INVERSE PROBLEMS

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- 1. Introduction. We call two problems inverses of one another if the formulation of each involves all or part of the solution of the other. Often, for historical reasons, one of the two problems has been studied extensively for some time, while the other is newer and not so well understood. In such cases, the former is called the **direct problem**, while the latter is called the **inverse problem**. As illustrations, we present the following three inverse problems. The corresponding direct problems, which are their solutions, are given in the appendix.
 - 1. What is the question to which the answer is "Washington Irving"?
 - 2. What is the question to which the answer is "Nine W"?
 - 3. What is the question to which the answer is "Chicken Sukiyaki"?

These examples demonstrate that inverse problems often have many solutions, and also that some particular solution is preferable to the others.

Some examples of inverse problems in mathematics are the following:

- 4. Find a polynomial p(x) of degree n with the roots x_1, \dots, x_n . This is inverse to the direct problem of finding the roots x_1, \dots, x_n of a given polynomial p(x) of degree n. In this case the inverse problem is easier, having the solution $p(x) = c(x x_1) \cdots (x x_n)$, which is not unique because $c \neq 0$ is an arbitrary constant.
- 5. Find a polynomial p(x) of degree n with given values y_1, \dots, y_n at x_1, \dots, x_n . The corresponding direct problem is to find the values y_1, \dots, y_n of a given polynomial p(x) at x_1, \dots, x_n . The inverse problem is called the Lagrange interpolation problem, while the direct problem is that of evaluation of a polynomial.
- 6. Given a real symmetric matrix A of order n, and n real numbers $\lambda_1, \dots, \lambda_n$, find a diagonal matrix D so that A + D has eigenvalues $\lambda_1, \dots, \lambda_n$. This is inverse to the direct problem of finding the eigenvalues $\lambda_1, \dots, \lambda_n$ of a given real symmetric matrix A + D.

A common inverse problem used on intelligence tests is this:

7. Given the first few members a_1 , a_2 , a_3 , a_4 of a sequence, find the law of formation of the sequence, i.e., find a_n for all positive integers n. Usually only the next few members a_5 , a_6 , a_7 are asked for as evidence that the law of formation has been found. The direct problem is to evaluate the first few members of a sequence a_n , given the law of formation. A well-known instance of this inverse problem is to find the next few members of the sequence which begins 4, 14, 34, 42. The solution is 59, 125, 145, since the sequence consists of the express stops on the 8th Avenue subway in New York. It is clear that such inverse problems have many solutions, and for this reason their use on intelligence tests has been criticized.

The main sources of inverse problems are science and engineering. Often these problems concern the determination of the properties of some inaccessible region from observations on the boundary of the region. Here are some examples:

8. Find the mass distribution $\rho(x)$ of matter within the earth, given the gravitational potential $\phi(x)$ for x on the surface of the earth. This is inverse to the direct problem of finding $\phi(x)$ given $\rho(x)$, which has the solution

$$\phi(x) = \frac{G}{4\pi} \int \rho(x')/|x-x'| dx'.$$

Here G is the gravitational constant and |x-x'| is the distance from x to x'. The inverse problem is

important in locating high or low density regions within the earth, which may contain ore or oil, from observations of anomalies in the gravitational potential on the earth's surface.

- 9. Find the intermolecular potential V(r) between two molecules a distance r apart, given the equation of state of a gas composed of such molecules. This is inverse to the direct problem of finding the equation of state, given the potential, which is a basic problem of statistical mechanics.
- 10. Find the intermolecular potential V(r) from scattering data; i.e., from information about the angle through which a molecule is scattered when it collides with another molecule. The direct problem is that of calculating the scattering angle, given the potential. These problems can be analyzed by either classical mechanics or quantum mechanics, and the two kinds of analysis are applicable in different physical situations.
- 11. Find the shape of a scattering object, given the intensity of light, of radar waves, or of sound waves it scatters in any direction. The direct problem is that of calculating the scattered light, radar or sound intensity in any direction from a given illuminated object. This problem is important in identifying objects in space from radar observations of them, and of identifying objects in the ocean from sonar observations.

In each of the seven following sections of this paper, an inverse problem which has arisen in physics will be analyzed.

2. Determination of the shape of a hill from travel time, and probing the ionosphere. Suppose we slide a particle up a frictionless hill with initial energy E, and measure the time T(E) required for it to return. If we vary E and measure T(E), can we determine the shape of the hill from it? This problem was formulated and solved by Abel in 1826. To analyze it we shall first formulate and solve the **direct problem:** Given the shape of the hill, find the travel time T(E).

Let s denote arclength along the hill and let the height of the hill at s be h(s) with h(0) = 0. We denote by m the mass of the particle, by g the acceleration of gravity, and by s(t) the position of the particle at time t. Then the equation of motion of the particle is

$$m\frac{d^2s(t)}{dt^2} = -\frac{dV(s)}{ds}.$$

Here V(s) = mgh(s) is the potential energy of the particle at s, so V(0) = 0. We shall measure s and t from the initial position and from the instant of release of the particle, respectively, and denote by v_0 its initial velocity. Then the initial conditions are

(2.2)
$$s(0) = 0, \quad \frac{ds(0)}{dt} = v_0.$$

We shall assume that $v_0 > 0$.

