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Equivalent Potentials

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An explicit construction is described for the entire class of potentials leading, for a particular angular momentum, to the same phase shift and energy spectrum as a given central potential. A similar procedure is applied to potentials with purely discrete spectra.

1. INTRODUCTION

LET us consider the Schrödinger equation

$$\varphi''(r)+E\varphi(r)=V_0(r)\varphi(r), \tag{1.1}$$

which describes the wave functions of a particle in a central field. In general, this equation leads to a discrete spectrum $E_i<0$ as well as a phase shift $\eta(E)$ for positive E. The question can then be asked whether this spectrum and phase shift can be reproduced by other "equivalent" potentials. In a previous paper[1] we have shown that in the case of m discrete eigenvalues the manifold of equivalent potentials is at most m-dimensional. We shall see in the present note that this manifold does in fact exist and can be easily constructed explicitly from the bound state solutions of the given potential V_0 [Eqs. (2.12), (2.10), and (2.29)]. The same is true for each higher angular momentum. However, under very general conditions, the phase shift and spectrum for any *two* angular momenta are compatible with at most one central potential.

The situation is similar in the case of a one-dimensional boundary value problem with a purely discrete spectrum. (We shall confine ourselves to the case where the wave function is required to vanish at the ends of the interval.) The equivalent potentials, i.e., potentials with the same spectrum, are then characterized by the values of a denumerably infinite set of parameters. Again explicit construction of these potentials is possible.

The case of a purely discrete spectrum has been the subject of an extensive investigation by Borg,[2] who confined himself to questions of existence and uniqueness. Very recently conditions for the existence of a boundary value problem corresponding to a given spectrum and given spectral constants [corresponding to our Γ_l, Eq. (3.5)] have been published by Gel'fand and Levitan.[3] The present work was stimulated by an interesting note[4] by Borg.

After completion of our investigation we received a manuscript by Holmberg,[5] which contains some of the results of the present paper.

2. SCATTERING PROBLEMS

We consider as an example the S-state radial Eq. (1.1) with a given potential $V_0(r)$ and corresponding spectrum $E_l=-\kappa_l^2$, $l=1, 2, \cdots, m$, and phase shift $\eta(k)$, $k=\sqrt{E}$.

Let $\psi_l(r)$ be the normalized bound state functions and $\psi(k, r)$ the continuum solutions normalized to $\sin(kr+\eta(k))$ at infinity. An infinitesimal change $\delta V(r)$ of the potential then produces the following changes of the eigenvalues and the phase shift:

$$\delta E_l=\int_0^\infty \delta V(r)[\psi_l(r)]^2dr, \tag{2.1}$$

$$\delta\eta(k)=-\frac{1}{k}\int_0^\infty \delta V(r)[\psi(k,r)]^2. \tag{2.2}$$

Thus the condition that the eigenvalues and phase shift remain unchanged is that $\delta V(r)$ be orthogonal to the squares of all the eigenfunctions.

We shall now verify that the functions $\psi_l'(r)\psi_l(r)$ have this property. Clearly,

$$\begin{aligned}
&\int_0^\infty \psi_l'\psi_l[\psi_m]^2dr\\
&=\frac{1}{2}\int_0^\infty \psi_l\psi_m[\psi_l'\psi_m+\psi_l\psi_m']dr\\
&\qquad+\frac{1}{2}\int_0^\infty \psi_l\psi_m[\psi_l'\psi_m-\psi_l\psi_m']dr\\
&=\frac{1}{2}\int_0^\infty \psi_l\psi_m[\psi_l\psi_m]'dr+\tfrac{1}{2}(E_l-E_m)\\
&\qquad\times\left[\int_0^\infty \psi_l(r')\psi_m(r')dr'\right]dr\\
&=\tfrac{1}{4}[\psi_l\psi_m]^2\Big|_0^\infty-\tfrac{1}{4}(E_l-E_m)\left[\int_r^\infty \psi_l\psi_m dr\right]^2=0,
\end{aligned} \tag{2.3}$$

where use has been made of the Schrödinger equation.

