Discrete States for Singular Potential Problems*†

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The solutions of the quantum mechanical wave equations for singular potentials are re-examined. It is shown that a set of orthonormal wave functions with complex energy eigenvalues ($E_n=W_n\pm\frac{1}{2}i\Gamma_n$) is obtained if certain natural analyticity requirements are imposed on the form of the potentials. In general, the result is interpreted in the following way: W_n is the most probable position of the energy level for various types of cutoff and Γ_n is a measure of the probable error.

1. INTRODUCTION

FOR nonsingular potentials, the solutions of the quantum mechanical wave equations are unique and of great value in the discussion of physical problems. Thus, an idealized, unbounded potential ($V=-Ze^2/r$) leads to a meaningful description of the hydrogen atom, even if the physical cutoff (finite proton size, etc.) is ignored. For singular potentials, such a correspondence between physical and idealized systems has not generally been found because the latter do not possess unique solutions unless the normalization requirement is supplemented (Sec. 3). The aims of this paper are: (a) to find some boundary condition which gives conventional results for nonsingular problems and unique discrete spectra for singular potentials; (b) to show that these singular levels are useful as approximations to many physical (cutoff) problems, even if the detailed location of the cutoff is unknown.

With these objectives in mind, the consequences of the following assumptions are investigated: (I) All physically realistic potentials are represented by functions of the coordinates which are analytic except at isolated poles and branch points. (II) All normalizable solutions of the quantum mechanical wave equations are meaningful and acceptable. Assumptions (I) and (II) do give standard results in all nonsingular problems (Sec. 2) and unambiguous point spectra for singular Hamiltonians. In the latter case, the ambiguity is removed because the wave function $\psi(-x)$ [or $\psi(-\mathbf{r})$] is determined in essentially a unique manner from $\psi(x)$ [or $\psi(\mathbf{r})$] by analytic continuation *around* the singularity (Sec. 4).

In general, the levels obtained by continuation have complex energies. The virial theorem suggests that these states correspond to the periodic or asymptotic orbits of classical singular problems. In the last section, it is shown that the complex eigenvalues contain information about the density of states for an indeterminate cutoff and can be used to approximate levels for repulsive core cutoff problems. This technique is possible because the logarithmic derivative of a wave function is large if the potential is singular and attractive, or if it is strongly repulsive; thus, solutions for the two cases can be joined smoothly.

2. NONSINGULAR POTENTIALS

Throughout the years attempts have been made to solve anomalous nonsingular problems by imposing new boundary conditions (together with the normalization requirement) on the solutions of the quantum mechanical wave equations.[1] In most cases, as pointed out by von Neumann and others,[2] the extra conditions are unnecessary and not generally applicable; von Neumann maintained that (II) is sufficient to give correct results if problems associated with the ordinary continuous spectrum are excluded.

As an example of this reasoning, consider the one-dimensional Schrödinger equation for an attractive potential:

$$V(x)=-V_0f(x)x^{-k},\quad f(0)=1.$$

Then

$$u''+[U_0f(x)x^{-k}-\eta^2]u=0, \tag{1}$$

where $U_0=2mV_0/\hbar^2$, and $\eta^2=-2mE/\hbar^2(\eta=i\lambda,\ E>0)$. If $0<x\ll1$, and $0<k<2$, the two linearly independent solutions of Eq. (1) behave like

$$\begin{aligned}u^{(1)}(x)&=x[1+O(x)],\\ u^{(2)}(x)&=[1+ax\ln x][1+O(x)].\end{aligned} \tag{2}$$

Both $u^{(1)}$ and $u^{(2)}$ are quadratically integrable near the origin, so that for any η, some linear combination is normalizable in the interval $0\leq x\leq\infty$ if $V(\infty)\geq0$. Thus, when $V(x)=-V_0x^{-1}$, $0<x\leq\infty$, $V(0)=\infty$, a continuum results if (II) gives the only restriction on $\psi=A[u^{(1)}+Bu^{(2)}]$ (several of the boundary conditions of reference 1 eliminate $u^{(2)}$, leading to a discrete spectrum). However, (I) cannot be used if the potential has an infinite discontinuity at the origin. In fact, the

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[1] G. Jaffe, Z. Physik **66**, 770 (1931); R. M. Langer and N. Rosen, Phys. Rev. **37**, 658 (1931); G. Araki, Progr. Theoret. Phys. Japan **3**, 97 (1948); G. Falk and H. Marschall, Z. Physik **131**, 269 (1952).
[2] J. von Neumann, *Mathematical Foundations of Quantum Mechanics* (Princeton University Press, Princeton, 1955), p. 29. See also K. Kodaira and T. Kato, Progr. Theoret. Phys. **3**, 439 (1948), T. Tits, J. Exptl. Theoret. Phys. U.S.S.R. **30**, 948 (1956) [translation: Soviet Phys. JETP **3**, 777 (1956)].

indeterminate result [for $V(0)=\infty$] is physically correct since classically a particle with infinite velocity impinges on an infinite barrier at $x=0$, and the situation is not well defined.

If the barrier at $x\leq 0$ is removed, the origin becomes an interior point and (II) is sufficient to determine the levels. All even states must have $\psi(x)=u^{(2)}(x)$ because $u^{(1)}$ (even) is a Green's function and not a solution of Eq. (1). Therefore, a unique discrete spectrum is found since $u^{(1)}(-x)=-u^{(1)}(x)$, $u^{(2)}(-x)=u^{(2)}(x)$ [this implies $V(x)=V(-x)$].

In anticipation of the singular potential discussion, it is significant to note that the same spectrum can be found without examining ψ *at* $x=0$, if assumption (I) is used. The potential may be represented as

$$V(x)=-V_0\lim_{\epsilon\to 0}(x^2+\epsilon^2)^{-\frac{1}{2}},$$

and $\psi(-x)$ can be obtained from $\psi(x)$ by analytic continuation around $x=0$. A branch cut must be crossed for $|x|>\epsilon$ so that the continuation is not unique; while solutions which are neither even nor odd may be selected, the ones consistent with $V(-x)=V(x)$ have $|u^{(1)}(-x)|=|u^{(1)}(x)|$, etc. The relative parity is determined by the requirement that the Wronskian,

$$W=u^{(1)}u^{(2)\prime}-u^{(2)}u^{(1)\prime}, \tag{3}$$

have the same constant value on both sides of the origin. If $u^{(1)}$ is odd, $u^{(2)}$ must be even, and this leads to the same discrete spectrum.

