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Determination of the shape of a potential barrier from the tunneling transmission coefficient

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Given the shape of a potential barrier $V(x)$, there is an explicit expression in the WKB approximation for the transmission coefficient for penetration of the barrier. The problem considered in this paper is to find the inverse relation, determining $V(x)$ from the transmission coefficient. It is shown that the width of the barrier at energy E can be determined if the transmission coefficient is known for energies between E and V_{max}, the barrier maximum. Other properties of the turning points can be deduced for potentials which can be written in terms of a parameter λ as $V(x) = V_0(x) - \lambda\phi(x)$, if the dependence of transmission coefficient on λ is known. For the specific case of field emission, one can find the potential $V(x)$ from the energy and field dependence of the transmission coefficient.

I. INTRODUCTION

A common problem in physics is utilizing experimental results to deduce some fundamental quantity. An example, for which refined techniques have been developed, is the determination of an interparticle interaction from scattering, spectral, transport, and thermodynamic data.[1-4] One tool often used in the "inversion" procedure is the Rydberg-Klein-Rees (RKR) method.[1-5] In this method, the width of an attractive potential $V(x)$ is expressed in terms of its bound-state spectrum via

$$x_2(E) - x_1(E) = \left(\frac{2}{m}\right)^{1/2} \hbar \int_{V_{min}}^{E} \frac{dn}{dE'} \frac{dE'}{(E-E')^{1/2}} . \tag{1.1}$$

Here the $x_i(E)$ are the classical turning points of the potential at energy E, V_{min} is the minimum value of $V(x)$, and $n(E)$ is the quantum number of a bound state expressed as a function of energy. [The equation is derived from the WKB approximation for the energy levels. The derivative dn/dE is not precisely specified by an observed spectrum $E(n)$ because of the spacing between the levels. In the tunneling problem, there is no such limitation.] Another useful relation is satisfied in the special case of the vibration-rotation spectrum of a diatomic molecule, for which the effective potential is of the form

$$V(x) = V_0(x) + \hbar^2 J(J+1)/2mx^2 , \tag{1.2}$$

where x is now the internuclear separation and m is the reduced mass. One finds[1-5]

$$\frac{1}{x_1(E)} - \frac{1}{x_2(E)} = \frac{2(2m)^{1/2}}{\hbar} \times \int_{V_{min}}^{E} \frac{(\partial E'/\partial\lambda)}{(\partial E'/\partial n)} \frac{dE'}{(E-E')^{1/2}} , \tag{1.3}$$

where $\lambda = J(J+1)$ and n is the vibrational quantum number. This relation can be combined with Eq. (1.1) to deduce the form of the attractive potential $V(x)$, given the spectrum $E(n,\lambda)$.

The problem considered in this paper is the derivation of an analogous inversion method for quantum-mechanical tunneling through a barrier. We consider the one-dimensional case of a barrier $V(x)$, of the simple form shown in Fig. 1. Although the discussion is one-dimensional, the applications we have in mind are to three-dimensional situations. Many problems (e.g., α decay) possess spherical symmetry so that an effective one-dimensional problem results; others (e.g., field emission) have translational invariance in two directions (to a good approximation) so that separation of variables leads to a one-dimensional equation.

This subject was treated earlier by Wheeler in connection with the problem of finding the shape of a double-minimum potential well from know-

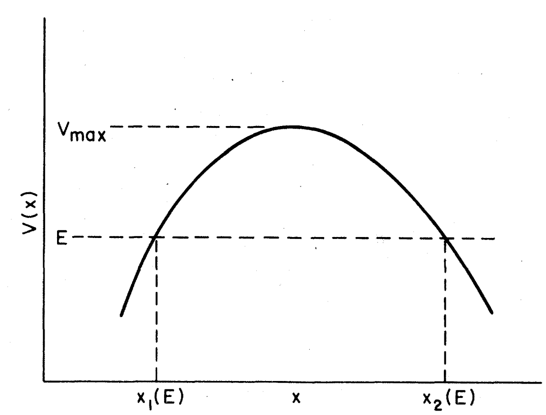

FIG. 1. Typical potential, with classical turning points indicated, for a particle of energy E incident on the barrier.

ledge of the bound-state spectrum.[1] One of our results is closely related to one of his, as described below.

