce a parameter s along the characteristics, the system of ordinary equations becomes

$$\frac{dx}{ds} = y',$$

$$\frac{dy}{ds} = -1,$$

$$\frac{d\phi}{ds} = \frac{-y''2\phi}{1 + (y')^2}. \tag{2.3}$$

Every surface generated by (2.3) is an integral surface of (2.1). A unique surface, however, may be defined from the initial value problem for (2.3). Let us define a space curve C by prescribing x, y and ϕ as a function of a parameter t (arc length) such that the projection C_0 of C on the x, y-plane coincides with the prescribed path of a particle. Now in the neighbourhood of C_0, we seek an integral surface $\phi(x, y)$ which passes through C; that is, a solution of (2.1) for which

$$\phi(t) = \phi(x(t), y(t))$$

holds identically in t. To solve the initial value problem, let us draw through each point of C a characteristic, that is, the solution of (2.3); this is possible in a unique way within a certain neighbourhood of C_0. We thus obtain a family of characteristics

$$\begin{aligned} x &= x(s, t), \\ y &= y(s, t), \\ \phi &= \phi(s, t). \end{aligned} \tag{2.4}$$

These curves will generate a surface $\phi(x, y)$ if, using the first two functions, we can express s and t in terms of x and y. To be able to do this, we must show that the Jacobian

$$\Delta = \frac{\partial x}{\partial s} \cdot \frac{\partial y}{\partial t} - \frac{\partial x}{\partial t} \cdot \frac{\partial y}{\partial s}$$

is non-vanishing. Using (2.3) we obtain

$$\Delta = y' y_t + x_t = y_t(1 + y'^2)/y'$$

which is non-vanishing for all values of y', and when $y_t \to 0$ then $y' \to 0$; the Jacobian is, therefore, non-vanishing. The geometrical interpretation of the above condition is that at every point on C_0, the projection of the tangent direction and the characteristic direction on the x, y-plane are distinct. In fact in our case, since

$$\frac{dx}{ds} = y'_{\text{Path}},$$

$$\frac{dy}{ds} = -1,$$

$$\left(\frac{dy}{dx}\right)_{\text{Char.}} = -1 \Big/ \left(\frac{dy}{dx}\right)_{\text{Path}}.$$

Hence

$$\left(\frac{dy}{dx}\right)_{\text{Char.}} \cdot \left(\frac{dy}{dx}\right)_{\text{Path}} = -1,$$

the base characteristics and the path of a particle are orthogonal. We therefore conclude that for any prescribed path (paths must not have double points) the solution of (2.1) may be obtained in a certain neighbourhood, therefore, $\partial\phi/\partial n$, the normal gradient, may be obtained. This establishes the theorem I.

We may recall that in the solution of (2.1) as the initial value problem, the potential $\phi = \phi_0$ has been prescribed arbitrarily along the path of a particle. This may now be chosen such that a group of particles moves along a set of paraxial paths that are prescribed again arbitrarily. The trajectory equation resulting from the paraxial approximation is given by Waters[2]).

$$2\phi_0 u'' + \phi_0' u' + (4\kappa^2\phi_0 + \phi_0'')u = 0, \tag{2.5}$$

where u is the normal distance of a particle from the central trajectory and κ is the curvature of the central trajectory. ϕ_0 is the axial potential. We may solve (2.5) for ϕ_0 if u and κ are known functions of t *). But unless the set of paths are suitably chosen, the potential ϕ_0 will be different for each individual path. The condition that the set of paths must satisfy so that a unique potential function ϕ may be obtained is as follows:

$$u = h(1 + a_1 t + a_2 t^2 + \ldots + a_n t^n), \tag{2.6}$$

where h is the height of starting point – by varying h we can obtain a whole set of paths **). If we substitute (2.6) into (2.5), we find that the resulting equation does not contain the constant h. Hence a set of paths defined by (2.6) gives rise to a unique potential function ϕ_0. This establishes the theorem II.

A simple case of considerable importance is where the x-axis is the central path. Then the equation (2.1) and (2.5) reduce to

$$\phi_y = 0 \tag{2.7}$$

and

$$2\phi_0 y'' + \phi_0' y' + \phi_0'' y = 0, \tag{2.8}$$

where now $y \equiv u$. It may be noted that any potential distribution

*) Initial conditions $\phi_0(0) = 1$ and $\phi_0'(0) = 1$.
This requires all particles to start with uniform energy.