More subtle difficulties are present in multidimensional problems. The two linearly independent S-state solutions for the hydrogen atom are $\psi_0^{(1)}(\mathbf{r})=u^{(1)}(r)/r$, $\psi_0^{(2)}(\mathbf{r})=u^{(2)}(r)/r$ where $u^{(1)}$ and $u^{(2)}$ are given by Eq. (2) for $r\ll 1$. The supplementary boundary conditions[1] have been proposed to eliminate $\psi_0^{(2)}$ because both series are quadratically integrable near the origin, and both are genuine solutions of the radial equation. However, Dirac has pointed out that $\psi_0^{(2)}$ is a Green's function, not a solution, for the three-dimensional Schrödinger equation[3]; hence it must be discarded. The use of spherical coordinates obscures this fact since the origin is treated as a boundary instead of an interior point.

The series $\psi_0^{(2)}$ can also be eliminated, as in the one-dimensional case, by using (I) without explicit examination of ψ *at* $r=0$. The reflected solution, $\psi(-\mathbf{r})$, is obtained from $\psi(\mathbf{r})$ by rotation in the complex (x,y,z) planes (Cartesian coordinates are used to avoid the additional singularity at the origin). Although the process of analytic continuation for functions of several complex variables is not completely understood (this is discussed further in Sec. 4), it can be established that $|\psi_0^{(1)}(-\mathbf{r})|=|\psi_0^{(1)}(\mathbf{r})|$, etc. The subsidiary condition that the Wronskian, $\mathbf{W}=\psi^{(1)}\nabla\psi^{(2)}-\psi^{(2)}\nabla\psi^{(1)}$, must satisfy $\nabla\cdot\mathbf{W}=0$ everywhere, leads to an integral relation,

$$\lim_{\epsilon\to 0}\left[\int\int dydzW_x(\epsilon,y,z)-\int\int_A dydzW_x(-\epsilon,y,z)\right]=0, \tag{4}$$

where the surface of integration is arbitrary. Equation (4) implies that

$$\lim_{\epsilon\to 0}[\psi^{(2)}/\psi^{(1)}]_{x=\epsilon}=-\lim_{\epsilon\to 0}[\psi^{(2)}/\psi^{(1)}]_{x=-\epsilon};$$

for the same energy, any two linearly independent solutions of a Schrödinger equation must have opposite parities, and $\psi_0^{(2)}$ can be eliminated.

For any nonsingular problem, two series with distinct, integral exponents can be found. If the singularity is not at a boundary, the eigenfunction must be $\psi=\psi^{(1)}$ *or* $\psi=\psi^{(2)}$, since only these choices have analytic properties consistent with (I) [$\psi=A(\psi^{(1)}+B\psi^{(2)})$ does not], and also satisfy $\nabla\cdot\mathbf{W}=0$. This leads to the conventional spectrum in every case. However, if the boundary is singular, (I) and (II) do not determine the spectrum and the Green's function argument also fails. Since the ambiguity should be present, (I) and (II) seem to represent correct boundary conditions, while those of reference 1 are incorrect.

3. SINGULAR POTENTIAL PROBLEM

Singular Hamiltonians ($k\geq 2$ in nonrelativistic equations) are characterized by wave functions with nonintegral exponents. For example, the choice $k=2$, $f(x)=[1+2\nu x/U_0]$ $(x>0)$ in Eq. (1) leads to the general solution

$$\psi(x)=A[u^{(+)}(x)+B_s(\eta)u^{(-)}(x)], \tag{5}$$

$$u^{(\pm)}(x)=e^{-\eta x}x^{\frac{1}{2}\pm s}\,{}_1F_1(\tfrac{1}{2}\pm s-\nu/\eta;\,1\pm 2s;\,2\eta x), \tag{6}$$

where $s=(\frac{1}{4}-U_0)^{\frac{1}{2}}$ and ${}_1F_1(a;c;z)$ is a confluent hypergeometric function. If $U_0>\frac{1}{4}$, s is imaginary ($s=i\sigma$) and therefore, for any U_0, $u^{(+)}$ and $u^{(-)}$ are quadratically integrable near the origin. The condition $\psi(\infty)=0$ is satisfied if

$$B_s(\eta)=-(2\eta)^{-2s}\frac{\Gamma(1+2s)}{\Gamma(1-2s)}\frac{\Gamma(\frac{1}{2}-s-\nu/\eta)}{\Gamma(\frac{1}{2}+s-\nu/\eta)}, \tag{7}$$

and in the interval $0\leq x\leq\infty$, there is a normalizable continuum. Moreover, both functions $\psi_0^{(\pm)}(\mathbf{r})=u^{(\pm)}(r)/r$ are solutions, not Green's functions, for the three-dimensional Schrödinger equation.

For $U_0<\frac{1}{4}$ and $k=2$, *ad hoc* boundary conditions have been used to obtain discrete bound states or unique scattering phase shifts.[4] However, when $U_0>\frac{1}{4}$

[3] P. A. M. Dirac, *Quantum Mechanics* (Clarendon Press, Oxford, 1947), p. 155. For a more general proof, see T. Kato, Trans. Am. Math. Soc. **70**, 195 (1951).

[4] G. H. Shortley, Phys. Rev. **38**, 120 (1931); N. F. Mott and H. S. W. Massey, *Theory of Atomic Collisions* (Clarendon Press, Oxford, 1949), p. 40.