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† On leave of absence from Carnegie Institute of Technology, Pittsburgh, Pennsylvania.
[1] R. Jost and W. Kohn, Phys. Rev. **87**, 979 (1952).
[2] G. Borg, Acta Math. **78**, 1 (1946).
[3] I. M. Gel'fand and B. M. Levitan, Doklady Akad. Nauk S.S.S.R. **77**, 557 (1951).
[4] G. Borg, Proceedings of the International Congress of Mathematics, Cambridge, Massachusetts, 1950, American Math. Soc. Providence, Rhode Island (unpublished).
[5] B. Holmberg, Nuovo cimento (to be published).

The same derivation holds when $\psi_m(r)$ is replaced by $\psi(k,r)$. This suggests that an m-dimensional manifold of potentials can be obtained from such infinitesimal increments by integration.

To carry out this integration it is convenient to work with the solutions $f(k,r)$, $\text{Im}(k)\leqslant 0$ defined by

$$\lim_{r\to\infty} e^{ikr}f(k,r)=1. \tag{2.4}$$

We fix our attention now on one of the bound state functions $f(-i\kappa_1,r)\equiv f_1(r)$ and look for the solution of the system of equations

$$\partial V(\lambda,r)/\partial\lambda = f_1(\lambda,r)f_1'(\lambda,r), \tag{2.5}$$

$$f_1''(\lambda,r)+E_1f_1(\lambda,r)=V(\lambda,r)f_1(\lambda,r) \tag{2.6}$$

with the boundary conditions

$$V(0,r)=V_0(r),\quad f_1(0,r)=f_1(r) \tag{2.7}$$

and

$$\lim_{r\to\infty} e^{\kappa_1 r}f_1(\lambda,r)=1. \tag{2.8}$$

Eliminating the potential from (2.5) and (2.6) gives

$$\frac{\partial}{\partial\lambda}\frac{f_1''(\lambda,r)}{f_1(\lambda,r)}=f_1'(\lambda,r)f_1(\lambda,r). \tag{2.9}$$

The solution of this equation satisfying (2.7) and (2.8) was obtained by a power series expansion in λ, every term being uniquely defined by the boundary conditions (2.7) and (2.8). The result is

$$f_1(\lambda,r)=f_1(r)/N(\lambda,r), \tag{2.10}$$

where

$$N(\lambda,r)=1+\frac{\lambda}{4}\int_r^\infty f_1^2(r')dr'. \tag{2.11}$$

By means of (2.6) this leads to the potential

$$V(\lambda,r)=V_0(r)+\frac{\lambda}{N}f_1(r)f_1'(r)+\frac{\lambda^2}{8N^2}[f_1(r)]^4. \tag{2.12}$$

It can be verified directly that (2.10) and (2.12) satisfy (2.5)–(2.8). Thus (2.12) constitutes a one parameter family of equivalent potentials. The conditions that the potential be regular requires that the variation of λ is restricted by

$$-4\left[\int_0^\infty f_1^2dr\right]^{-1}<\lambda<\infty.$$

To obtain further insight we shall construct explicitly the solutions $f(\lambda;k,r)$, for any k with $\text{Im}(k)\leqslant 0$, corresponding to this family of phase equivalent potentials. An increment δV of the potential leads to

$$\delta f(k,r)=-\int_r^\infty G(k,r,r')\delta V(r')f(k,r')dr', \tag{2.13}$$

where the Greens function $G(k,r,r')$ is the solution of (1.1) defined by the initial values

$$G(k,r,r)=0,\quad \left[\frac{\partial}{\partial r}G(k,r,r')\right]_{r=r'}=1.^{6} \tag{2.14}$$

From (2.5) and (2.13) one has therefore the equation

$$\frac{\partial f(\lambda;k,r)}{\partial\lambda}=-\int_r^\infty G(\lambda;k,r,r')f(\lambda;k,r')\times f_1(\lambda;r')f_1'(\lambda;r')dr'. \tag{2.15}$$

The integral can be evaluated in analogy with (2.3) by using the fact that G is a solution of the Schrödinger equation in r'.[7] The result simplifies by means of (2.14) and the equation

$$\left[\frac{\partial}{\partial r'}G(k,r,r')\right]_{r=r'}=-1 \tag{2.16}$$

to give

$$\frac{\partial f(\lambda;k,r)}{\partial\lambda}=-\frac{1}{4(k^2+\kappa_1^2)}f_1(\lambda;r)\times[f_1(\lambda;r)f'(\lambda;k,r)-f_1'(\lambda;r)f(\lambda;k,r)], \tag{2.17}$$

or equivalently,

$$\frac{\partial f(\lambda;k,r)}{\partial\lambda}=-\tfrac{1}{4}f_1(\lambda;r)\int_r^\infty f_1(\lambda;r')f(\lambda;k,r')dr'. \tag{2.18}$$