For the tunneling problem, the input to an inversion procedure is the transmission coefficient $T(E)$, the ratio of the flux transmitted through the barrier to the flux incident. We know that in the WKB type of approximation[6,7,9]

$$T(E) = \{1 + \exp[(8m)^{1/2} f(E)/\hbar]\}^{-1} , \tag{1.4}$$

where

$$f(E) = \int_{x_1}^{x_2} [V(x) - E]^{1/2} dx . \tag{1.5}$$

For many applications $E \ll V_{max}$, the maximum of $V(x)$, so that the argument of the exponential is large. In that case, the one can be neglected in Eq. (1.4). Here we consider the more general case, including the region $E > V_{max}$ for which the turning points become complex. The problem is: given $T(E)$, or equivalently $f(E)$, what can be inferred about $V(x)$?

In Sec. II, considering $E < V_{max}$, we first derive a relation between $x_2(E) - x_1(E)$ and the function $f(E)$. We next treat the case where V depends linearly on some parameter λ so that we have

$$V(x) = V_0(x) - \lambda\phi(x) . \tag{1.6}$$

In such situations, the dependence of $T(E, \lambda)$ on λ can be utilized to deduce other properties of the turning points. An example is field emission from a metal, for which λ is proportional to the electric field at the surface. Then it is shown that $x_2^2(E, \lambda) - x_1^2(E, \lambda)$ can be obtained from knowledge of $\partial f(E, \lambda)/\partial\lambda$. Regarding the function f as input, we are then able to compute x_1 and x_2 individually. Thus the barrier shape can be deduced from measurement of the electric field and energy dependence of the transmission coefficient.

In Sec. III, we derive analogous results for the case $E > V_{max}$. In Sec. IV, we address the bound-state problem described above and derive a generalization of Eq. (1.3) for potentials in the form given in Eq. (1.6).

II. INVERSION IN THE REGION $E < V_{max}$

Our first goal is a result for the width of the barrier at energy E. One can write

$$x_2(E) - x_1(E) = \frac{1}{\pi} \int_{x_1}^{x_2} dx \int_E^{V(x)} \frac{dE'}{\{[E' - E][V(x) - E']\}^{1/2}} \tag{2.1}$$

because the E' integral is identically π. We assume that $V(x)$ has only one extremum (a maximum) between $x_1(E)$ and $x_2(E)$, as shown in Fig. 1. It is easy to change the order of integration in Eq. (2.1), the domain remaining as the region of Fig. 1 between the dashed line at E and the $V(x)$ curve. We find

$$x_2(E) - x_1(E) = \frac{1}{\pi} \int_E^{V_{max}} dE' \int_{x_1(E')}^{x_2(E')} \frac{dx}{\{[E' - E][V(x) - E']\}^{1/2}} \tag{2.2a}$$

and

$$x_2(E) - x_1(E) = -\frac{2}{\pi} \int_E^{V_{max}} \frac{df}{dE'} \frac{dE'}{(E' - E)^{1/2}} . \tag{2.2b}$$

This is our first main result. Its significance is that knowledge of the transmission coefficient [hence, $f(E)$ from Eq. (1.4)] for energies between E and V_{max} enables one to derive the barrier width at energy E. The similarity of Eq. (2.2b) to Eq. (1.1) for the bound-state problem occurs because the Bohr-Sommerfeld-quantization condition expresses the quantum number n in terms of an integral similar to that in Eq. (1.5) but with $[E - V(x)]^{1/2}$ as the integrand.

This result is closely related to one found by Wheeler.[1] Thus, Eq. (2.2b) can be obtained by partially integrating his Eq. (85) and substituting into his Eq. (89).