($k=2$) or $k>2$ (all U_0), the functions $u^{(\pm)}$ differ only in phase and the extra conditions do not clarify the situation. Some authors have concluded that singular problems have no meaning in quantum mechanics although they are meaningful in classical physics.[5] Case has suggested that one should consider only an orthogonal set of solutions.[6] This additional restriction on the spectrum (the singular Hamiltonian is not self-adjoint) is equivalent to the requirement that probability current density be conserved for an arbitrary superposition of eigenfunctions. As shown by Case, solutions with eigenvalues η_n and η_m will be orthogonal if and only if

$$B_s^*(\eta_n)-B_s(\eta_m)=0, \qquad U_0<\tfrac{1}{4},\ k=2, \quad (8)$$

$$B_{i\sigma}^*(\eta_n)B_{i\sigma}(\eta_m)=1, \quad U_0>\tfrac{1}{4},\ k=2 \text{ or } k>2. \quad (9)$$

Since $|B_{i\sigma}|=1$ [$(u^{(+)})^*=u^{(-)}$ for these problems], we may write $B_{i\sigma}(\eta)=\exp[2i\gamma_\sigma(\eta)]$ and Eq. (9) becomes $\gamma_\sigma(\eta_m)=\gamma_\sigma(\eta_n)+N\pi$, $N=0, \pm1, \pm2, \cdots$. Thus, if one chooses any η_0 or λ_0 (presumably corresponding to a definite cutoff at some x_0), an orthonormal set of eigenfunctions is determined.[7]

The function $B_s(\eta)$ of Eq. (7) is periodic with an infinite number of poles and zeros at $(\frac{1}{2}\pm s-\nu/\eta)=-n$, $n=0, 1, 2, \cdots$. Moreover, for almost every η_0 there is a finite lowest solution with $B_s(\eta_0)=B_s(\eta_{\max})$. Thus, if $U_0<\frac{1}{4}$ the spectrum is generally bounded from below, and there are an infinite number of negative energy states. However, when $U_0>\frac{1}{4}$, $\gamma_\sigma(\eta)$ is given by

$$\gamma_\sigma(\eta)=\tfrac{1}{2}\pi-\sigma\ln 2\eta+\arg\Gamma(1+2i\sigma)+\arg\Gamma(\tfrac{1}{2}-i\sigma-\nu/\eta), \quad (10)$$

and it can be seen that there is no lower bound to the spectrum for any η_0 because the term $(\sigma\ln 2\eta)$ is monotonically increasing.

Case asserted that eigenvalue formulas for singular potentials always contain an arbitrary constant. Furthermore, although spectra associated with the Dirac equation have finite lower bounds, Case concluded that the use of a singular potential in the Schrödinger equation is academic since the spectrum is always unbounded from below, if $U_0>\frac{1}{4}$ or $k>2$. Vogt and Wannier[8] criticized the first of these conclusions; they pointed out that in many cases only one value of η_0 is likely to be relevant. This idea is discussed further in Sec. 5, however, it will be demonstrated here that unbounded spectra are not a general feature of the Schrödinger equation.

Consider $k=2$, $f(x)=x^2\csc^2x$ for $0<x<\pi/2$ and $f(0)=f(\pi/2)=\infty$. The two linearly independent solutions of Eq. (1) are hypergeometric functions,

$$u^{(\pm)}(x)=(\sin x)^{\frac{1}{2}\pm s}\times {}_2F_1(\tfrac{1}{4}\pm\tfrac{1}{2}s+\tfrac{1}{2}i\eta, \tfrac{1}{4}\pm\tfrac{1}{2}s-\tfrac{1}{2}i\eta; 1\pm s; \sin^2x), \quad (11)$$

and $\psi(\pi/2)=0$ if

$$B_s(\eta)=-\frac{\Gamma(1+s)}{\Gamma(1-s)}\frac{\Gamma(\frac{3}{4}-\frac{1}{2}s-\frac{1}{2}i\eta)}{\Gamma(\frac{3}{4}+\frac{1}{2}s-\frac{1}{2}i\eta)}\frac{\Gamma(\frac{3}{4}-\frac{1}{2}s+\frac{1}{2}i\eta)}{\Gamma(\frac{3}{4}+\frac{1}{2}s+\frac{1}{2}i\eta)}. \quad (12)$$

Using the expansion

$$\Gamma(x+iy)=\Gamma(x)\prod_{n=1}^{\infty}\left[1+\frac{y^2}{(x-1+n)^2}\right]^{-\frac{1}{2}} \times\exp\left\{i\left[-\gamma y+\frac{y}{n}-\tan^{-1}\left(\frac{y}{x-1+n}\right)\right]\right\}, \quad (13)$$

where γ is Euler's constant, Eq. (9) becomes

$$B_s(\eta)=\frac{\Gamma(1+s)}{\Gamma(1-s)}\frac{\Gamma^2(\frac{3}{4}-\frac{1}{2}s)}{\Gamma^2(\frac{3}{4}+\frac{1}{2}s)} \times\prod_{n=1}^{\infty}\left[1+\frac{\eta^2}{(\frac{3}{2}+s+2n)^2}\right]\times\left[1+\frac{\eta^2}{(\frac{3}{2}-s+2n)^2}\right]^{-1}. \quad (14)$$

The infinite product is a monotonic function of $\eta(U_0<\frac{1}{4})$, and for any choice of B_0 there is at most one root, $B_s(\eta)=B_0$. In general, $\eta=\infty$ is not a solution. When $U_0>\frac{1}{4}$, the spectrum for Eq. (12) differs markedly from that of Eq. (10). The function $\gamma_\sigma(\eta)$ for Eq. (12) is shown in Fig. 1[9]; as $\eta\to\infty$, $\gamma_\sigma(\eta)\to[\pi/2-\arg\Gamma(1+i\sigma)]$ and the spectrum is generally bounded from below.

It is desirable to find a criterion to predict which potentials have generally bounded spectra and which ones have $\eta=\infty$ as a solution for any η_0. A distinction can perhaps be made on the basis of the classical virial theorem. All periodic or asymptotic orbits for classical problems have

$$E_{\text{per}}=\langle V\rangle+\tfrac{1}{2}\langle x\,dV/dx\rangle. \quad (15)$$

If $f(x)=1+\alpha x(\alpha>0)$, $-\infty\leq E_{\text{per}}\leq 0$, but when $f(x)=x^2\csc^2x$, $E_{\text{per}}=V_0\langle\csc^2x[x\operatorname{ctn}x-1]\rangle$ so that $-\frac{1}{3}V_0\leq E_{\text{per}}\leq\infty$. In classical physics, singular periodic orbits have negative energies for the long range potential and have $E_{\text{per}}>-\frac{1}{3}V_0$ for the short-range force. In quantum mechanics, this result is reflected by the form of $\gamma_\sigma(\eta)$; when $f(x)=1+\alpha x$, the density of possible states (with an indeterminate cutoff) is large for $-\infty<E<0$, but if $f(x)=x^2\csc^2x$, the density of periodic negative

[5] E. C. Kemble, *Principles of Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1937), p. 198; P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill Book Company, Inc., New York, 1953), p. 1666.