By putting $r=0$ in (2.18) one obtains

$$\partial f(\lambda;k)/\partial\lambda=0 \tag{2.19}$$

or

$$f(\lambda;k)=f(0,k)\equiv f(k). \tag{2.20}$$

Since $f(\lambda;k)$ determines the spectrum and phase shift, this equation confirms again the fact that we are dealing with a family of equivalent potentials. On the other hand, (2.17) leads to the interesting equation

$$\frac{\partial f'(\lambda;k,0)}{\partial\lambda}=-\frac{1}{4(k^2+\kappa_1^2)}[f_1'(\lambda;0)]^2f(k), \tag{2.21}$$

which shows that all the $f_l'(\lambda;0)\equiv f'(\lambda;-i\kappa_l,0)$ stay constant except one, namely, $f_1'(\lambda;0)\equiv f'(\lambda;-i\kappa_1,0)$. This latter is according to (2.10) given by

$$f_1'(\lambda;0)=f_1'(0)\bigg/\left[1+\frac{\lambda}{4}\int_0^\infty[f_1(r)]^2dr\right]. \tag{2.22}$$

[6] $G(k,r,r')$ can be written as

$$G(k,r,r')=u(k,r)v(k,r')-u(k,r')v(k,r),$$

where u and v are those solutions of (1.1) defined by the initial values $u(k,0)=0$, $u'(k,0)=1$; $v(k,0)=1$, $v'(k,0)=0$.

[7] For this purpose one evaluates $\int_a^b\chi^2f_1f_1'dr$ where $\chi=\alpha G+\beta f$, as in (2.3) and then picks out the coefficient of $\alpha\beta$.

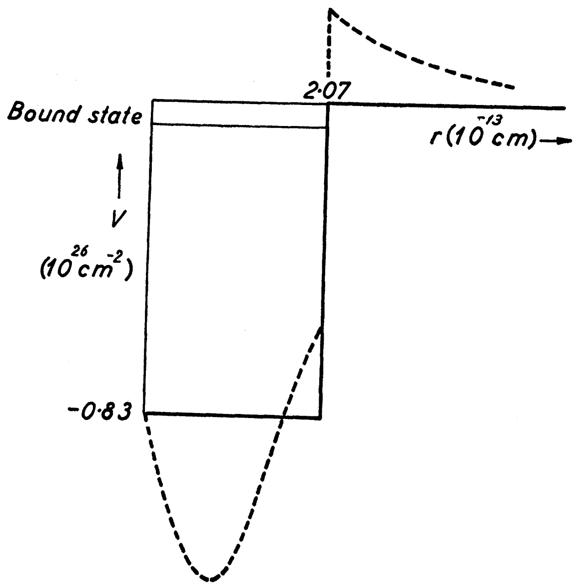

FIG. 1. The deuteron square well (——) and an equivalent potential (-----).

Introducing

$$\frac{1}{\Gamma_1(\lambda)} \equiv \int_0^\infty [f_1(\lambda; r)]^2 dr = \frac{1}{2i\kappa_1} \dot{f}(-i\kappa_1) f_1'(\lambda, 0), \quad (2.23)$$

where

$$\dot{f}(k) \equiv df(k)/dk \quad (2.24)$$

and the Schrödinger equation has been used, leads to

$$\lambda = 4[\Gamma_1(\lambda) - \Gamma_1(0)]. \quad (2.25)$$

As λ varies over its admissible range $-4\Gamma_1(0) < \lambda < \infty$, $\Gamma_1(\lambda)$ takes on all the values $0 < \Gamma_1(\lambda) < \infty$. Let us now generalize the definition (2.23) to the other bound state wave functions,

$$\frac{1}{\Gamma_l(\lambda)} \equiv \int_0^\infty [f_l(\lambda, r)]^2 dr = \frac{1}{2i\kappa_l} \dot{f}(-i\kappa_l) f'(\lambda, 0). \quad (2.26)$$

Then we have the following result: Each equivalent potential of the manifold (2.12) is characterized by the value of Γ_1, which varies in the range $0 < \Gamma_1 < \infty$ while all the other Γ_l are constant.