**) Note that $u'(0) = ha_1$ i.e. $\propto$ height of starting point.

that is symmetric about the x-axis satisfies (2.7). Therefore, in order to obtain the potential at any point $P(x, y)$, we observe that

$$\phi(x, y) = \mathrm{Re}\,(\phi_0(x + iy)), \tag{2.9}$$

(see ref. 3 p. 689). We hope that the function $\phi_0(x + iy)$ has no singularity in the neighbourhood of the x-axis.

§ 3. *Efficient source.* Here we shall illustrate an application of the theory of the inverse problem to the design of an efficient ion source for the mass spectrometer. The efficiency of ion beam transmission is defined as the ratio of number of ions withdrawn from the source to the total number of ions formed in the source in unit time. It is usually less than one percent. The present ion source, consisting of a stack of parallel plates carrying coplaner and parallel slits, produces a divergent beam of which a large fraction is lost at the collimating slits. Therefore, in order to minimize the losses, we must form a convergent beam.

A few examples of convergent beams are shown in fig. 1. We may now apply the theory of the inverse problem to obtain the appropriate potential distribution. A class of converging paths may be represented by

$$y = h \exp(-bx^n), \tag{3.1}$$

where h is the height of starting point, and b and n are constants. Substituting in (2.8) we obtain

$$\phi_0'' - bnx^{n-1}\,\phi_0' + \frac{2(1 + bnx^n - n)}{x^2}\, bnx^n\phi_0 = 0. \tag{3.2}$$

The above equation reduces to a particularly simple form for $b = 1$ and $n = 1$

$$\phi_0'' - \phi_0' + 2\phi_0 = 0, \tag{3.3}$$

whose solution is given by

$$\phi_0 = A \exp\,(x/2) \sin \tfrac{1}{2}\sqrt{7}(x - B), \tag{3.4}$$

where A and B are arbitrary constants. The axial potential given by (3.4) is an oscillatory function with increasing amplitude. Further, since ϕ_0 changes sign, a given particle cannot be guided along the path $y = \exp(-x)$ over an arbitrary length. The particle suffers a total reflection at the points where $\phi_0 = 0$. These are known as mirror points and such paths as incomplete paths. In general it was found that the class of converging paths represented by (3.1) are incomplete. Therefore they are not of our interest.

We may notice that equation (2.8) is almost symmetrical in ϕ_0 and y. Now, if we assume the paths to be oscillatory functions with increasing amplitude, the axial potential turns out to be an exponentially decreasing function. In particular if we desire the paths to be

$$y = A \exp(-x/4) \sin \tfrac{1}{4}\sqrt{7}(x - B), \tag{3.5}$$

that is, damped oscillatory paths, the axial potential is given by

$$\phi_0 = \exp(x). \tag{3.6}$$

Therefore, the class of converging paths represented by (3.5) (fig. 1b) are complete (i.e. no mirror points).

Though the first system as compared to the second system is not of much practical importance on account of the presence of the mirror points, it is interesting to consider both systems for comparison because in the next section we shall see that, from the point of stability, the second system is to be favoured. The potential distributions for the above two sets of convergent paths are shown in figures 2 and 3.

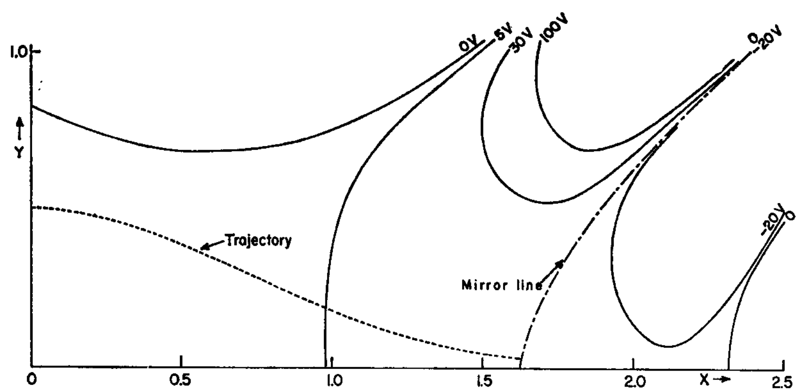

Fig. 2. System I. Potential distribution for converging paths.