We now multiply (2.1) by ds/dt and integrate to get the energy equation

(2.3)
$$\frac{1}{2} m \left(\frac{ds}{dt}\right)^2 + V(s) = E.$$

In (2.3) E is the total energy of the particle, given by

$$(2.4) E = \frac{1}{2} m v_0^2.$$

Next we solve (2.3) for $(ds/dt)^{-1}$ choosing the positive square root because $v_0 > 0$, and integrate using (2.2) to get

(2.5)
$$t = \left(\frac{m}{2}\right)^{1/2} \int_0^s \left[E - V(s')\right]^{-1/2} ds', \qquad 0 \le t \le \frac{1}{2} T(E).$$

This equation yields the solution in the form t = t(s) from s = 0 until s reaches the value $s_1(E)$, which is the smallest value of $s \ge 0$ at which E - V(s) = 0. The corresponding value of t, which we shall call

 $\frac{1}{2}T(E)$, is given by setting $s = s_1(E)$ in (2.5). Thus

(2.6)
$$T(E) = (2m)^{1/2} \int_0^{s_1(E)} [E - V(s')]^{-1/2} ds'.$$

At the instant T(E)/2 the particle velocity vanishes, and then the velocity becomes negative. Thus the solution for $t \ge T(E)/2$ is obtained by using the negative square root in solving (2.3). The result can be written in the form

(2.7)
$$t = \frac{1}{2} T(E) + \left(\frac{m}{2}\right)^{1/2} \int_{s}^{s_1(E)} \left[E - V(s')\right]^{-1/2} ds', \quad \frac{1}{2} T(E) \le t.$$

By setting s = 0 in (2.7), we see that the time at which the particle returns to its initial position s = 0 is just T(E) given by (2.6). Thus (2.6) yields the solution of the direct problem. We see that it is defined only for those values of E for which $s_1(E)$ exists. These are just the values of E in the interval $0 \le E \le V_m = \sup_{s \ge 0} V(s)$. For $E > V_m$ the particle never returns to s = 0, so we can set $T(E) = \infty$ for $E > V_m$.

Now we can consider the inverse problem: Given the travel time T(E) for $E \ge 0$, find the shape of the hill, i.e., find the potential V(s) for $s \ge 0$. Once we know V(s) then the height of the hill is given by h(s) = V(s)/mg. To find the equation of the hill in cartesian coordinates we write it parametrically as x(s), y(s). Then y(s) = h(s), while x(s) is related to y(s) by the arclength condition $(dx/ds)^2 + (dy/ds)^2 = 1$. Solving this equation for dx/ds and integrating yields

(2.8)
$$x(s) = x(0) + \int_0^s \left(1 - \left[\frac{dh(s')}{ds}\right]^2\right)^{1/2} ds', \qquad s \ge 0.$$

This shows that the shape of the hill can be determined readily once V(s) is found, so it suffices to find V(s).

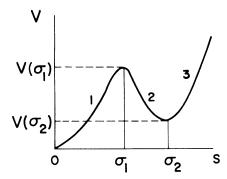


Fig. 1. A potential V(s) which is increasing in the interval $0 \le s < \sigma_1$, decreasing in $\sigma_1 < s < \sigma_2$ and increasing again in $\sigma_2 < s$. The inverse function is called $s_1(V)$ in the first interval, $s_2(V)$ in the second interval and $s_3(V)$ in the third interval.

To find V(s) we shall start with (2.6), which relates T(E) to V(s). It is a nonlinear integral equation for V. We can convert it into a linear integral equation by introducing V instead of s as the integration variable. This change of integration variable must be made separately in each interval within which V(s) is monotonic. Therefore we first consider the first such interval, $0 \le s \le \sigma_1$ and suppose that V(s) is monotone increasing within it. (See Fig. 1.) Let $s = s_1(V)$ denote the inverse of V(s) within this interval, within which $0 \le V \le V(\sigma_1)$. Then we can rewrite (2.6) in this interval in the form

(2.9)
$$T(E) = (2m)^{1/2} \int_{0}^{E} [E - V]^{-1/2} \frac{ds_{1}(V)}{dV} dV, \qquad 0 \le E \le V(\sigma_{1}).$$

Eq. (2.9) is a Volterra integral equation of the first kind for ds_1/dV , and with the kernel $(E-V)^{-1/2}$ it is called an Abel equation. Its solution for $ds_1(V)/dV$ is

(2.10)
$$\frac{ds_1(V)}{dV} = \frac{T(0)}{(2mV)^{1/2}\pi} + \frac{1}{(2m)^{1/2}\pi} \int_0^V (V - E)^{-1/2} T'(E) dE.$$

This can be verified by substitution into (2.9). Finally integrating (2.10) from 0 to V yields, after an integration

(2.11)
$$s_1 = \frac{1}{(2m)^{1/2}\pi} \int_0^V (V - E)^{-1/2} T(E) dE, \qquad 0 \le V \le V(\sigma_1).$$

This is the solution of the inverse problem for V(s) in the interval $0 \le s \le \sigma_1$. It was obtained by Abel. If $V(\sigma_1) = \infty$, it is the complete solution. This solution applies to a particle in any potential, not only a gravitational one.