[6] K. M. Case, Phys. Rev. **80**, 797 (1950).

[7] For all of these cases, the "continuous" spectra are examples of limit circle problems. [See E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations* (McGraw-Hill Book Company, New York, Inc., 1955), Chap. 9.] In an unpublished manuscript Professor E. Gerjuoy has examined anomalous quantum mechanical problems and shown that the specification of a real η_0 corresponds to choosing one point on the limit circle. He has also noted that this makes the problem self-adjoint.

[8] E. Vogt and G. H. Wannier Phys. Rev. **95**, 1190 (1954).

[9] H. Salzer *et al.*, National Bureau of Standards, Applied Mathematics Series 34 (U. S. Government Printing Office, Washington, D. C., 1954).

energy states is vanishingly small. The classical argument based on Eq. (15) gives no information about nonperiodic, localized states with $E\simeq-\infty$. A similar gap is present in the quantum mechanical discussion since the asymptotic formulas used to determine $B_{i\sigma}(\eta)$ are meaningless in this limit, and an intricate study of the solutions as $\eta\to\infty$ would be needed to discuss these states.

When Eq. (15) is applied to potentials with $k>2$, $f(x)=1$, $E_{\rm per}=(\frac{1}{2}k-1)V_0\langle x^{-k}\rangle$, suggesting that singular orbits have $E_{\rm per}>0$ (all classical examples do fall in this range[10]). For these problems, the functions $\gamma_\sigma(\eta)$ are not well known since the solutions are represented by semiconvergent power series with three term recursion relations. However, on the basis of the above correspondence, it is reasonable to expect that $\gamma_\sigma(\eta)$ is independent of η as $\eta\to\infty$, so that for $k>2$ the spectrum is also generally bounded from below.

4. ANALYTIC CONTINUATION

The eigenvalue formulas of the last section represent non-unique, discrete levels because only one boundary condition, $\psi(\infty)=0$, has been imposed. If the other end point is not singular, more information should be obtainable from the requirement, $\psi(-\infty)=0$.

The discussion of Sec. 2 indicates that the use of assumption (I) to define $\psi(-x)$ leads to meaningful spectra. Since $f(x)/x^2=\csc^2x$ is an analytic function of $\sin x$ for $0<x<\pi/2$, $\psi(-x)$ is determined by setting $z=|\sin x|\exp i\theta$ in Eq. (11) and rotating from $\theta=0$ to $\theta=\pi$. The continuation is straightforward because neither $u^{(+)}$ nor $u^{(-)}$ contain logarithms and both series converge for $|z|<1$. (A branch cut must be crossed; this cut may be taken at $\theta=\pi/2$ for both $u^{(+)}$, $u^{(-)}$.) The most general result is $u^{(+)}(-x)=Cu^{(+)}(x)$, $u^{(-)}(-x)=Du^{(-)}(x)$ and the Wronskian is constant over the interval $-\frac{1}{2}\pi<x<\frac{1}{2}\pi$ if $CD=-1$.

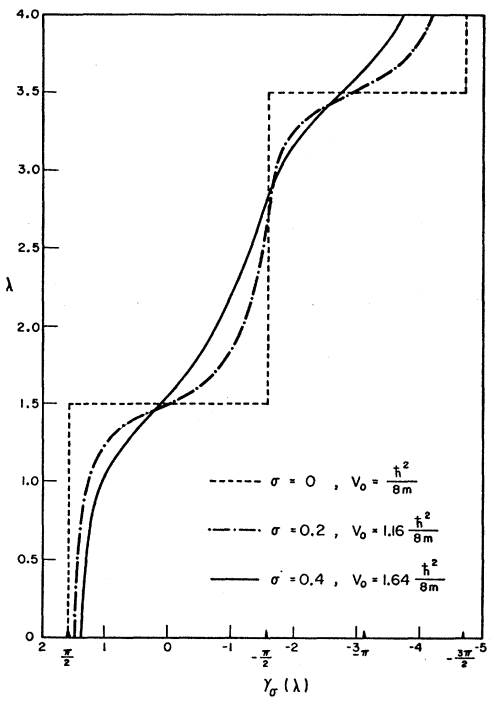

FIG. 1. The phase function $\gamma_\sigma(\lambda)[=\cos^{-1}\mathrm{Re}(-u^{(+)}/u^{(-)})_{x=\frac{1}{2}\pi}]$ for the potential $V(x)=-V_0\csc^2x$, $V(0)=V(\pi/2)=\infty$. The dimensionless parameters are defined by: $V_0=\hbar^2(\sigma^2+\frac{1}{4})/2m$, $E=\hbar^2\lambda^2/2m$.

This analysis is sufficient to show that $\psi(\pm\frac{1}{2}\pi)=0$ only if $B=0$ ($\psi=u^{(+)}$) or $B=\infty$ ($\psi=u^{(-)}$). The corresponding roots of Eq. (12) for $U_0<\frac{1}{4}$ are,

$$\left.\begin{aligned}\lambda_n^{(-)2}&=(\tfrac{3}{2}-s+2n)^2,\quad \psi=u^{(-)}\\ \lambda_n^{(+)2}&=(\tfrac{3}{4}+s+2n)^2,\quad \psi=u^{(+)}\end{aligned}\right\}n=0,\,1,\,2,\,\cdots. \tag{16}$$

It is natural to choose branches so that $C=i\exp(\pi is)$, $D=i\exp(-\pi is)$.[11] Then as $U_0\to0$, $s\to\frac{1}{2}$, and the eigenfunctions and eigenvalues go over into those for a free particle. When U_0 increases from zero to $\frac{1}{4}$, the eigenvalues for $\psi=u^{(-)}$ increase in magnitude; the problem is thus not of Sturm-Liouville class, although the $\psi_n^{(\pm)}$ do form an orthonormal set.[12]