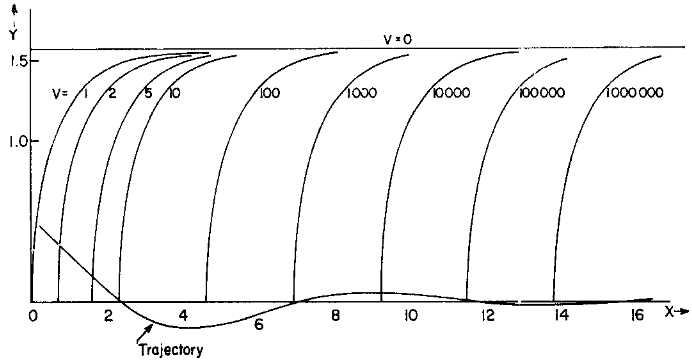

Fig. 3. System II. Potential distribution for damped oscillatory paths.

§ 4. *Stability analysis.* The basic assumptions in the theory of the inverse problem are such that the particles start with the same initial energy and in a direction proportional to the height of the starting point *). These assumptions are but rarely satisfied in a real source, for thermal energy spread is bound to exist. The present section is devoted to the study of the effect of abnormal initial conditions – the conditions not satisfying the requirement of the theory. One of the serious consequences of the abnormal initial conditions is that such particles may deviate considerably from their projected paths, leading to an unstable situation. The two systems discussed in section 3 provide the examples of the unstable and stable systems.

The paraxial trajectory equation of a particle whose initial energy differs from the mean by ε is given by

$$2(\phi_0 + \varepsilon)\, y'' + \phi_0' y' + \phi_0'' y = 0, \tag{4.1}$$

where ϕ_0 is the solution of

$$2\phi_0 y_0'' + \phi_0' y_0' + \phi_0'' y_0 = 0, \tag{4.1'}$$

where y_0 is the specified path of a normal particle. We may express the solution of (4.1) following the method suggested by Poincaré[4]) as

$$y = y_0 + \varepsilon y_1 + \varepsilon^2 y_2 + \dots + \varepsilon^n y_n, \tag{4.2}$$

where $y_1, y_2, \dots, y_n$ are known as the perturbation functions.

*) See footnotes on page 5.

Substituting (4.2) into (4.1) and equating the coefficients of ε^m, $m = 1 \ldots n$ to zero, we obtain a system of differential equations;

$$
\begin{aligned}
&2\phi_0 y_1'' + \phi_0' y_1' + \phi_0'' y_1 + 2y_0'' = 0,\\
&2\phi_0 y_2'' + \phi_0' y_2' + \phi_0'' y_2 + 2y_1'' = 0,\\
&\cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\\
&\cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\\
&2\phi_0 y_n'' + \phi_0' y_n' + \phi_0'' y_n + 2y_{n-1}'' = 0.
\end{aligned}
\tag{4.3}
$$

All perturbation functions may be required to satisfy the initial conditions

$$
\begin{aligned}
y_n &= 0,\\
y_n' &= 0,
\end{aligned}
$$

while the principal solution y_0 satisfies the given initial conditions. Let u_0 and v_0 be the fundamental solutions of (4.1) satisfying the initial conditions $u_0 = 1$, $u_0' = 0$, $v_0 = 0$, $v_0' = 1$, so that we may write

$$y_0 = au_0 + bv_0,$$

where a and b are the initial conditions. Now the first perturbation function may be written as *)

$$y_1 = v_0 \int \frac{-2y_0'' u_0}{\Delta(u_0, v_0)}\, \mathrm{d}x - u_0 \int \frac{-2y_0'' v_0}{\Delta(u_0, v_0)}\, \mathrm{d}x, \tag{4.4}$$

where

$$\Delta(u_0, v_0) = (u_0 v_0' - v_0 u_0')\, 2\phi_0.$$

Substituting for y_0'' into (4.4) we obtain

$$
\begin{aligned}
y_1 = a\left[+ v_0 \int \frac{-2u_0'' u_0}{\Delta(u_0, v_0)}\, \mathrm{d}x - u_0 \int \frac{-2u_0'' v_0}{\Delta(u_0, v_0)}\, \mathrm{d}x\right] + \\
+ b\left[v_0 \int \frac{-2v_0'' u_0}{\Delta(u_0, v_0)}\, \mathrm{d}x - u_0 \int \frac{-2v_0'' v_0}{\Delta(u_0, v_0)}\, \mathrm{d}x\right].
\end{aligned}
\tag{4.5}
$$