A method like that described here is used to find the electron density n(s) at height s above the earth in the ionosphere. The method is to send up a radio wave of angular frequency ω , and to measure the time $T(\omega)$ required for it to return to the ground from the ionosphere. The group velocity c_s of a wave of frequency ω in an electron plasma, like the ionosphere, is $c_s = c\omega^{-1}[\omega^2 - \omega_p^2(s)]^{1/2}$. Here c is the velocity of light in vacuum and $\omega_p^2(s) = 4\pi e^2 n(s)/m$ is the plasma frequency, where e and e are the charge and mass of an electron, respectively. Thus the time for a wave to travel from e oup to the first point e is e0, where e0 and then back down to e0 is

(2.12)
$$T(\omega) = 2 \int_{0}^{s_{1}(\omega)} \frac{ds}{c_{g}} = \frac{2\omega}{c} \int_{0}^{s_{1}(\omega)} \left[\omega^{2} - \omega_{p}^{2}(s)\right]^{-1/2} ds.$$

This is of the form (2.6) and therefore its solution is of the form (2.11):

$$(2.13) s_1(\omega) = \frac{c}{\pi} \int_0^{\omega_p^2} \left[\omega_p^2 - \omega^2 \right]^{-1/2} T(\omega) d\omega.$$

3. The nonmonotonic case. Now we suppose that $V(\sigma_1)$ is finite, and that V is decreasing in the interval $\sigma_1 < s < \sigma_2$ and then increasing in the next interval $\sigma_2 < \sigma < \sigma_3$. (See Fig. 1.) We denote by $s_2(V)$ and $s_3(V)$ the inverses of V(s) in these two intervals, respectively. Then we can write (2.6) in the form

(3.1)
$$T(E) = (2m)^{1/2} \left[\int_0^{V(\sigma_1)} (E - V)^{-1/2} \frac{ds_1}{dV} dV - \int_{V(\sigma_2)}^{V(\sigma_1)} (E - V)^{-1/2} \frac{ds_2}{dV} dV + \int_{V(\sigma_2)}^{E} (E - V)^{-1/2} \frac{ds_3}{dV} dV \right].$$

Next we define w(V), the width at depth V of the "potential well," by

(3.2)
$$w(V) = s_3(V) - s_2(V), \quad V(\sigma_2) \le V \le V(\sigma_1).$$

In writing (3.2) we assume that $E \ge V(\sigma_1)$. Then we can rewrite (3.1) as

(3.3)
$$T(E) = (2m)^{1/2} \left[\int_0^{V(\sigma_1)} (E - V)^{-1/2} \frac{ds_1}{dV} dV + \int_{V(\sigma_1)}^E (E - V)^{-1/2} \frac{ds_3}{dV} dV + \int_{V(\sigma_2)}^{V(\sigma_1)} (E - V)^{-1/2} \frac{dw}{dV} dV \right].$$

The formula (3.3) shows that T(E) involves only the width function w(V) of the well, and does not depend upon its two sides $s_2(V)$ and $s_3(V)$ separately. Therefore it is not possible to obtain these sides from T(E). However, as we shall soon see, it is not even possible to determine w(V) from T(E).

Let us regard (3.3) as an integral equation for ds_3/dV in the range $V \ge V(\sigma_1)$. Then it is of the same form as (2.9) with T(E) replaced by T(E) plus the integrals involving ds_1/dV and dw/dV, and with the lower limit replaced by $V(\sigma_1)$. Therefore the solution is given by (2.10) with the same replacement. After integration, the solution becomes

$$(3.4) s_3(V) = s_3[V(\sigma_1)] + \frac{1}{\pi} \int_{V(\sigma_1)}^{V} (V - E)^{-1/2} \left[(2m)^{-1/2} T(E) - \int_{0}^{V(\sigma_1)} (E - z)^{-1/2} \frac{ds_1}{dz} dz \right]$$

$$- \int_{V(\sigma_2)}^{V(\sigma_1)} (E - z)^{-1/2} \frac{dw}{dz} dz dE, V(\sigma_1) \leq V.$$

This form of the solution can be simplified with the aid of the integral formula

(3.5)
$$\int_{V(\sigma_1)}^{V} (V-E)^{-1/2} (E-z)^{-1/2} dE = 2 \sin^{-1} \left(\frac{E-z}{V-z} \right)^{1/2} \Big|_{V(\sigma_1)}^{V} = \pi - 2 \sin^{-1} \left[\frac{V(\sigma_1)-z}{V-z} \right]^{1/2}.$$