As a specific example of Eq. (2.2), consider the case of a parabolic potential (a good approximation for most potentials for energy near the maximum), $V(x) = V_{max} - \alpha^2 x^2$. From Eq. (1.5) we find

$$f(E) = \pi(V_{max} - E)/2\alpha , \tag{2.3}$$

so that Eq. (2.2b) gives $x_2 - x_1 = 2(V_{max} - E)^{1/2}/\alpha$, as expected. The vanishing of f as $E \to V_{max}$ must occur in general. It corresponds to a transmission coefficient of $\frac{1}{2}$, according to Eq. (1.4); this permits clear identification of the upper limit in Eq. (2.2) from the input data. Deviations from the linear dependence of f on E will occur for energies sufficiently far below V_{max} for the parabolic approximation to fail.

Further information can be derived if the potential can be written in the form of Eq. (1.6). We do not assume that $\lambda\phi(x)$ is either a perturbation or an external field term (although these are special cases). An example that does not fall into either category is α decay, for which $\lambda\phi(x) \propto l(l+1)/x^2$, the angular-momentum contribution to the effective potential for radial motion. Now the reasoning is

$$\int_{x_1(E,\lambda)}^{x_2(E,\lambda)} \phi(x)\,dx = \frac{1}{\pi}\int_{x_1}^{x_2} \phi(x)\,dx \int_E^{V(x)} \frac{dE'}{\{[E'-E][V(x)-E']\}^{1/2}}$$

$$= \frac{1}{\pi}\int_E^{V_{\max}} dE' \int_{x_1(E',\lambda)}^{x_2(E',\lambda)} \frac{\phi(x)\,dx}{\{[E'-E][V(x)-E']\}^{1/2}} = -\frac{2}{\pi}\int_E^{V_{\max}} \frac{\partial f(E',\lambda)}{\partial\lambda}\frac{dE'}{(E'-E)^{1/2}}\,. \tag{2.4}$$

This relation, our second main result, is useful in evaluating $V(x)$ from $f(E,\lambda)$, provided the function $\phi(x)$ is known.

As a straightforward and potentially useful application of Eq. (2.4), we consider the case of field emission. Here $V_0(x)$ of Eq. (1.6) is the one-electron potential due to the ions, most generally calculated self-consistently to include screening.[8] The field-dependent term usually considered for this problem is $Fex=\lambda\phi(x)$, where F is the electric field at the surface. From Eq. (2.4) we have

$$x_2^2(E,F)-x_1^2(E,F) = -\frac{4}{\pi e}\int_E^{V_{\max}}\left(\frac{\partial f(E'F)}{\partial F}\right)\frac{dE'}{(E'-E)^{1/2}}\,. \tag{2.5}$$

When combined with Eq. (2.2b) for x_2-x_1, this relation is capable of yielding the individual values x_1 and x_2. Thus, measurement of the transmission coefficient, which yields $f(E,F)$ as a function of energy and electric field, can, in principle, determine the barrier shape completely.

III. INVERSION IN THE REGION $E > V_{\max}$

The program described above uses only the transmission coefficient for energy $E< V_{\max}$ to find the potential. It is interesting to see what information is available from values of $T(E)$ for $E> V_{\max}$. The conventions for evaluating $f(E)$ are[9] to use the branch of $[V(x)-E]^{1/2}$ which has argument near $\frac{1}{2}\pi$, with $x_1=b_1-ib_2=x_2^*$ and $b_2>0$. The function f vanishes for $E=V_{\max}$ and monotonically decreases with increasing E above the barrier. With these conventions, the argument proceeds as in the case $E<V_{\max}$, but the manipulations involve complex variables. As a first step one writes

$$x_2(E)-x_1(E) = \frac{1}{\pi}\int_{x_1}^{x_2} dx \int_{V(x)}^{E} \frac{dE'}{\{[E'-V(x)](E-E')\}^{1/2}}\,.$$