Furthermore, we may note that if one potential of this family satisfies the conditions

$$\int_0^\infty r|V(r)|dr < \infty \quad (2.27)$$

and

$$\int_0^\infty r^2|V(r)|dr < \infty, \quad (2.28)$$

then, by (2.10), so do all the others.

In reference 1 we have proved that under the two last conditions a potential is uniquely defined by its phase, its discrete eigenvalues, and the m positive parameters Γ_l. It is therefore clear that by repeating the above construction (2.12) using the other discrete energy levels, we obtain the complete m-dimensional manifold of equivalent potentials. This construction can be explicitly performed since one can write down explicitly all the bound state functions for an arbitrary λ. In fact, integration of (2.18) leads to the following expression for the solution corresponding to arbitrary k:

$$f(\lambda; k, r) = f(0; k, r) - \frac{\lambda}{4N} f_1(r) \int_r^\infty f_1(r') f(0; k, r') dr', \quad (2.29)$$

which can be easily verified. It will be noticed that in the final equations (2.10), (2.12), and (2.29) the normalization of f_1 is irrelevant since it can be absorbed into the parameter λ.

For any higher angular momentum l, the results are completely analogous to those for S-states. Equations (2.10), (2.12), and (2.29), with the f's now denoting solutions of the radial equation for the given l, remain uncharged and lead to the totality of potentials equivalent for the l under consideration.

The following question then arises naturally: Given a potential V_0, is there another potential V_1 which leaves the spectrum and phase shifts corresponding to two angular momenta, say $l=0$ and $l=1$, unchanged?

Let us first consider the usual case where none of the S-eigenvalues $E_{i,S}$ coincide with a P-eigenvalue $E_{j,P}$. From our construction [see Eq. (2.12)] it follows that any potential V_S equivalent with V_0 as far as S-states are concerned has the property

$$\lim_{r\to\infty} V_S - V_0 / e^{-2\kappa_S r} = \text{constant}, \quad (2.30)$$

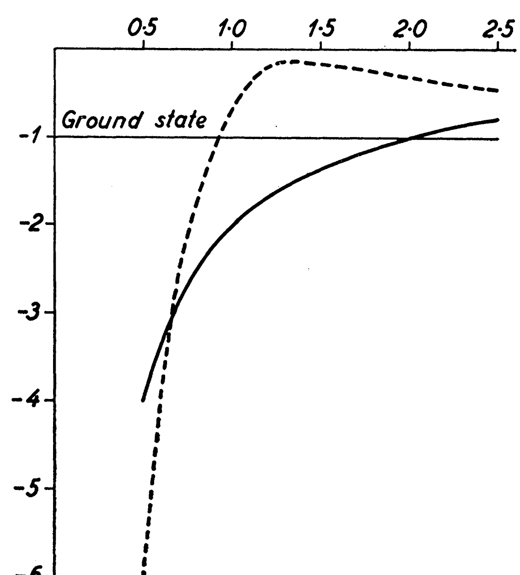

FIG. 2. The Coulomb potential (——) and an equivalent potential (-----).

where κ_S is the positive root of the smallest $|E_{i,S}|$ used in the construction of V_S. A corresponding result holds for any V_P reproducing the P-spectrum and phase shift. Since all $E_{i,S} \neq E_{j,P}$, $\kappa_S \neq \kappa_P$ so that $V_S \neq V_P$ unless $V_S = V_P = V_0$.

The same result can be obtained even when some of the eigenvalues coincide, provided that V_0 has an asymptotic expansion of the form

$$\sum_{3}^{\infty} a_r r^{-n}.^{8}$$

It can then be shown[9] that $f_{i,S}$ and $f_{j,P}$ have different asymptotic expansions and hence so do $V_S - V_0$ and $V_P - V_0$.

It is clear that even if V_0 falls off at infinity only like r^{-1}, Eqs. (2.10), (2.12), and (2.29) still lead to equivalent potentials.

Examples of potentials equivalent for S-states are shown in Figs. 1 and 2. They have been constructed by using the ground-state wave functions.