When (3.5) is used in (3.4), the solution can be written in the simpler form

$$(3.6) s_3(V) = \frac{1}{(2m)^{1/2}\pi} \int_{V(\sigma_1)}^{V} (V - E)^{-1/2} T(E) dE + \frac{2}{\pi} \int_{0}^{V(\sigma_1)} \frac{ds_1}{dz} \sin^{-1} \left[\frac{V(\sigma_1) - z}{V - z} \right]^{1/2} dz + \frac{2}{\pi} \int_{V(\sigma_2)}^{V(\sigma_1)} \frac{dw}{dz} \sin^{-1} \left[\frac{V(\sigma_1) - z}{V - z} \right]^{1/2} dz, V(\sigma_1) \leq V.$$

The result (3.4) or (3.6) shows that $s_3(V)$ is not unique, since w(V) can be chosen arbitrarily. For each choice of w(V), $s_3(V)$ is determined uniquely in the range $V \ge V(\sigma_1)$, up to the next local maximum of V(s). The function ds_1/dV in (3.4) is given by (2.10) in terms of T(E).

The preceding considerations can be applied at once to a potential V(s) with any number of local maxima and minima, but we shall not do that.

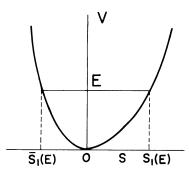


Fig. 2. A potential V(s) which increases as |s| increases. The intersections of the graph with the horizontal line at height E are the roots $s_1(E)$ and $\bar{s}_1(E)$ of the equation V(s) = E.

4. Determination of a potential from the period of oscillation. Let us now consider a particle in a potential well. (See Fig. 2.) Its motion is still governed by (2.1) with the initial conditions (2.2). Therefore the results (2.3)-(2.7) apply, so the particle travels to the right until it reaches the point $s_1(E)$ at the time T(E)/2 and then it travels to the left, returning to the origin at the time T(E). Its velocity at the origin is $-v_0$, so it will continue past the origin until it reaches a point $\bar{s}_1(E)$ where E - V(s) = 0, at a time we shall call $T(E) + \frac{1}{2}\bar{T}(E)$. Then its velocity reverses sign and it travels to the right, reaching the origin again at the time $T(E) + \bar{T}(E)$ with the velocity v_0 . Thereafter the motion repeats periodically, since the position and velocity have returned to their initial values s = 0 and $ds/dt = v_0$.

The period P(E) of this periodic motion is $P(E) = T(E) + \bar{T}(E)$, since the initial conditions first recur at this time. Now T(E) is given by (2.6), and $\bar{T}(E)$ is given by the corresponding expression with $s_1(E)$ replaced by $\bar{s}_1(E)$, and with the negative square root. Thus the period is given by

$$(4.1) \quad P(E) = T(E) + \bar{T}(E) = (2m)^{1/2} \int_0^{s_1(E)} [E - V(s)]^{-1/2} ds - (2m)^{1/2} \int_0^{\bar{s}_1(E)} [E - V(s)]^{-1/2} ds$$

$$= (2m)^{1/2} \int_{\bar{s}_1(E)}^{s_1(E)} [E - V(s)]^{-1/2} ds.$$

Here $s_1(E)$ and $\bar{s}_1(E)$ are respectively the smallest (in absolute value) positive and negative roots of the equation V(s) = E.

The result (4.1) is the solution of the following problem, which we shall call the **direct problem:** Given a potential well V(s), find the period P(E) of oscillation of a particle with energy E. It is important to note that in general the period does vary with E, since in the often studied case of small amplitude oscillations, the period is independent of E. We shall return to this point later. Now we shall pose the **inverse problem:** Given the period of oscillation P(E) of a particle with energy E in a potential V(s), find the potential.

To solve the inverse problem, let us consider first the case in which V(s) is symmetric, V(s) = V(-s). In this case it is clear that $\bar{s}_1(E) = -s_1(E)$ and then $\bar{T}(E) = T(E)$. Thus the period is just P(E) = 2T(E), where T(E) is given by (2.6). The problem of finding V(s) was solved in Section 2 for the case in which V(s) is monotonic increasing for s > 0. The solution is given by (2.11). The inverse problem for this symmetric monotonic case was first posed and solved by B. F. Kimball (1932). The symmetric nonmonotonic case is treated in Section 3.

Next, let us consider the nonsymmetric case. For simplicity we shall assume that V(s) is monotone increasing as |s| increases. Then we can introduce the two inverses $s_1(V) > 0$ and $\bar{s}_1(V) < 0$ of V(s), and write (4.1) in the form

(4.2)
$$P(E) = (2m)^{1/2} \int_0^E (E - V)^{-1/2} \frac{ds_1}{dV} dV - (2m)^{1/2} \int_0^E (E - V)^{-1/2} \frac{d\bar{s}_1}{dV} dV$$
$$= (2m)^{1/2} \int_0^E (E - V)^{-1/2} \frac{dw}{dV} dV.$$

In writing the last form of the expression for P(E), we have again introduced w(V), the width of the well at height V, defined by $w(V) = s_1(V) - \bar{s}_1(V)$. This form shows that P(E) depends only upon w(V), and not upon the separate sides of the well, $s_1(V)$ and $\bar{s}_1(V)$. Therefore it is not possible to obtain these sides from P(E), but only the width.

