

Inversion of Gamow's Formula and Inverse Scattering

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Abstract

We present a pedagogical description of the inversion of Gamow's tunnelling formula and we compare it with the corresponding classical problem. We also discuss the issue of uniqueness in the solution and the result is compared with that obtained by the method of Gel'fand and Levitan. We hope that the article will be a valuable source to students who have studied classical mechanics and have some familiarity with quantum mechanics.

1 Introduction

Eugen Merzbacher has commented that [1] "among all the successes of quantum mechanics as it evolved in the third decade of the 20th century, none was more impressive than the understanding of the tunnel effect—the penetration of matter waves and the transmission of particles through a high potential barrier." The tunnel effect provided a straightforward and remarkable explanation of the radioactive α -decay of nuclei. George Gamow was one of the—although not the sole—protagonists in the discovery of the theory of α -decay [1, 2] and the basic formula, equation (1), that underlies tunnelling through a potential barrier is often referred to as—perhaps unjustly—**Gamow's penetrability factor** (see, for example, p. 62 of [3]).

Leaving aside Gamow's mischievous account of history, this article will discuss how knowledge of the tunnelling behavior of a potential can be used to determine the potential itself. The quantum mechanical problem will also be contrasted with the classical version in order to gain further insight.

2 Classical vs Quantum Problem

2.1 The Classical Problem

The classical, one-dimensional inverse scattering problem is probably best exemplified by the two systems depicted in figure 1.

To the left of figure 1 is a particle oscillating in an attractive potential with single minimum, set to zero and occurring at the origin. Conservation of energy gives the period,

$$T(E) = \sqrt{2m} \int_{x_1(E)}^{x_2(E)} \frac{dx}{\sqrt{E - U(x)}},$$

where $x_1(E)$ and $x_2(E)$ are the turning points for the energy E . The inverse problem is to determine the form of the potential, $U(x)$, given the period as a function of energy, $T(E)$. The solution is well known and may be found in many standard texts on classical mechanics (see,

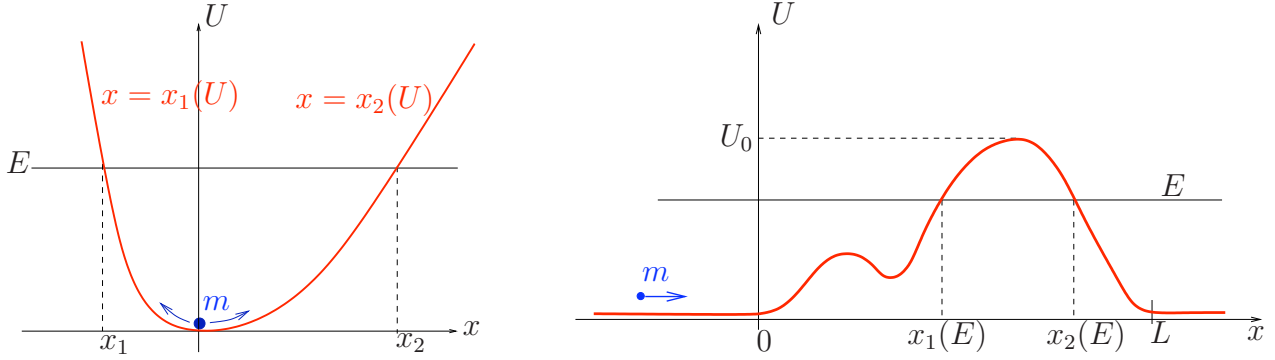


Figure 1: A particle in a potential well (attractive force field) performs oscillations; a particle on a potential barrier (repulsive force field) will either overcome the potential if it has enough energy ($E > U_0$) or will reflect back if it does not have enough energy $E < U_0$.

for example [4]). Treating x as a function of U rather than U a function of x , the above may be turned into Abel's integral equation. Since $U(x)$ is not one-to-one this requires splitting its domain at the origin and defining the two functions $x_1(U)$ and $x_2(U)$ as per figure 1. The result is

$$x_2(U) - x_1(U) = \frac{1}{\pi\sqrt{2m}} \int_0^U \frac{T(E)dE}{\sqrt{U-E}}.$$

We find that the solution cannot be determined uniquely unless the additional, assumption that the potential is even, is introduced. In this case

$$x(\tilde{U}) = \frac{1}{2\pi\sqrt{2m}} \int_0^{\tilde{U}} \frac{T(E)dE}{\sqrt{\tilde{U}-E}},$$

where we have denoted the unique, even solution by $\tilde{U}(x)$.