When $U_0>\frac{1}{4}$, the continuation yields

$$C=\pm i\exp(\pm\pi\sigma),\quad D=\pm i\exp(\mp\pi\sigma).$$

No matter which branch is chosen, if it is consistent with the restriction $CD=-1$, it will again lead to the eigenvalue formulas $B_{i\sigma}(\lambda)=0$, $B_{i\sigma}(\lambda)=\infty$. These equations have *only* complex roots:

$$\lambda_n^{(\pm)2}=[\tfrac{3}{2}\pm i\sigma+2n]^2=[(\tfrac{3}{2}+2n)^2-\sigma^2]\pm2i\sigma[\tfrac{3}{2}+2n]. \tag{17}$$

The energies are of the form $E_n=W_n\pm\frac{1}{2}i\Gamma_n$ and the complete spectrum for this problem is plotted in Fig. 2. For $8mV_0/\hbar^2>1$, the W_n are given by solid lines and the dotted curves represent $W_n\pm\frac{1}{2}\Gamma_n$. The complex energies clearly describe nonstationary states with lifetimes $\tau_n=\hbar/\Gamma_n$ and $(C^*C)\neq1$, etc., so that $|\psi^{(\pm)}|^2$ is asymmetric. The asymmetry is not inconsistent with $[R_x,H]_-=0$ since there is a source or sink at the origin. The reflected wave functions, $R_x\psi^{(\pm)}$, are also eigenfunctions, and if the initial position of the particle is unknown, an even or odd mixture can be considered.

When these techniques are applied to the long range problem [Eq. (6)], $f(x)$ is defined as $[1+2\nu U_0^{-1}\times\lim_{\epsilon\to0}(x^2+\epsilon^2)^{\frac{1}{2}}]$ so that $V(x)$ is even. Postulates (I) and (II) lead to $B_s(\eta)=0$, $B_s(\eta)=\infty$, and the discrete

[10] See, for instance, E. T. Whittaker, *Analytical Dynamics* (Dover Publications, New York, 1944), Chap. IV.

[11] Although $\psi^{(+)}$ and $\psi^{(-)}$ have phase changes upon reflection, $|\psi|^2$ is symmetric. Since the reflection operator, R_x, commutes with the Hamiltonian, $R_x\psi^{(+)}$ and $R_x\psi^{(-)}$ are also eigenfunctions of H; however, R_x on $R_x\psi$ represents a complex rotation inverse to that of R_x on ψ. An even or odd mixture of the degenerate solutions, ψ and $R_x\psi$, can also be constructed.

[12] It is useful to choose C, $D=\pm1$ when comparison is made with a cut-off problem. See Sec. 5 below and F. L. Scarf, Bull. Am. Phys. Soc., Ser. II, 3, 60 (1958).

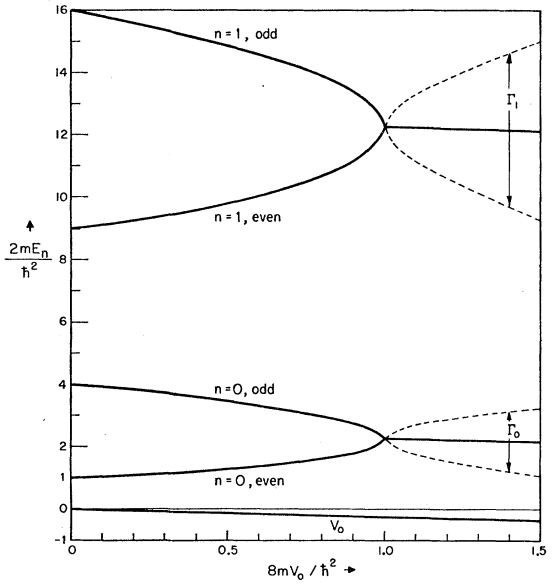

FIG. 2. First four levels for the potential $V(x)=-V_0\csc^2 x$, $|x|<\pi/2$, $V(\pm\pi/2)=\infty$. For $V_0\leq\hbar^2/8m$, the levels are stationary. For $V_0>\hbar^2/8m$, the levels are quasi-stationary. The dotted lines are $W_n\pm\frac{1}{2}\Gamma_n$, where Γ_n is the width of the nth state.

eigenvalues are

$$\eta_n^{(\pm)}=\nu[n+\tfrac{1}{2}\pm s]^{-1}, \quad n=0, 1, 2, \cdots. \tag{18}$$

In any problem for which it is sensible to consider adiabatic variations of U_0, the $\eta_n^{(-)}$ ($B=\infty$) must be discarded since none of the $u_n^{(-)}$ are solutions of Eq. (1) when U_0 is zero.

For $k>2$, $f(x)=1$ and $\sigma^2=U_0$, two linearly independent solutions of Eq. (1) are

$$u^{(\pm)}(x)=x^{k/4}g^{(\pm)}(x)\exp\left\{\pm i\left[\frac{2\sigma}{(k-2)x^{\frac{1}{2}k-1}}\right]\right\}, \tag{19}$$

where the $g^{(\pm)}$ are complex conjugate functions represented by semiconvergent series of the form

$$\sum_{n=0}^{\infty} A_n^{(\pm)}x^{n(\frac{1}{2}k-1)}.$$

The solutions $u^{(+)}$ and $u^{(-)}$ have distinct continuations as $\arg(x)$ is rotated from 0 to π; therefore, an arbitrary linear combination $\psi=A[u^{(+)}+Bu^{(-)}]$ with $\psi(\infty)=0$, will not generally satisfy $\psi(-\infty)=0$. However, if the Stokes phenomenon does not mix solutions, $g^{(+)}(-x)=Cg^{(+)}(x)$, $g^{(-)}(-x)=Dg^{(-)}(x)$ and $\psi(-\infty)=0$ implies $B=0$ or $B=\infty$, so that $\lambda_n^{(\pm)}=(a_n\pm ib_n)$. In any case, a unique discrete spectrum will be found if (I) and (II) are used along with the requirement that the Wronskian be constant.

Complications arise in multidimensional problems. For physical interactions, $V(\mathbf{r})$ is usually defined as a regular function of the curvilinear coordinates except at isolated singular points. However, the non-Cartesian coordinate systems themselves introduce additional singularities. It is therefore desirable to discuss singular problems in Cartesian coordinates, even if the equations are not separable for these variables. With this point of view, the solution of a partial differential equation is regarded as a function of several complex variables (x,y,z) which is analytic except at the singular points of the potential. The solution is defined as $\psi(\mathbf{r}_0)$ (r_0 is an ordinary point) plus its analytic continuations to all $\mathbf{r}$. Much work has been done in this field, however, it does not seem to have been carried far enough to discuss rigorously the very singular cases of interest here.[13] A nonrigorous justification of analytic continuation in multidimensional problems must suffice.