Eq. (4.2) is an Abel equation for dw/dV which is of the form (2.9) with w and P replacing s_1 and T, respectively. Therefore the solution is given by (2.11) with the same replacements, i.e.,

(4.3)
$$w(V) = \frac{1}{(2m)^{1/2}\pi} \int_{0}^{V} (V - E)^{-1/2} P(E) dE, \quad 0 \le V.$$

In the symmetric case $\bar{s}_1(V) = -s_1(V)$ so $w(V) = 2s_1(E)$ and P(E) = 2T(E). Then (4.3) becomes identical with (2.11). It is always possible to assume that the well is symmetric, and then (2.11) yields the unique symmetric solution. However, whether or not the solution is symmetric is not determined by P(E); only the width is determined.

As an application of (4.3), we shall find w(V) when the period P(E) is constant, independent of E. Then (4.3) yields

$$(4.4) w(V) = \frac{P}{\pi} \left[\frac{2V}{m} \right]^{1/2}.$$

Solving (4.4) for V yields

$$(4.5) V = \frac{m}{2} \left[\frac{\pi w}{P} \right]^2.$$

Thus, if and only if V is proportional to w^2 is the period constant, independent of E. In the symmetric case when $w = 2s_1$, (4.5) is just the quadratic potential which arises in the analysis of small amplitude oscillations.

The results of this section are due to J. B. Keller (1962). They can be extended to the case in which V(s) is not a monotone function of |s| by the method of Section 3, but we shall not carry out that extension.

5. Inverse transit time problem. We shall again consider a particle moving in the potential V(s), governed by (2.1) with the initial condition (2.2). We now pose the following direct problem: Find the transit time $\tau(E)$ required for a particle of energy E to travel from s = 0 to s = L > 0. From the analysis of Section 3, we know that the particle will reach L if and only if E satisfies the condition

$$(5.1) E > V_m = \sup_{0 \le s \le L} V(s).$$

When (5.1) is satisfied, $\tau(E)$ is obtained by setting s = L in the solution (2.5), which yields

(5.2)
$$\tau(E) = \left[\frac{m}{2}\right]^{1/2} \int_{0}^{L} [E - V(s)]^{-1/2} ds, \qquad E > V_{m}.$$

From the solution (5.2) of the direct problem, we see that $\tau(E)$ is a decreasing function of E. A series expansion of τ can be obtained by expanding the integrand with the aid of the binomial theorem, and integrating term by term. This yields with binomial coefficients c_n

(5.3)
$$\tau(E) = \left[\frac{m}{2E}\right]^{1/2} \sum_{n=0}^{\infty} c_n E^{-n} \int_0^L V^n(s) ds, \qquad E > V_m.$$

Now we can formulate the **inverse problem:** Given the transit time $\tau(E)$ for $E > V_m$, find the potential V(s). In order that this problem have a solution, the given $\tau(E)$ must possess an expansion of the form (5.3), which we shall write as follows:

(5.4)
$$\tau(E) = \left[\frac{m}{2E}\right]^{1/2} \sum_{n=0}^{\infty} c_n E^{-n} \tau_n, \qquad E > V_m.$$

By comparing (5.3) with (5.4), we see that the coefficients τ_n in the expansion of the given function $\tau(E)$ are related to the unknown function V(s) by the relations

(5.5)
$$\tau_n = \int_0^L V^n(s) ds, \qquad n = 0, 1, \cdots.$$

To find V(s) from (5.2) or (5.5), we shall assume that V(s) is monotone increasing. Then we can rewrite (5.2) and (5.5) as follows:

(5.6)
$$\tau(E) = \left(\frac{m}{2}\right)^{1/2} \int_0^{V(L)} (E - V)^{-1/2} \frac{ds}{dV} dV, \qquad E > V(L) = V_m.$$

(5.7)
$$\tau_{n} = \int_{0}^{V(L)} V^{n} \frac{ds}{dV} dV, \qquad n = 0, 1, \cdots.$$

Eq. (5.6) is a linear integral equation for ds/dV, called a Fredholm equation of the first kind. It differs from the Volterra equation (2.9) by having a fixed upper limit of integration, rather than a variable limit. Because of this difference we cannot solve it explicitly, as we did (2.9). Therefore we shall instead try to find ds/dV from (5.7).