To the right of figure 1 is a particle incident on a potential barrier that is confined to the interval $[0, L]$. The problem of determining the potential given the time of traversal of the potential as a function of energy has been solved by Lazenby and Griffiths [5]. The forward and backward scattering data are defined respectively as,

$$T(E) = \sqrt{\frac{m}{2}} \int_0^L \frac{dx}{\sqrt{E-U(x)}}, \quad \text{if } E > U_0,$$

$$R(E) = \sqrt{\frac{m}{2}} \int_0^{x_1(E)} \frac{dx}{\sqrt{E-U(x)}}, \quad \text{if } E \leq U_0,$$

where $x_1(E)$ is the left turning point. The former applies when the particle has energy exceeding U_0 , the maximum of the potential, and gives the time required for the particle to traverse the potential. The latter applies when $E \leq U_0$ and gives the time required for the particle to reach the turning point $x_1(E)$ or half the time taken for the particle to return to the origin.

The solutions to the barrier equations are quite similar to that of the previous system. The most important feature is that a class of potentials are obtained. There is, however, a unique solution with the property that it increases monotonically over the interval $[0, L]$ (and drops

discontinuously to zero at L). Lazenby and Griffiths call this the *canonical* potential and use it to represent the class of solutions. For instance the inversion of the backward scattering data is given by

$$x(\tilde{U}) = \frac{1}{\pi} \sqrt{\frac{2}{m}} \int_0^{\tilde{U}} \frac{R(E) dE}{\sqrt{\tilde{U} - E}},$$

where \tilde{U} is the canonical potential.

In their paper, Lazenby and Griffiths remark that it is curious that the above solutions are not determined uniquely whereas in the quantum mechanical analogue the solution is unique. It is further remarked that “given the transmission coefficient T (the probability that the particle will surpass the barrier) as a function of energy E , (the potential) may be recovered by the method of Gel’fand and Levitan”. As will be discussed, this statement is not accurate as it stands. The transmission coefficient alone is not sufficient to determine the potential. The transmission amplitude however is a complex function and carries more information. All this will be clarified in the following.

2.2 The Quantum Mechanical Problem

The quantum mechanical problem is depicted in figure 2.

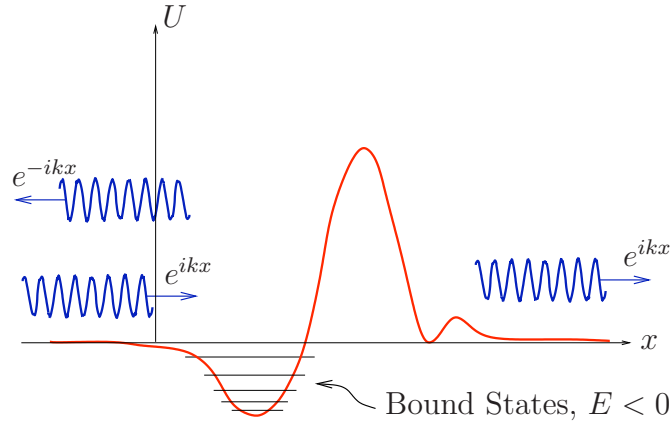


Figure 2: Quantum mechanical scattering of a right-moving particle that approaches a potential from left. It is assumed that the potential vanishes at large distances and, therefore, bound states appear only if there is a region with $U < 0$ and appear only for negative energies.

A particle is incident from the left, say, on a potential which limits to a constant as $x \rightarrow \pm\infty$, which we will set to zero. If the potential approaches zero (a constant) rapidly enough, the asymptotic form of the wavefunction for $x \rightarrow \pm\infty$ are plane waves:

$$\psi(x) \sim \begin{cases} e^{ikx} + b(k) e^{-ikx}, & x \rightarrow -\infty, \\ a(k) e^{ikx}, & x \rightarrow +\infty, \end{cases}$$

where the energy of the particle $E > 0$ and

$$k = \sqrt{\frac{2mE}{\hbar^2}}.$$

If there exists an interval over which $U(x) < 0$, then there is a discrete spectrum E_n corresponding to bound states:

$$\psi(x) \sim \begin{cases} c_n e^{+\kappa_n x}, & x \rightarrow -\infty, \\ d_n e^{-\kappa_n x}, & x \rightarrow +\infty, \end{cases}$$

where $E_n < 0$ and

$$\kappa_n = \sqrt{\frac{-2mE_n}{\hbar^2}}.$$

The scattering data for the inverse problem is comprised of the asymptotic coefficients $b(k)$ and c_n as well as the discrete eigenvalues κ_n . The potential is then uniquely constructed by way of the method of Gel'fand and Levitan [6] outlined in figure 3 below.

$$\begin{array}{c}
 b(k), (c_n, \kappa_n) \\
 \downarrow \\
 F(X) = \sum c_n^2 e^{-\kappa_n X} + \frac{1}{2\pi} \int_{-\infty}^{+\infty} b(k) e^{ikX} dk \\
 \downarrow \\
 K(x, z) + F(x+z) + \int_x^{+\infty} K(x, y) F(y+z) dy = 0 \\
 \downarrow \\
 U(x) = -2 \frac{d}{dx} K(x, x)
 \end{array}$$

Figure 3: The Gel'fand and Levitan method in a nutshell.