Consider, for example, $V(\rho,\theta,z)=-U_0\hbar^2(1+2\nu\rho/U_0)/2m\rho^2$ and let $\psi(\rho,\theta,z)=R(\rho)\Theta(\theta)Z(z)/\rho^{\frac{1}{2}}$. All states with $L_\theta=l\hbar$, $k_z=0$, $R_l(\infty)=0$, have $R_l(\rho)=A[u_l^{(+)}(\rho)+B_{sl}(\eta)u_l^{(-)}(\rho)]$ where $u_l^{(\pm)}(\rho)$ and $B_s(\eta)$ are defined by Eqs. (6) and (7), and $s_l^2=l^2-U_0$. For $s_l\geq\frac{1}{2}$, B must be zero if ψ is to be normalized, but if $s_l<\frac{1}{2}$ and ρ is defined as $|(x^2+y^2)^{\frac{1}{2}}|$, there is no restriction on B. However, if $\rho=\lim_{\epsilon\to 0}(x^2+y^2+\epsilon^2)^{\frac{1}{2}}$, then ψ is an analytic function of x, y, z except for isolated singularities and branch cuts, and $\psi(\pm x, \pm y, z)$ is obtained from $\psi(x,y,z)$ by rotation of $\arg(x)$ and/or $\arg(y)$. If $\psi^{(+)}$ and $\psi^{(-)}$ correspond to $B=0$, ∞, respectively, then

$$\begin{aligned}\psi^{(+)}(-x,y,z)&=\pm\psi^{(+)}(x,y,z), && |x|<y\\ &=\pm C\psi^{(+)}(x,y,z), && |x|>y;\\ \psi^{(-)}(-x,y,z)&=\pm\psi^{(-)}(x,y,z), && |x|<y\\ &=\pm D\psi^{(-)}(x,y,z), && |x|>y,\end{aligned} \tag{20}$$

and $\psi^{(+)}(-x,-y,z)=\pm C\psi^{(+)}(x,y,z)$, etc. for all (x,y). An even or odd mixture of ψ plus its reflection about the line $x=-y$ can be used to reproduce the θ dependence. However, since $\psi^{(+)}$ and $\psi^{(-)}$ must have negative relative parity [Eq. (4)], only $\psi^{(+)}$ *or* $\psi^{(-)}$ may be used to describe a state of given l. In practice, $\psi_l^{(+)}$ is retained since $\psi_0^{(-)}$ tends to a Green's function as $U_0\to 0$.

The details of this discussion are not rigorously justified but the main results seem well founded. Only series with distinct exponents can be taken as solutions of the eigenvalue problem consistent with (I), (II) [a combination such as $r^{\frac{1}{2}}\cos(\sigma\ln r+\gamma)$ or $r^{\frac{1}{4}k}\cos(\sigma r^{1-\frac{1}{2}k}+\gamma)$ is ruled out]. Equation (4) insures that the two solutions do not combine so that $B=0$ or $B=\infty$.

These ideas can also be applied to the relativistic wave equations. For example, the two linearly independent sets of solutions for a Dirac electron in a Coulomb field behave as $r^{-1\pm s_j}$ [$s_j^2=(j+\frac{1}{2})^2-\alpha Z$] near the origin. If $s_j>\frac{1}{2}$, the more singular set is eliminated

[13] For a summary of the ideas behind this approach to such problems and its present limitations, see the discussion by F. John in *Proceedings of the Symposium on Spectral Theory and Differential Problems* (Oklahoma Agricultural and Mechanical Press, Stillwater, 1951), p. 113.

because it cannot be normalized, and the energies are

$$E_{nj}/mc^2=[1+\alpha^2Z^2/(n-j-\tfrac{1}{2}+s_j)^2]^{-\frac{1}{2}},$$
$$n=1, 2, 3, \cdots; \quad j=\tfrac{1}{2}, \tfrac{3}{2}, \cdots. \quad (21)$$

However, the problem is singular for $\alpha Z>(j+\frac{1}{2})^2-\frac{1}{4}$ and $s_{\frac{1}{2}}$ is imaginary when $\alpha Z>1$. The technique outlined above leads to Eq. (21) for all Z, with s_j replaced by $i\sigma_j$ if $\alpha Z>(j+\frac{1}{2})^2$. Thus, for $j=\frac{1}{2}$, $Z>137$, $E_{n\frac{1}{2}}=(W_{n\frac{1}{2}}\pm\frac{1}{2}i\Gamma_{n\frac{1}{2}})$, and

$$W_{n\frac{1}{2}}/mc^2=\frac{(n-1)[A_n(\sigma)+1]^{\frac{1}{2}}+\sigma[A_n(\sigma)-1]^{\frac{1}{2}}}{\sqrt{2}A_n(\sigma)(n^2-2n+2)^{\frac{1}{2}}}, \quad (22)$$

$$\Gamma_{n\frac{1}{2}}/2mc^2=\frac{\sigma[A_n(\sigma)+1]^{\frac{1}{2}}-(n-1)[A_n(\sigma)-1]^{\frac{1}{2}}}{\sqrt{2}A_n(\sigma)(n^2-2n+2)^{\frac{1}{2}}}, \quad (23)$$

where $A_n^2(\sigma)=1+4\sigma^2(n-1)^2(n^2-2n+2)^{-2}$. In Fig. 3, the four lowest roots of Eqs. (21) and (22) are plotted. The higher levels are smoothly varying functions of Z in the region $Z\simeq137$; if $n\gg\sigma$, $W_{n\frac{1}{2}}/mc^2\simeq(n-1)\times(n^2-2n+2)^{-\frac{1}{2}}$ and $\Gamma_{n\frac{1}{2}}/2mc^2\simeq\sigma(n^2-2n+2)^{-\frac{1}{2}}$, so that $W_n\gg\Gamma_n$. In common with spectra for other long-range singular problems, only the lowest levels have appreciable widths (for $\alpha Z=1.4$, $\Gamma_{n\frac{1}{2}}/2mc^2=0.635, 0.220, 0.065, 0.025$ as n goes from 1 to 4) since for high n, the electron has a large orbit and the motion is insensitive to the singularity at the origin.