The integral in (5.7) is called the *n*th moment of ds/dV. Thus the problem of finding ds/dV is equivalent to that of finding a function from all its moments. This classical problem is called the **moment problem.** One aspect of it is to determine whether a given set of numbers τ_n are the moments of some function. We shall assume that they are, because of the manner in which they are determined. Then it remains to find ds/dV from them. Because (5.7) is a linear relation between ds/dV and τ_n , it follows that ds/dV is a linear function of the τ_n . Thus we shall seek ds/dV in the form

(5.8)
$$\frac{ds}{dV} = \sum_{n=0}^{\infty} \tau_n g_n(V).$$

The functions $g_n(V)$ are to be determined in such a way that (5.7) holds. This leads to the condition

(5.9)
$$\int_{0}^{V(L)} V^{n} g_{j}(V) dV = \delta_{nj}.$$

Eq. (5.9) can be satisfied by choosing for $g_n(V)$ an appropriate polynomial of degree n. To find this polynomial it is convenient to introduce the orthonormal polynomials $\phi_n(V)$ of degree n, which satisfy

(5.10)
$$\int_0^{V(L)} \phi_n(V) \phi_j(V) dV = \delta_{nj}.$$

Then we express V^n and $g_n(V)$ in terms of the ϕ_n as follows:

(5.11)
$$V^{n} = \sum_{i=0}^{\infty} c_{ni}\phi_{j}(V), \qquad c_{nj} = \int_{0}^{V(L)} V^{n}\phi_{j}(V)dV,$$

(5.12)
$$g_k(V) = \sum_{j=0}^{\infty} g_{kj} \phi_j(V).$$

Substitution of (5.11) and (5.12) into (5.9), and then using (5.10), yields for the g_{kj} the equations

$$(5.13) \sum_{i=0}^{\infty} c_{ni}g_{kj} = \delta_{nk}.$$

It follows from (5.11) that the matrix c_{nj} is triangular, i.e., $c_{nj} = 0$ for j > n, and therefore (5.13) can be solved recursively for the g_{kj} . Then $g_n(V)$ is given by (5.12) and ds/dV is given by (5.8). Integrating (5.8) yields finally

(5.14)
$$s(V) = \sum_{n=0}^{\infty} \tau_n \int_0^V g_n(V') dV'.$$

The foregoing analysis yields the unique monotone increasing solution V(s) of (5.2). It is clear from (5.2), however, that any function equimeasurable with this solution is also a solution. Thus the inverse problem has many solutions, and we have found a particular one of them.

6. Inverse eigenvalue problem. In quantum mechanics the wave function $\psi(x)$ of a particle of mass m in a potential V(x) satisfies the Schrödinger equation

(6.1)
$$\psi_{xx} + \frac{2m}{\hbar^2} [E - V(x)] \psi = 0, \quad -\infty < x < \infty.$$

Here \hbar is Planck's constant divided by 2π , and E is the energy of the particle. Let us suppose that V(x) is a monotonic increasing function of |x|, tending to $+\infty$ as |x| becomes infinite. Then (6.1) has a quadratically integrable solution, not identically zero, if and only if E is equal to one of the discrete set of eigenvalues E_n , $n = 0, 1, \cdots$ of the equation (6.1). The eigenvalues tend to $+\infty$ as n increases, and they can be labelled so that $E_{n+1} \ge E_n$.

The direct problem is that of finding the E_n , given V(x). This problem can be solved asymptotically for large values of E_n by the so-called WKB method. In this method one seeks a solution of (6.1) of the form $\psi(x) \sim A(x) \sin s(x)$. By first ignoring derivatives of A, one gets an equation for s. Then by keeping A_x but ignoring A_{xx} , one gets an equation for A. This leads to the following asymptotic form of ψ :

(6.2)
$$\psi(x) \sim [E - V(x)]^{-1/4} \sin \left\{ \frac{\pi}{4} + \int_{\bar{x}_1(E)}^x \left[\frac{2m}{\hbar^2} \left[E - V(x') \right] \right]^{1/2} dx' \right\}, \quad \bar{x}_1(E) < x < x_1(E).$$

This result holds only between the two roots $\bar{x}_1(E)$ and $x_1(E)$ of V(x) = E, and the constant $\pi/4$ results from matching (6.2) to a boundary layer solution valid around $\bar{x}_1(E)$. A similar matching to a boundary layer solution valid around $x_1(E)$ leads to the condition

(6.3)
$$(2m)^{1/2} \int_{\bar{x}_1(E)}^{x_1(E)} \left[E - V(X) \right]^{1/2} dx = \left(n + \frac{1}{2} \right) \pi \hbar, \qquad n = 0, 1, \cdots.$$

This equation (6.3) can be viewed as an equation for the determination of E_n , and thus provides an asymptotic solution to the **direct problem**. The **inverse problem** is that of finding the potential V(x) given the eigenvalues E_n , $n = 0, 1, \cdots$. To solve it, we shall begin with (6.3), which holds asymptotically with $E = E_n$ and n a large integer. We interpolate the given values E_n by a smooth function E(n), defined for all real $n \ge 0$. Then we assume that (6.3) holds for all $n \ge 0$ with E = E(n), and (6.3) becomes an integral equation for V(x). Differentiating (6.3) with respect to n and dividing by dE/dn yields

(6.4)
$$2\pi\hbar \left[\frac{dE}{dn}\right]^{-1} = (2m)^{1/2} \int_{\bar{x}_1(E)}^{x_1(E)} \left[E - V(x)\right]^{-1/2} dx.$$

If we set $P(E) = h(dE/dn)^{-1}$, (6.4) becomes identical with (4.1). Therefore (6.4) has the solution (4.3) for the width w(V) of the potential, which is all that can be determined from E(n). This nonuniqueness is to be expected from the general theory of the inverse eigenvalue problem, and it is not a consequence of our method of approximate solution. If the potential is even, V(-x) = V(x), then $w(V) = 2x_1(E)$ and the potential is unique. When the eigenvalues $E_n = (n + \frac{1}{2})h\omega$ are used in (4.3), and V(x) is assumed to be even, the potential $V(x) = \omega^2 m x^2/2$ is obtained, which is exactly that which yields these eigenvalues.

