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Singular Potentials in Nonrelativistic Quantum Mechanics.

K. MEETZ

II. Institut für Theoretische Physik der Universität Hamburg

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Summary. — The mathematical aspects of singular potentials in nonrelativistic quantum mechanics are studied in terms of the self-adjoint transformations related to singular differential operators in the space $L_2(0, \infty)$. The physical content is expressed by the spectral decompositions and for attractive potentials found to be determined only up to a parameter defining a particular extension. In general it is not possible to determine a specific extension by a cut-off procedure.

1. – Introduction.

The recent work of FEINBERG and PAIS [1,2] has made it desirable to study the formal techniques applied by them to unrenormalizable field theories on the firmer ground of singular potential scattering [3-5]. Unfortunately the mathematical implications of singular potentials in nonrelativistic quantum mechanics have not been worked out in such detail as in the more familiar case, although a first step in this direction has been done by the work of CASE [6] and SCARF [7]. This may be due to the fact that attractive potentials singular as $r^{-\alpha}$ ($\alpha \geqslant 2$) are of a rather academic interest from the physical point of view, because in general they do not lead to a Hamiltonian bounded inferiorly.

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(1) G. FEINBERG and A. PAIS: *Phys. Rev.*, **131**, 2724 (1963).
(2) G. FEINBERG and A. PAIS: *Phys. Rev.*, **133** B, 477 (1964).
(3) N. KHURI and A. PAIS: *Singular Potentials and Peratization, I*, preprint.
(4) A. PAIS and T. T. WU: *Singular Potentials and Peratization, II*, preprint.
(5) A. PAIS and T. T. WU: *Scattering Formalism for Singular Potential Theory*, preprint.
(6) K. M. CASE: *Phys. Rev.*, **80**, 797 (1950).
(7) F. L. SCARF: *Phys. Rev.*, **109**, 2170 (1958).

This does not mean that the mathematical situation is obscure. Singular differential operators are either self-adjoint or give rise to a well-defined class of self-adjoint extensions in the Hilbert space of square-integrable functions $L_2(0, \infty)$ (Sect. **2** and **3**). The corresponding resolutions of the identity are discussed in Sect. **4** in terms of scattering solutions and bound-state wave functions. Analyticity properties in the coupling constant g^2 are displayed by a spectral representation of the resolvent in the complex g^2-plane. Finally it is shown (Sect. **5**) that it is not possible to fix a specific self-adjoint extension by a cut-off procedure, except in a special range of coupling-constant values for the potential r^{-2}. This leaves the « physical » content of Hamiltonians not bounded below undetermined up to a parameter fixing the extension.

2. – Singular differential operators.

In order to study the possible meaning of singular potentials in quantum mechanics we begin with some results from the theory of singular differential operators. An exhaustive treatment of the subject can be found in Stone's book [8], from which we have borrowed the general statements of this Section.

We consider the differential operator

$$L = -\frac{\mathrm{d}^2}{\mathrm{d}z^2} + g^2 V(z) \tag{2.1}$$

in the interval $(0, \infty)$. The potential function $V(z)$ shall be integrable over every closed interval interior to $(0, \infty)$. To avoid complications not of interest in our context we assume $V(z) > 0$. The point $z = \infty$ is a singular point of the operator (2.1) and the point $z = 0$ is said to be singular, if the integral

$$\int_0^a \mathrm{d}z\,|V(z)|\,, \qquad a > 0\,, \tag{2.2}$$

does not exist. This is the case we are interested in.

The operator L defines a linear transformation H^* in the space $L_2(0, \infty)$ with domain D^*. D^* is essentially the set of all functions $f \in L_2(0, \infty)$ such that $Lf \in L_2(0, \infty)$. For $f, g \in D^*$ we have

$$(g, Lf) = [g, f]_0^\infty + (Lg, f)\,, \tag{2.3}$$

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[8] M. H. Stone: *Linear Transformations in Hilbert Space*, in *Ann. Math. Soc.* (New York, 1932).

where the limits

$$[g,f]_0^\infty = \lim_{b\to\infty}(-\bar{g}f' + \bar{g}'f)|_{z=b} - \lim_{a\to 0}(-\bar{g}f' + \bar{g}'f)|_{z=a} \tag{2.4}$$

do exist ($\bar{g}$ is the complex conjugate of g). If D is the set of all $f \in D^*$ such that

$$[g,f]_0^\infty = 0 \qquad \text{for every } g \in D^*, \tag{2.5}$$

then the operator L with domain D defines a symmetric transformation H in $L_2(0,\infty)$ with adjoint H^*.

For physical interpretation H needs to be self-adjoint or a physically reasonable self-adjoint extension has to be given. To find out whether H is self-adjoint or not we consider the solution $w(z,k)$ of the differential equation

$$Lw = -\frac{d^2w}{dz^2} + g^2 V(z) w = k^2 w, \tag{2.6}$$

where k is in the upper half-plane ($\operatorname{Im} k > 0$). We call n_0 or n_∞ the number of linear independent solutions of (2.6) which belong to $L_2(0,a)$ or $L_2(a,\infty)$, where a is arbitrary > 0. The number n of independent solutions in $L_2(0,\infty)$ is

$$n = n_0 + n_\infty - 2. \tag{2.7}$$

It is called the « deficiency-index » of the transformation H. The numbers n_0 and n_∞ are independent of k in the upper half-plane and may have the values 1, 2 each. Hence $n = 0, 1, 2$.