Now compare each of the brackets on the right-hand side of (4.5) with (4.4). Each of them represents a perturbation function corre-

*) To obtain this, see ref. 3, p. 530. In 5.2.19 let $c_1 = c_2 = 0$ because of our initial conditions.

sponding to one of the fundamental solutions, u_0 and v_0; hence we may write

$$y_1 = au_1 + bv_1,$$

where u_1 and v_1 are the first fundamental perturbation functions corresponding to the fundamental solutions u_0 and v_0 respectively. Following a similar procedure, we can show that

$$y_n = au_n + bv_n$$

for all values of n. The fundamental perturbation functions may be obtained by solving the system of differential equations given by (4.1) and (4.3) numerically. The above method of taking into account the effect of the abnormal initial conditions has the following two advantages:

(i) fundamental perturbation functions are easily computed on a digital computer;

(ii) it is not necessary to compute the perturbation functions for each set of initial conditions as in the original method or slightly different method due to Moulton[5]).

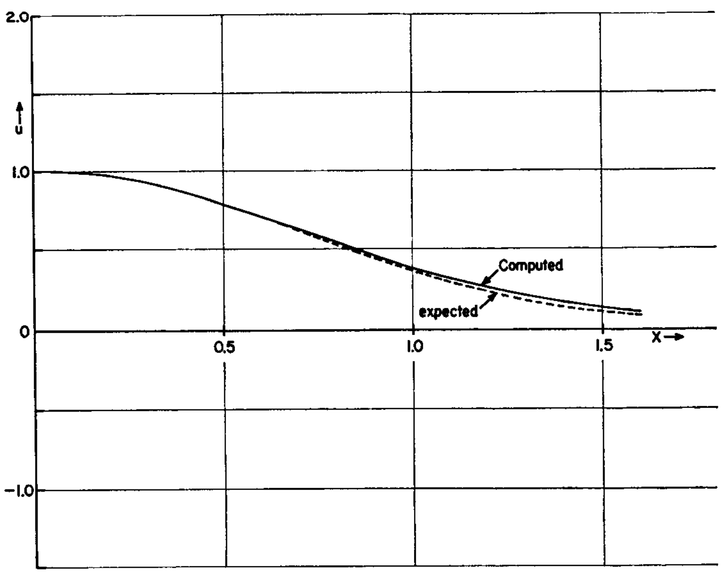

Fig. 4. System I. First fundamental solution (u_0).

For the sake of simplicity we specify the normal initial conditions as

$$y_0 = a,$$
$$y_0' = 0,$$

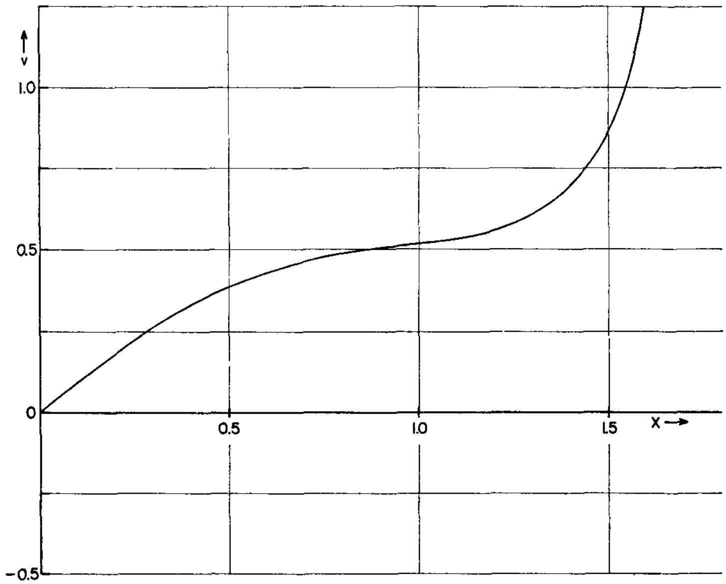

Fig. 5. System I. Second fundamental solution (v_0).