The scattering data is used to construct the auxiliary function $F(X)$. The auxiliary function is then used to define a linear Fredholm integral equation, called the **Marchenko equation**, for a second auxiliary function $K(x, z)$ (third entry). The potential is then determined by taking the directional derivative along the line $z = x$.

3 Gamow's Formula and its Inversion

3.1 Gamow's Formula

The applicable situation is illustrated in figure 4. A particle is incident on a potential barrier with a *single* maximum, U_0 (at $x = 0$, say), with energy E less than U_0 . It is known that in quantum mechanics there can be a finite probability for the particle to exceed the potential despite the fact that $E < U_0$.

Gamow's tunnelling formula gives a good approximation to the transmission coefficient, $T(E)$, giving the probability for the particle to surpass the barrier.

$$T(E) = \exp\left(-\frac{2}{\hbar} \int_{x_1(E)}^{x_2(E)} \sqrt{2m(U(x) - E)} dx\right). \quad (1)$$

This formula can be proved easily by considering the barrier as an infinite sum of infinitely thin rectangular barriers (p. 219 of [7]). However, this method, although it provides the correct

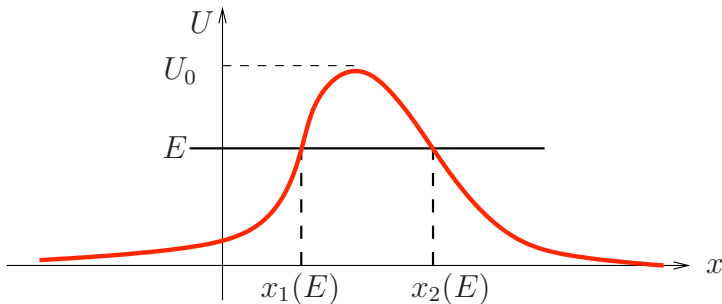


Figure 4: A particle incident on a potential barrier has a finite probability to overcome the barrier even if its energy E is below the maximum U_0 of the barrier.

result, is mathematically inconsistent. A mathematically sound proof can be given using the JWKB approximation (p. 507 of [7]).

In what follows, $T(E)$ will play the role analogous to the classical scattering data.

3.2 Inversion of Gamow's Formula

Let us take up the task of inverting Gamow's formula. By differentiating and, once again, rewriting in terms of the inverse functions $x_1(U)$ and $x_2(U)$ (we have again split the domain of $U(x)$ at the origin), we find

$$\frac{\hbar}{\sqrt{2m}} \frac{1}{T(E)} \frac{dT}{dE} = \int_{x_1(E)}^{x_2(E)} \frac{dx}{\sqrt{U-E}} = \int_E^{U_0} \left(\frac{dx_1}{dU} - \frac{dx_2}{dU} \right) \frac{dU}{\sqrt{U-E}}. \quad (2)$$

The above equation is nearly in the form of Abel's equation

$$\int_0^E \frac{\phi(U)}{\sqrt{E-U}} dU = f(E).$$

However, it differs in that the position of the parameter and the variable have been switched in the root, and in that the limits of the integral are from the variable to a constant rather than zero to the variable:

$$\int_E^a \frac{\phi(U)}{\sqrt{U-E}} dU = f(E).$$

Consequently, the preferred approach of applying the Laplace transform to the equation and making use of the convolution theorem fails. However, Abel's equation can be solved by composition with a kernel [4]. We can, in fact, apply this process with some modification. We divide both sides by $\sqrt{E-\alpha}$, where $0 \leq \alpha \leq U_0$, and integrate with respect to E from α to U_0 :

$$\begin{aligned} \frac{\hbar}{\sqrt{2m}} \int_{\alpha}^{U_0} \frac{dT/dE}{T(E)\sqrt{E-\alpha}} dE &= \int_{\alpha}^{U_0} \frac{dE}{\sqrt{E-\alpha}} \int_E^{U_0} \left(\frac{dx_1}{dU} - \frac{dx_2}{dU} \right) \frac{dU}{\sqrt{U-E}} \\ &= \int_{\alpha}^{U_0} \left(\frac{dx_1}{dU} - \frac{dx_2}{dU} \right) dU \int_{\alpha}^U \frac{dE}{\sqrt{(U-E)(E-\alpha)}}, \end{aligned}$$