The fact that (6.4) coincides with (4.1) when $P(E) = 2\pi\hbar (dE/dn)^{-1}$ is an instance of the correspondence principle, according to which certain results of quantum mechanics are asymptotically equal to the corresponding results of classical mechanics at high energies. In the present case, the quantum mechanical frequency of oscillation ν associated with the energies E_{n+1} and E_n is given by $\hbar\nu = E_{n+1} - E \sim dE_n/dn$. Thus the period $\nu^{-1} \sim \hbar (dE/dn)^{-1}$ is asymptotic to the classical period P(E).

7. Inverse scattering problem. Suppose a moving particle is repelled from a fixed scattering center by a force derivable from a potential V(r), where r is distance from the center. Then the path of the moving particle is a curve which lies in the plane containing the center, the initial position of the moving particle, and its initial velocity. This path can be found by solving Newton's equations of motion for the particle. The result is that the path is like a hyperbola, with one asymptote along which it comes in from infinity and another asymptote along which it goes out again to infinity.

To describe the path, it is convenient to introduce polar coordinates r, θ in the plane of the path, with origin at the center. Let the incoming asymptote be the line y = b, x < 0 so that the particle comes in from $x = -\infty$ parallel to the x-axis and at distance b above it. The distance b is called the **impact parameter** of the particle. Then the direction of the outgoing asymptote, determined by solving the equations of motion, is found to be

(7.1)
$$\theta(b) = \pi - 2 \int_{r_0}^{\infty} \left[b^{-2} - r^{-2} - V(r) E^{-1} b^{-2} \right]^{-1/2} r^{-2} dr.$$

Here E < V(0) is the energy of the particle, and r_0 is the largest root of the bracketed expression in the integrand.

Suppose a uniform beam of particles of energy E is incident from $x = -\infty$. The number scattered in the directions from θ to $\theta + d\theta$ is denoted $-\sigma(\theta)2\pi \sin\theta d\theta$ apart from a constant factor, and $\sigma(\theta)$ is called the differential scattering cross-section. These particles are incident in the annular ring of area $2\pi bdb$ bounded by the impact parameters b and b + db and their number is proportional to this area. By equating the incoming and outgoing numbers of particles we get $-\sigma(\theta)2\pi \sin\theta d\theta = 2\pi bdb$, from which

(7.2)
$$\sigma(\theta) = -\frac{b}{\sin \theta} \frac{db}{d\theta}.$$

By using (7.1) to eliminate b from (7.2), we obtain the solution of the **direct scattering problem**, which is to find $\sigma(\theta)$ given V(r) and E.

The inverse scattering problem is to find V(r), given $\sigma(\theta)$ and E. To solve it we follow Keller, Kay and Shmoys (1956). First we integrate (7.2) to get

(7.3)
$$\int_{\theta}^{\pi} \sigma(\theta) \sin \theta d\theta = b^2/2.$$

Here we have used the fact that $\sigma(0) = \pi$, which follows from (7.1). Now (7.3) determines $\theta(b)$. Therefore we may now consider the inverse problem of finding V(r), given $\theta(b)$ and E. To solve it, we shall consider (7.1) to be an integral equation for V(r).

Let $x = b^{-2}$ and let us consider $\theta(x)$ to be a function of x. Similarly, let $u = r^{-1}$ and let us consider V(u) to be a function of u. Then we can write (7.1) as

(7.4)
$$\theta(x) = \pi - 2 \int_0^{u_0} \{x[1 - V(u)E^{-1}] - u^2\}^{-1/2} du, \qquad u_0 = r_0^{-1}.$$

Now we define v(u), w(u) and g(w) by

(7.5)
$$v(u) = 1 - V(u)E^{-1}, \qquad w(u) = u^2 v^{-1}(u), \qquad g(w) = v^{-1/2} \frac{du}{dw}.$$

Then we can put (7.4) in the form

(7.6)
$$\frac{1}{2} \left[\pi - \theta(x) \right] = \int_0^x (x - w)^{-1/2} g(w) dw.$$

The Abel equation (7.6) has the solution

(7.7)
$$g(w) = \frac{d}{dw} \left[\frac{1}{2\pi} \int_0^w \frac{\pi - \theta(x)}{(w - x)^{1/2}} dx \right].$$

From the definitions (7.5) of v and g we obtain by integration

(7.8)
$$v = \exp \int_0^\infty [2g(w)w^{-1/2} - w^{-1}]dw.$$

Finally by using (7.7) in (7.8) we get

(7.9)
$$v = \exp\left\{\frac{1}{\pi} \int_0^w (w')^{-1/2} \int_0^{\theta(w')} [w' - x(\theta)]^{-1/2} d\theta dw'\right\}.$$