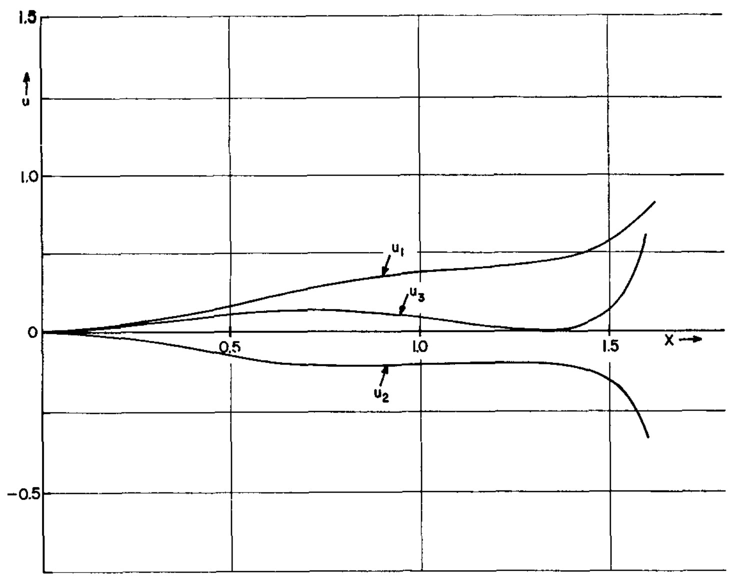

Fig. 6. System I. Perturbation functions (u_n).

and the initial average energy $\phi_0(0) = 1$. Then the trajectory of a particle with given abnormal initial conditions $y_0' = b$ and $\phi_0(0) = 1 + \varepsilon$ is given by

$$\tilde{y} = au_0 + bv_0 + a \sum_1^m \varepsilon^n u_n + b \sum_1^m \varepsilon^n v_n. \tag{4.6}$$

All perturbation functions are illustrated in figures 4 to 11. The fundamental perturbation functions for System I increase monotonically in the region where the particles are accelerated, and outside this region they tend to oscillate (not shown in the figures). Hence the abnormal initial conditions are amplified to a stage when the particle trajectories deviate so much from their projected paths

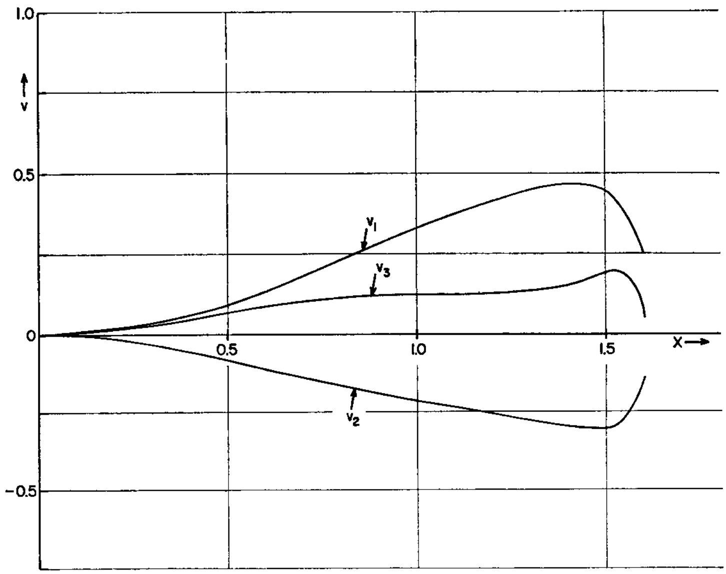

Fig. 7. System I. Perturbation functions (v_n).

that it leads to an unstable situation (fig. 12). The system II, on the other hand, is characterized by damped oscillatory perturbation functions (figs. 9 to 11) so that the abnormal initial conditions are damped out, leading to a stable situation (fig. 13).