5. CONCLUSION

Using assumptions (I) and (II), we have found unique discrete spectra for essentially all quantum mechanical problems. The results are mathematically reasonable and they agree with conventional predictions in nonsingular cases. Furthermore, (I) is not independent of von Neumann's assertion if the term "solution" is understood to mean "solution in the complex plane." However, the spectra have no *a priori* significance for singular problems; they have meaning only to the extent that they correspond to results for physical, bounded-potential problems.

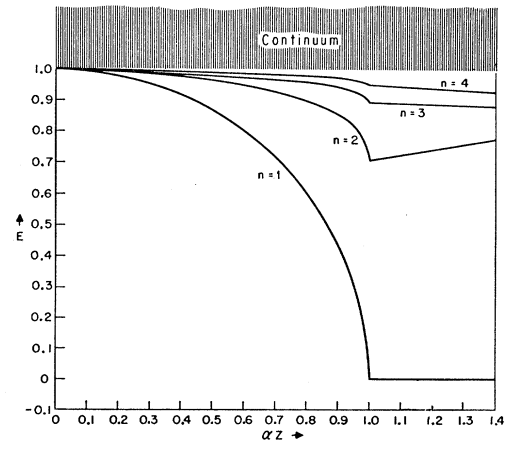

FIG. 3. The first four S states of an electron in a Coulomb field, as given by the Dirac equation. For $\alpha Z>1$, only $\mathrm{Re}(E_n)$ is shown. It can be seen that this quantity varies smoothly with Z if n is large; the corresponding widths [Eq. (23)] are found to be small.

Consider a cutoff at $x=x_0$ so that the inside wave function has a logarithmic derivative $D_i(x_0)=(\psi_i'/\psi_i)_{x=x_0}$. Since the Wronskian must be constant, $D_i(x_0)=D_0(x_0)$. For $k=2$ and $U_0<\frac{1}{4}$, it can be verified that eigenvalues corresponding to $B_s=0$, $B_s=\infty$ will be obtained if $x_0D_i=\frac{1}{2}\pm s$ ($x_0\ll1$). A constant repulsive core cutoff $[V(x)=\hbar^2V_1/2m, |x|<x_0]$ has even and odd states with

$$x_0D_i(x_0)=\begin{cases}x_0[V_1+\lambda^2]^{\frac{1}{2}}\tanh[V_1+\lambda^2]^{\frac{1}{2}}x_0\\ x_0[V_1+\lambda^2]^{\frac{1}{2}}\operatorname{ctnh}[V_1+\lambda^2]^{\frac{1}{2}}x_0\end{cases}, \quad (24)$$

and if $s\simeq\frac{1}{2}$ or $s\simeq0$, one can readily choose $V_1=U_1(U_0)/x_0^2$ so that $B_s(\text{even})\to\infty$, $B_s(\text{odd})\to0$ as $x_0\to0$. (For s not near 0 or $\frac{1}{2}$, V_1 must be x dependent to obtain these results exactly.) Thus, the energies found in Sec. 4 for $k=2$, $U_0<\frac{1}{4}$ correspond exactly to those for a specific set of repulsive core cutoffs in the limit $x_0\to0$, and can be used to approximate levels for any finite repulsive core.

When $U_0>\frac{1}{4}$, the exact solutions are not so useful. The equation $x_0D_i(x_0)=\frac{1}{2}\pm i\sigma$, which implies $E_n=W_n\pm\frac{1}{2}i\Gamma_n$, can be satisfied if V_1 is complex, or if $W_n\to-\infty$ as $x_0\to0$ so that $\lim_{x_0\to0}[x_0^2\eta^2(x_0)]$ remains finite. When V_1 is real, the outside wave function is $\psi_0=x^{\frac{1}{2}}\cos[\sigma\ln x+\gamma_\sigma(\lambda)]$, $x\ll1$, and the (real) eigenvalues are solutions of

$$\gamma_\sigma(\lambda_n)=\sigma\ln(1/x_0)+P\tan^{-1}[(\tfrac{1}{2}-x_0D_i)/\sigma]+n\pi, \quad (25)$$

where P is the principal value. Since x_0D_i is independent of λ for $x_0\ll1$, the finite eigenvalues are determined by the variation of γ_σ. The most probable values of λ_n occur at the maxima of $\partial\gamma/\partial\lambda$, and the probable deviations from these values are measured by the widths of the maxima. From Fig. 1, it can be seen that the inflection points decrease slowly as σ increases, and that the widths of the $\partial\gamma/\partial\lambda$ peaks are zero at $\sigma=0$ and increase with σ. For $\sigma\ln(1/x_0)<\pi$, the lowest level corresponds to the lowest inflection point of Fig. 1.

When Figs. 1 and 2 are compared, it can be verified that if $\partial\gamma/\partial\lambda=0$, $E\simeq W_n$, and that the Γ_n measure the deviations. This feature is not accidental. In any problem for which $B_{i\sigma}(\lambda)=0, \infty$ has roots $\lambda_n^{(\pm)}=(a_n\pm ib_n)$, $\mathrm{Re}(B)$ will have maxima on the real axis near $\lambda=a_n$; the width of each maximum corresponds to b_n. Therefore, for any problem, $\gamma_\sigma(\lambda)$ $(=P\cos[\mathrm{Re}B_\sigma(\lambda)]+n\pi)$ has the step-like λ dependence, and roughly the same σ dependence as that exhibited in Fig. 1.