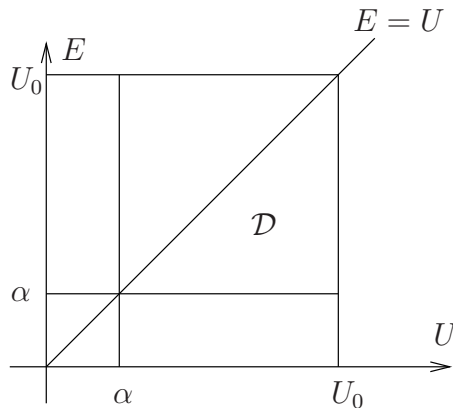


Figure 5: Our integral is defined on the triangular domain \mathcal{D} .

where in the second line we have changed the order of integration (see figure 5).

In the appendix we show that

$$\int_{\alpha}^U \frac{dE}{\sqrt{(U-E)(E-\alpha)}} = \pi .$$

Therefore

$$\frac{\hbar}{\sqrt{2m}} \int_{\alpha}^{U_0} \frac{dT/dE}{T(E)\sqrt{E-\alpha}} dE = \pi \int_{\alpha}^{U_0} \left(\frac{dx_1}{dU} - \frac{dx_2}{dU} \right) dU ,$$

and finally:

$$x_1(U) - x_2(U) = -\frac{\hbar}{\pi\sqrt{2m}} \int_U^{U_0} \frac{dT(E)/dE}{T(E)\sqrt{E-U}} dE , \quad (3)$$

where we have used the fact that $x_1(U_0) - x_2(U_0) = 0$. We see that the solution is quite similar in form to the classical result, and again the solution is not unique. Rather, we have obtained a family of potentials which all result in the same transmission coefficient.

3.3 An Example: Cold Emission

Although the photoelectric effect has become the most popular example of emission of electrons by metals, easily recognized and studied by students, it is not the only phenomenon in which electrons are emitted by metals. Electrons can be emitted by metals at room temperature by the application of an external electric field \mathcal{E} . To contrast with the emission of electrons when a metal is heated, this phenomenon is termed **cold emission**. It was first explained by Fowler and Nordheim [9].

When an external field is applied, an electron in the metal sees a potential

$$U(x) = U_0 - e\mathcal{E}x , \quad (4)$$

where x is the distance from the wall of the metal. This description ignores the fact that a positive image charge will appear at the surface of the metal as the electron is removed, and

thus an additional Coulomb attraction will be established. For an electron of energy E we find, using Gamow's formula (1),

$$T(E) = e^{-a(U_0-E)^{3/2}}, \quad (5)$$

with

$$a = \frac{4\sqrt{2m}}{3e\mathcal{E}\hbar}.$$

Equation (5) is known as the **Fowler-Nordheim** equation. The quantity $U_0 - E$ is known as the **work function**.

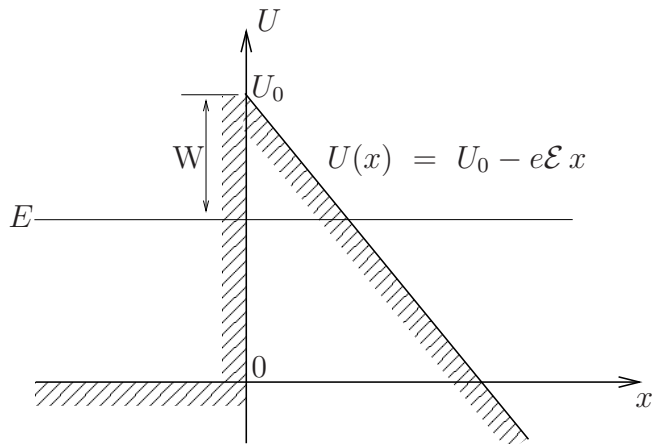


Figure 6: Model potential for cold emission. E is typically taken as the fermi energy. W is the work function of the metal.

We shall now assume that the Fowler-Nordheim equation is known—say from experimental data. Can we find the potential that reproduces it?