§ 5. *Conclusion.* We have shown that given a set of paths which satisfy certain conditions (equation (2.6)) a unique potential distribution can be found so as to guide the particles along these paths.

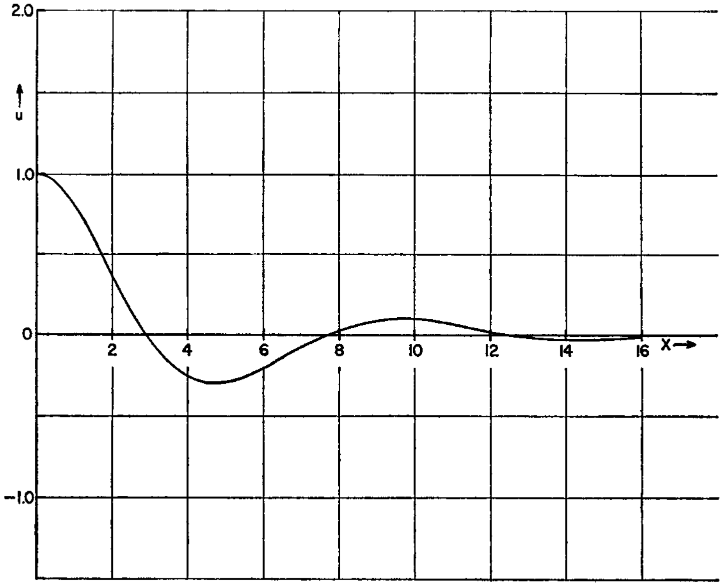

Fig. 8. System II. First fundamental solution (u_0).

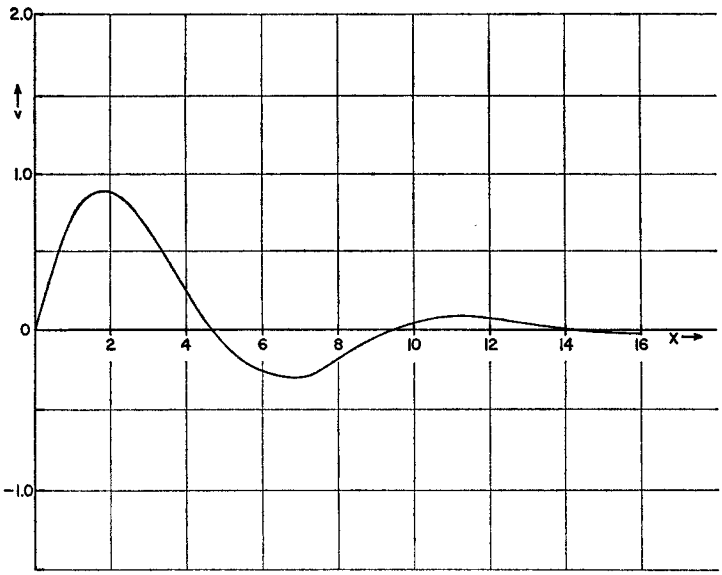

Fig. 9. System II. Second fundamental solution (v_0).

An application of the theory of the inverse problem to the design of an efficient ion source for a mass spectrometer is given. Although in principle one may choose any set of converging paths and find the appropriate potential distribution, for the system to be stable, the set of paths must belong to the class of damped oscillatory

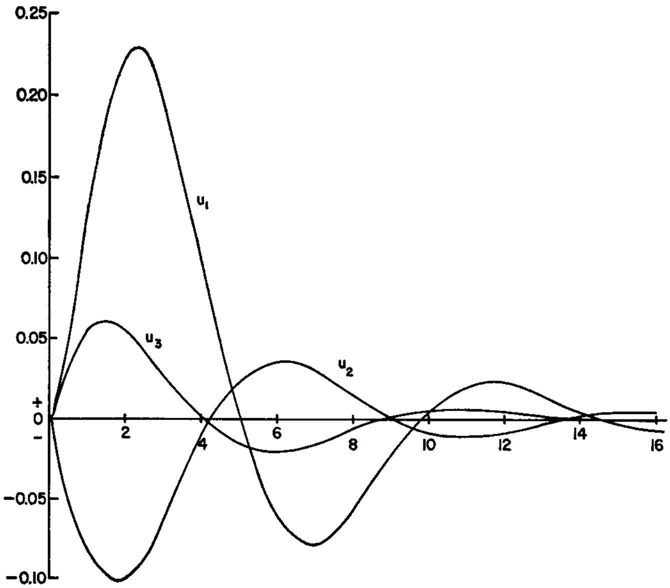

Fig. 10. System II. Perturbation functions (u_n).