Thus, energies $E_m\simeq W_n\pm\frac{1}{2}\Gamma_n$ will be found for any repulsive core if $2\sigma\ll1$; if $q\pi<\sigma\ln(1/x_0)\leq(q+1)\pi$, then $m=q+n$, and there are $(2q)$ negative energy states. In Fig. 4, levels are shown for such a cutoff with $q=0$. The energies are between $W_0+\frac{1}{2}\Gamma_0$ and $W_0-\frac{1}{2}\Gamma_0$, and the degeneracy predicted by Eq. (17) is actually

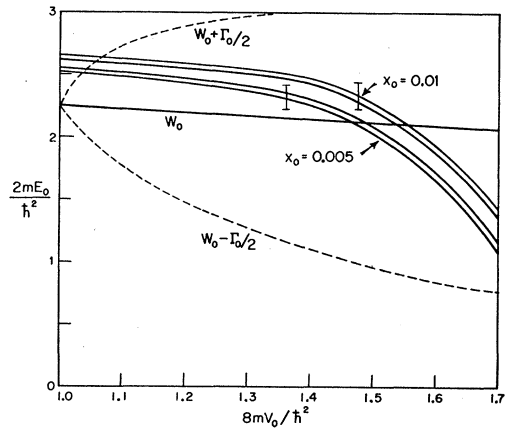

FIG. 4. The lowest levels ($n=0$, even and odd) for $V=-V_0\csc^2 x$, $x_0\leq|x|<\pi/2$; $V(\pm\pi/2)=\infty$; $V=\pi V_0/x_0^2$, $|x|<x_0$. The functions W_0, $W_0\pm\Gamma_0/2$ are taken from Fig. 2 (note change in scale). The vertical bars represent values of σ which satisfy $\sigma\ln(1/x_0)=\pi$. It can be seen that the $n=0$ levels are bounded by $W_0\pm\Gamma_0/2$ considerably beyond these limiting values of σ.

present to a high degree. It should be noted that for fixed σ, the $n=0$ levels of Fig. 4 will be the $n=(q)$ levels when the cutoff is at $x_q=x_0\exp(-q\pi\sigma)$; there will then be $(2q)$ states with $E\simeq-|V(x_q)|$.

When k is greater than two, $B_s=0$, ∞ implies

$$x_0D_i(x_0)=\tfrac{1}{4}k[1\pm(4i\sigma/kx_0{}^{\frac{1}{2}k-1})], \tag{26}$$

if the higher terms in the power series can be neglected in the region $x_0\ll1$. Again there can be an exact solution of Eq. (26) only if V is complex, $|x|<x_0$. For real inside potentials there are two approximate solutions. When $(4\sigma/kx_0{}^{\frac{1}{2}k-1})\ll1$, then $x_0D_i\simeq k/4$, and $V(x)$ must be of the form $\hbar^2V_1/2mx_0{}^2$ for $|x|<x_0$. For small σ the outside wave function is almost real and $\Gamma_n\ll W_n$ so that the situation is similar to that shown in Fig. 4. However, when $(4\sigma/kx_0{}^{\frac{1}{2}k-1})\gg1$, Eq. (26) is approximately satisfied when the inside cutoff is horizontal $[V(x)=-\hbar^2U_0/2mx_0{}^k,\ |x|<x_0]$ so that $\psi_i=\exp(ikx)$.

In the general case, if $V(x)$, $|x|<x_0$, is real, the outside wave function is $\psi_{\text{out}}(x)\simeq x^{\frac{1}{2}k}\cos[2\sigma x^{1-\frac{1}{2}k}/(k-2)+\gamma_\sigma(\lambda)]$ and the (real) energies are roots of

$$\gamma_\sigma(\lambda)=2\sigma/(k-2)x_0{}^{\frac{1}{2}k-1}-P\tan^{-1}[(x_0D_i-k/4)x_0{}^{\frac{1}{2}k-1}/\sigma]+n\pi. \tag{27}$$

If $2\sigma\ll1$, then $E_m\simeq W_n\pm\frac{1}{2}\Gamma_n$ where $m=q+n$ and

$$q\pi<2\sigma/(k-2)x_0{}^{\frac{1}{2}k-1}\leq(q+1)\pi.$$

The WKB method, which can be applied if $k>2$, tends to confirm these results.[14] For $E=0$, $p(x)dx$ can be integrated from x_0 to ∞. The WKB quantization rule gives $E_n=0$ if

$$(n+\tfrac{1}{2})\pi=\sigma/(k-2)x_0{}^{\frac{1}{2}k-1}. \tag{28}$$

Thus, there are no negative energy states for $2\sigma/(k-2)x_0{}^{\frac{1}{2}k-1}<\pi$, which is in agreement with the prediction of Eq. (27). Equation (28) also sets the lowest maximum of $\partial\gamma/\partial\lambda$ above zero energy as predicted by the classical virial theorem.

It can be concluded that the complex energies found by using assumptions (I) and (II) give definite information concerning the density of possible levels. If the singular potential is not too strong and the cutoff distance not too small, the essential singularity in the wave function does not appear, and the energies for a repulsive core are $E_n\simeq W_n\pm\frac{1}{2}\Gamma_n$. In the other extreme, if x_0 is very small, there are many levels clustered near $\eta^2=U_0/x_0{}^k$. For a very small, oscillating or fluctuating x_0, there is an effective continuum with $\langle E_n\rangle=W_n$. In this case, the complex E_n might be interpreted as energies of weakly quantized continuum states.‡

ACKNOWLEDGMENTS

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[14] The WKB method is rigorously applicable if $\hbar^2|Qp^{-2}|\ll1$, $Q=\frac{3}{4}(p'/p)^2-p''/2p$, $p^2=2m(E-V)$ (see Kemble, reference 5, p. 96). If $V=-V_0x^{-k}$ and $k>2$, $|Qp^{-2}|\to0$ as $x\to0$. When a long-range nonsingular force acts together with the short-range singular one, $\hbar^2|Qp^{-2}|$ is small for all x so that the WKB approximation is accurate.

‡ *Note added in proof.*—In a recent discussion, F. G. Werner and J. A. Wheeler [Phys. Rev. **109**, 126 (1958)] have accurately calculated $E_{1,\frac{1}{2}}$ for $V(r)=-\alpha Z/b$ $(r<b)$ at $Z=170$. They found $E_{1,\frac{1}{2}}=-1.85\ mc^2$ for a range of b near $0.03\hbar/mc$. Equations (22) and (23) describe a problem with $V(r)\simeq+\alpha Z/b$ $(r<b)$ and should lead to much smaller binding energies than the above, with little dependence on b; we find $E_{1,\frac{1}{2}}=(-1.0\pm0.49)mc^2$. Since the properties of the $n=1$ state are most sensitive to the type of cutoff and the precise value of b, the relatively close agreement between these two numbers indicates that Eqs. (22) and (23) will lead to useful approximations to $E_{n,j}$, $n\gg1$, for almost any cutoff.