According to our formula (3)

$$x_1(U) - x_2(U) = -\frac{2}{\pi e\mathcal{E}} \int_U^{U_0} \sqrt{\frac{U_0 - E}{E - U}} dE.$$

This is an elementary integral and we compute it in the appendix. The result is

$$x_1(U) - x_2(U) = -\frac{1}{e\mathcal{E}} (U_0 - U).$$

The reader may believe that we have recovered the potential (4). Unfortunately, this is not the case as any two functions $x_1(U)$ and $x_2(U)$ that differ by the above amount are solutions of the inverse problem. The the cold emission potential is recovered if we assume that $x_1(U) = 0$.

3.4 The Issue of Uniqueness

The reader, at this point, may believe that the apparent conflict of our result with that which would have obtained by the method of Gel'fand-Levitan is due to the approximations used to produce formula (1). However, a moment's reflection will reveal that this cannot be so. The

mathematical statement of the problem is independent of the underlying physics which can be left aside.

The answer to this puzzle is quite simple. The method of Gel'fand and Levitan makes use of the amplitude $b(k)$ (in the situation were considering there is no bound spectrum) which is a *complex* quantity. However, in our case we make use of T which is a *real* quantity— $T = |a(k)|^2$ with $|a(k)|^2 + |b(k)|^2 = 1$. Thus, we have lost information about regarding phase.

Given the transmission coefficient $T(E)$, $b(k)$ can be anything of the form

$$b(k) = \sqrt{1 - T(E(k))} e^{if(k)} ,$$

where $f(k)$ is a real-valued function. Each distinct potential among the family of our solutions, corresponds to a different choice of $f(k)$.

4 Discussion and Conclusion

We have found that, in quantum mechanics, $T(E)$, the probability for transmission and the analog of the classical scattering data, does not uniquely determine the potential, just as it is in classical mechanics. However, quantum mechanics does afford us an additional set of data, the phase difference $f(k)$, which corresponds to measurements of time delay (p.138 of [8]). It is only with both these sets of data that we can uniquely determine the potential.

The approximate nature of Gamow's formula is an irrelevant feature for the problem we have studied. However, a different kind of question may be asked which makes this feature relevant: Assuming that the potential barrier is even and a unique solution $U(x)$ can be found, what is the error in determining the potential? That is, how close is the solution $U(x)$ to the real potential, $U_{real}(x)$, that gave the experimental data $T(E)$? This question remains open.

Finally, toward proving our result, we have succeeded in solving a modified version of Abel's equation: Given the integral equation,

$$\int_E^a \frac{\phi(U)}{\sqrt{U-E}} dU = f(E) ,$$

where $f(E)$ is a known function and $\phi(U)$ is an unknown function, we have shown that the solution is given by

$$\phi(U) = -\frac{1}{\pi} \frac{d}{dU} \int_U^a \frac{f(E)}{\sqrt{E-U}} dE .$$

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Appendix

The integrals

$$I = \int \frac{dE}{\sqrt{(\beta - E)(E - \alpha)}}, \quad J = \int \frac{\sqrt{\beta - E}}{\sqrt{E - \alpha}} dE$$

which have appeared in our article are elementary, but their calculation is somewhat lengthy. We present their calculation here.

Introducing the substitution

$$u^2 = \sqrt{\frac{\beta - E}{E - \alpha}}$$

in J , we can rewrite it as

$$J = -2(\beta - \alpha) \int \frac{u^2}{(1 + u^2)^2} du = -2(\beta - \alpha) \left[\int \frac{1}{1 + u^2} du - \int \frac{1}{(1 + u^2)^2} du \right].$$

However,

$$\frac{1}{\lambda} \tan^{-1} \frac{u}{\lambda} = \int \frac{1}{\lambda^2 + u^2}.$$

Therefore,

$$J = -2(\beta - \alpha) \left[\tan^{-1} u - \frac{1}{2} \frac{\partial}{\partial \lambda} \left(\frac{1}{\lambda} \tan^{-1} \frac{u}{\lambda} \right) \Big|_{\lambda=1} \right],$$

and, finally,

$$J = \sqrt{(E - \alpha)(\beta - E)} - (\beta - \alpha) \tan^{-1} \sqrt{\frac{\beta - E}{E - \alpha}}.$$

It is immediate that

$$\int_{\alpha}^{\beta} \sqrt{\frac{\beta - E}{E - \alpha}} dE = (\beta - \alpha) \frac{\pi}{2}.$$

Using Leibnitz's rule for the differentiation of integrals depending on a parameter, we can also easily obtain

$$\int_{\alpha}^{\beta} \frac{dE}{\sqrt{(\beta - E)(E - \alpha)}} = 2 \frac{\partial I}{\partial \beta} = \pi.$$

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