Here, $V(x)$ is understood to have a small imaginary part, E is chosen real and greater than ReV, and the argument of the square root is near zero. We conjecture that, for the class of potentials we deal with, the order of integration can be changed with the same limits occurring as in Eq. (2.2a). Then we have

$$x_2(E)-x_1(E) = \frac{1}{\pi}\int_{V_{\max}}^{E} dE' \int_{x_1(E')}^{x_2(E')} \frac{dx}{\{[E'-V(x)](E-E')\}^{1/2}}\,.$$

The factors in the denominator can be rearranged,

$$x_2(E)-x_1(E) = \frac{i}{\pi}\int_{V_{\max}}^{E} \frac{dE'}{(E-E')^{1/2}} \int_{x_1(E')}^{x_2(E')} \frac{dx}{[V(x)-E']^{1/2}}\,,$$

where the argument of $(E-E')^{1/2}$ is zero and that of $[V(x)-E']^{1/2}$ is near $\frac{1}{2}\pi$. The x integration is now seen to be related to df/dE; the result is

$$x_2(E)-x_1(E) = -\frac{2i}{\pi}\int_{V_{\max}}^{E} \frac{df}{dE'}\frac{dE'}{(E-E')^{1/2}}\,. \tag{3.1}$$

Note that the left-hand side is $2i\,\mathrm{Im}x_2=2ib_2$. In the case when $V(x)$ can be written as in Eq. (1.6), one obtains similarly

$$\int_{x_1(E,\lambda)}^{x_2(E,\lambda)} \phi(x)\,dx = -\frac{2i}{\pi}\int_{V_{\max}}^{E} \frac{\partial f(E',\lambda)}{\partial\lambda}\frac{dE'}{(E-E')^{1/2}}\,. \tag{3.2}$$

For the case of the parabolic barrier considered in Sec. II, one obtains Eq. (2.3) in the $E>V_{\max}$ region as well. It may be possible, as in the field-emission case described in Sec. II, to find a $\phi(x)$, which yields the individual turning points through Eqs. (3.1) and (3.2). This would provide a line in the complex x plane, mirror symmetric about the real axis, on which $V(x)$ is known. By Taylor expansion about the intercept on the real axis, one could deduce $V(x)$ along the real axis and provide information about the form of $V(x)$ with x real from data for $E>V_{\max}$. There are, thus, two independent approaches to finding $V(x)$ from knowledge of $f(E,\lambda)$, one depending on values of f in $E<V_{\max}$ and the other depending on values in the range $E>V_{\max}$.

IV. BOUND-STATE PROBLEM

The method used above applies also in the bound-state problem and it leads to a generalization of Eq. (1.3). For a potential well $V(x)$, the quantum number n in the WKB approximation is given by

$$\frac{(n+\frac{1}{2})\hbar\pi}{(2m)^{1/2}} = \int_{x_1}^{x_2} [E - V(x)]^{1/2}\, dx . \tag{4.1}$$

This equation defines the function $n(E)$; the eigenvalues occur when n is an integer or zero. Equation (1.1) may be easily derived by a procedure very similar to that used in Sec. II. If $V(x)$ can be written in terms of a parameter λ as in Eq. (1.6), manipulations similar to those of Sec. II can be performed with Eq. (4.1), leading immediately to

$$\int_{x_1}^{x_2} \phi(x)\, dx = \left(\frac{2}{m}\right)^{1/2} \hbar \int_{V_{\min}}^{E} \frac{\partial n}{\partial \lambda} \frac{dE'}{(E-E')^{1/2}}$$
$$= -\left(\frac{2}{m}\right)^{1/2} \hbar \int_{V_{\min}}^{E} \frac{(\partial E'/\partial\lambda)\, dE'}{(\partial E'/\partial n)(E-E')^{1/2}} . \tag{4.2}$$

This supposes that $V(x)$ has only the one extremum at $V_{\min}$. This specializes to Eq. (1.3) when one treats the potential of Eq. (1.2). Equation (4.2) could also be used for image-potential-induced surface states of insulators.[10] In this problem the potential $\lambda\phi(x)$ would be that due to an electric field, which produces a linear Stark effect.[10,11]

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