3. POTENTIALS WITH PURELY DISCRETE SPECTRUM

The boundary value problems which lead to purely discrete spectra fall into several subcases. We shall not make an extensive study of all of these but only exemplify the situation by discussing in some detail the case

$$\varphi''(r) + E\varphi(r) = V_0(r)\varphi(r), \tag{3.1}$$

$$\varphi(0) = \varphi(1) = 0, \tag{3.2}$$

where $V_0(r)$ is regular. We shall make a brief reference to the case of an infinite interval.

A solution of (3.1) which plays the same role as our previous function $f(k,r)$ of (2.4) can be chosen as $g(E,r)$ defined by the initial conditions

$$g(E,0) = 0, \quad g'(E,0) = 1. \tag{3.3}$$

The eigenvalues E_l of (3.1) and (3.2) are defined by

$$g(E_l, 1) = 0. \tag{3.4}$$

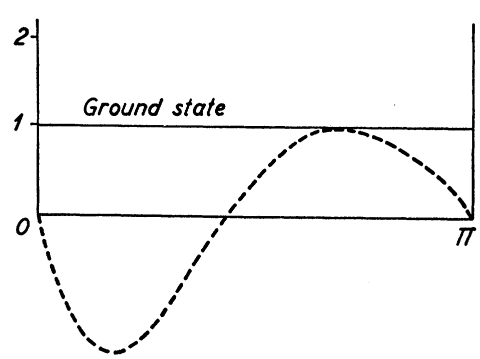

FIG. 3. The one-dimensional box (——) and an equivalent potential (-----).

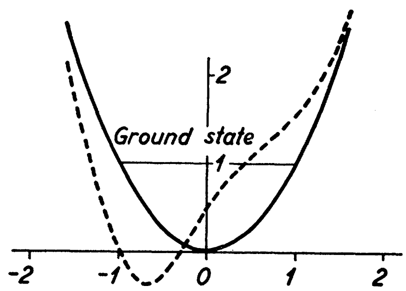

FIG. 4. The harmonic oscillator potential (——) and an equivalent potential (-----).

The eigenfunctions are $g(E_l, r) \equiv g_l(r)$, and we call

$$\frac{1}{\Gamma_l} \equiv \int^1 g_l^2 dr = g_l'(1)\dot{g}(E_l, 1), \tag{3.5}$$

where

$$\dot{g}(E,r) \equiv \partial g(E,r)/\partial E. \tag{3.6}$$

Again the expression $g_l' g_l$ is orthogonal to all the squares of the eigenfunctions and therefore—just as in Sec. 2—gives rise to a one parameter family of equivalent potentials

$$V(\lambda, r) = V_0(r) + \frac{\lambda}{4} g_1'(r) g_1(r) + \frac{\lambda^2}{8N^2}[g_1(r)]^2, \tag{3.7}$$

$$N(\lambda, r) = 1 - \frac{\lambda}{4}\int_0^r [g_1(r')]^2 dr', \tag{3.8}$$

with the solutions

$$g(\lambda; E, r) = g(0; E, r) + \frac{\lambda}{4N} g_1(r) \int_0^r g_1(r') g(0; E, r') dr'. \tag{3.9}$$

From (3.9) and (3.5) it follows that the Γ_l, $l \neq 1$ are independent of λ whereas Γ_1 varies from 0 to ∞ as λ varies from $-4\Gamma_1(0)$ to ∞. Again the manifolds of potentials and solutions, (3.7) and (3.9) are independent of the normalization of $g_1(r)$.

By an obvious modification of appendix II of reference 1 it can be shown that in the present case an equivalent potential is completely determined by the infinite set of parameters Γ_l, $l = 1, 2, \cdots$. Hence, by repeating the above construction procedure using the other eigenvalues any equivalent potential can be constructed.[10]

Also for the case of an infinite interval (e.g., the harmonic oscillator) Eqs. (3.7) to (3.9) lead to equivalent potentials, the normalization of $g_1(r)$ being arbitrary.

Potentials equivalent to a one-dimensional "box" and to a harmonic oscillator potential are shown in Figs. 3 and 4. They have been constructed by means of the ground-state wave functions.

It is a pleasure to thank Professor Niels Bohr for extending to us the hospitality of his institute.

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[8] The a_n may, of course, all vanish as, for example, for cut-off or exponentially decreasing potentials.

[9] W. Sternberg, Math. Ann. **81**, 119 (1920).

[10] We assume here, without proof, that the process of adjusting successive Γ_l converges, under reasonable conditions, as $l \to \infty$.