This result, together with the definitions (7.5) of v and w, determines the potential V(r). As an example let us apply our result to the Rutherford scattering cross-section

(7.10)
$$\sigma(\theta) = \frac{e^2}{16E^2 \sin^4(\theta/2)},$$

where e is a constant. We obtain V = e/r, the Coulomb potential from which (7.10) comes. As a second example, we consider

(7.11)
$$\sigma(\theta) = \frac{e\left[1 - \frac{\theta}{\pi}\right]}{\pi E \sin\theta \left(\frac{\theta}{\pi}\right)^2 \left[2 - \frac{\theta}{\pi}\right]^2}.$$

From the equations above we get the inverse square potential $V = e/r^2$, which gives rise to (7.11).

8. Inversion of thermodynamic data. A problem of statistical mechanics is to determine the equation of state of a gas in terms of the potential V(r) between the molecules of the gas. If the number density n of the gas is small, the equation of state is found to be

(8.1)
$$\frac{p}{nRT} = 1 - 2\pi b(kT)n + O(n^2).$$

Here p is the pressure, T is the temperature, R is the gas constant, k is Boltzmann's constant and

(8.2)
$$b(kT) = \int_{0}^{\infty} [1 - e^{-V(r)/kT}] r^{2} dr.$$

The expansion (8.1) is called the virial expansion of the equation of state, and b is called the second virial coefficient.

The inverse problem which we consider, following J. B. Keller and B. Zumino (1959), is to determine V(r) given the equation of state. Since the equation of state can be obtained by thermodynamic measurements, this problem is that of finding the intermolecular potential from thermodynamic data. If the equation of state is known, then in particular b(kT) is known. Therefore we shall consider the **inverse problem** of finding V(r) given b(kT). The solution of the **direct problem** is given by (8.2), which we shall use as an integral equation for V(r).

Let us set $\mu = (kT)^{-1}$ and $v = r^3$, and regard $b = b(\mu)$ as a function of μ and V = V(v) as a function of v. Then we can write (8.2) in the form

(8.3)
$$b(\mu) = \frac{1}{3} \int_0^\infty \left[1 - e^{-\mu V(v)}\right] dv.$$

Differentiation of (8.3) with respect to μ yields

(8.4)
$$b'(\mu) = \frac{1}{3} \int_0^\infty V(v) e^{-\mu V(v)} dv.$$

We first suppose that V(v) is monotone decreasing from $V(0) = \infty$ to $V(\infty) = 0$, and introduce V as integration variable. Then we write (8.4) as

(8.5)
$$-3b'(\mu) = \int_0^\infty e^{-\mu V} V(dV/dv)^{-1} dV.$$

Equation (8.5) expresses $-3b'(\mu)$ as a Laplace transform of $V(dV/dv)^{-1}$. Thus if L^{-1} denotes the inverse Laplace transform, the solution of (8.5) is

$$(8.6) V(dV/dv)^{-1} = L^{-1}[-3b'(\mu)].$$

The solution of (8.6) which vanishes at $v = \infty$ is given by

(8.7)
$$v = 3 \int_{V}^{\infty} L^{-1}[b'(\mu)] \frac{dV'}{V'}.$$

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Thus when V(r) is monotonically decreasing, it is determined uniquely by b(kT), and (8.7) yields it explicitly.

If V is not monotone then it is not uniquely determined by b(kT). In fact, all equimeasurable functions V(v) yield the same function $b(\mu)$, as (8.3) shows. Let us suppose that V is not monotonic, but has the form shown in Fig. 3, which is typical of intermolecular potentials. Then we proceed as above, introducing V separately as the integration variable on each of the two monotonic branches of V(v). We find that (8.7) holds as before for V > 0. However for V < 0 we find instead

(8.8)
$$v_2(V) - v_1(V) = 3 \int_{V_0}^{V} L^{-1}[b'(\mu)] \frac{dV'}{V'}.$$

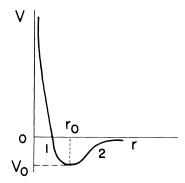


Fig. 3. A typical intermolecular potential V(r) which is decreasing in the interval $0 < r < r_0$ and increasing for $r > r_0$. The inverse is $r_1(V)$ in the first interval and $r_2(V)$ in the second interval.

Here $v_2(V)$ and $v_1(V)$ are the larger and smaller inverses of V(v), and V_0 is the minimum of V. As (8.8) shows, only the volume $4\pi/3[r_2^3(V)-r_1^3(V)]$ of the region where the potential is less than V is determined.

Appendix.

- 1. What is the capital of the United States, Max?
- 2. Do you spell your name with a "V," Herr Wagner?
- 3. What is the name of the sole surviving Kamikaze pilot?

Supported by the Office of Naval Research under Contract No. N00014-67-A-0467-0006 and at the Applied Mathematics Summer Institute under N00014-67-A-0467-0027.

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