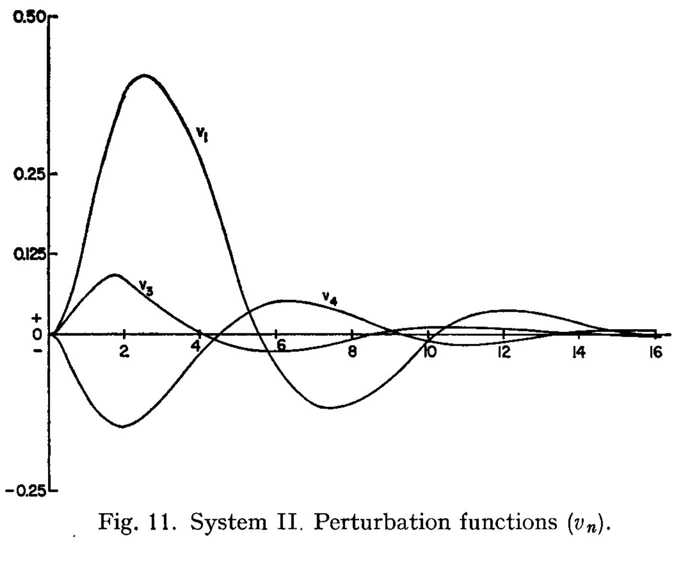

Fig. 11. System II. Perturbation functions (v_n).

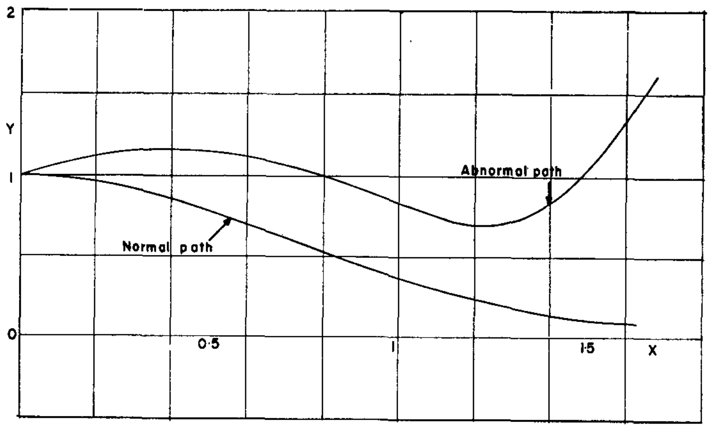

Fig. 12. System I. Unstable abnormal path.

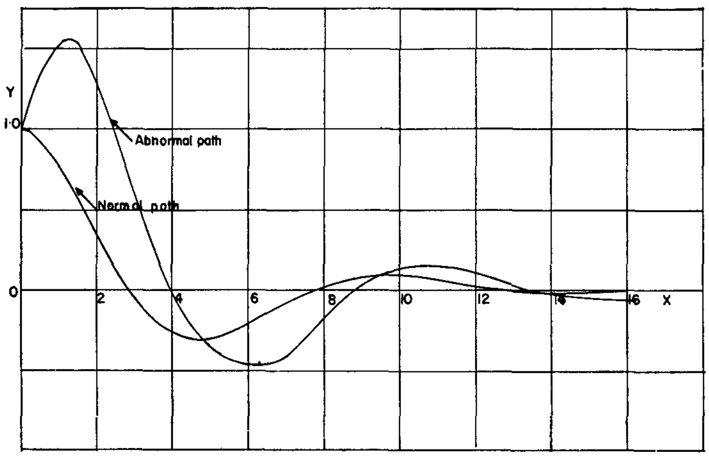

Fig. 13. System II. Stable abnormal path.

functions and also the chosen set of paths must be complete, i.e. without any mirror points. Fortunately, the damped oscillatory paths are complete and stable; and hence they are ideally suited for the formation of convergent beam of charged particles.

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