It has been shown by VON NEUMANN [9] that the domain D^* can be decomposed in the form

$$D^* = D \oplus D_{k^2} \oplus D_{\bar{k}^2}. \tag{2.8}$$

D_{k^2} and $D_{\bar{k}^2}$ are the linear manifolds in $L_2(0,\infty)$ belonging to the eigenvalues k^2 and $\bar{k}^2$ of (2.6). Because

$$\dim D_{k^2} = \dim D_{\bar{k}^2} = n, \tag{2.9}$$

H is clearly self-adjoint for $n = 0$, while for $n = 1, 2$ self-adjoint extensions have to be constructed.

We now determine the numbers n_∞ and n_0 for certain classes of potentials.

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[9] N. I. ACHIESER and I. M. GLASSMANN: *Theorie der linearen Operatoren im Hilbert Raum* (Berlin, 1958).

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For a potential with the property

$$(2.10)\qquad \int_b^\infty dz\, z\,|V(z)|<\infty\,, \qquad b>0\,,$$

there exists only one solution of (2.6) in $L_2(0,\infty)$ for $\operatorname{Im} k>0$. We call it $f(z,g,-k)$ and define it in the usual way by the Volterra integral equation

$$(2.11)\qquad \begin{cases} f(z,g,-k)=\exp[ikz]+g^2\int_z^\infty d\zeta\,\dfrac{\sin k(\zeta-z)}{k}\,V(\zeta)f(\zeta,g,-k)\,,\\ f(z,g,k)=\bar f(z,\bar g,-\bar k)\,. \end{cases}$$

The second solution

$$(2.12)\qquad f(z,g,k)=f(z,g,-k\exp[i\pi])\,,\qquad W\big(f(z,g,k),f(z,g,-k)\big)=2ik$$

(W means the Wronskian determinant) is not in $L_2(a,\infty)$ and we have $n_\infty=1$. The solutions for the potential

$$(2.13)\qquad g^2V(z)=\frac{\nu^2-\frac14}{z^2}$$

are

$$(2.14)\qquad \begin{cases} f(z,\nu,-k)=\sqrt{\dfrac{\pi kz}{2}}\,H_\nu^{(1)}(kz)\exp\left[i\dfrac{\pi}{2}\left(\nu+\dfrac12\right)\right],\\ f(z,\nu,k)=\sqrt{\dfrac{\pi kz}{2}}\,H_\nu^{(2)}(kz)\exp\left[-i\dfrac{\pi}{2}\left(\nu+\dfrac12\right)\right], \end{cases}$$

where $H_\nu^{(1)}$ and $H_\nu^{(2)}$ are the Hankel functions of first and second kind. $f(z,\nu,-k)$ is in $L_2(a,\infty)$, and $f(z,\nu,k)$ is not, independent of the value ν. Again $n_\infty=1$. To determine n_0 for the potential (2.13) we look at the general solution of (2.6):

$$(2.15)\qquad w(z,\nu,k)=\alpha\sqrt{z}\,J_\nu(kz)+\beta\sqrt{z}\,N_\nu(kz)$$

in terms of the Bessel function J_ν and the Neumann function N_ν.

If $\nu\geqslant1$, only $\sqrt{z}J_\nu(kz)$ is in $L_2(0,a)$ and we have $n_0=1$. But for $0\leqslant\nu<1$ and purely imaginary values of $\nu=i\gamma$ (γ real) every solution (2.15) is in

$L_2(0, a)$ and $n_0 = 2$. Hence the transformation H is self-adjoint for a repulsive potential (2.13) with $\nu^2 \geqslant 1$ $(n = 0)$, while for $\nu^2 < 1$ we have to look for possible extensions $(n = 1)$. It is a peculiar property of the potential (2.13) that H has the deficiency-index 1 in the range $\frac{1}{4} \leqslant \nu^2 < 1$, where the potential is repulsive.

We now turn to potentials that are more singular than z^{-2} at the origin. For the sake of simplicity we assume the form

$$V(z) = \frac{1}{z^\alpha} + V'(z) ,$$

where

$$\int_0^b \mathrm{d}z\, z\, |V'(z)| < \infty \qquad \text{for } b > 0 \tag{2.16}$$

and $\alpha > 2$. The transformation

$$z' = \frac{1}{z}, \qquad w\left(\frac{1}{z'}\right) = \tilde{w}(z') = \frac{1}{z'}\,\tilde{v}(z') \tag{2.17}$$

of (2.6) leads to the differential equation

$$-\frac{\mathrm{d}^2\tilde{v}}{\mathrm{d}z'^2} + g^2\left(z'^{\alpha-4} + \frac{1}{z'^4}\,V'\left(\frac{1}{z'}\right)\right)\tilde{v} = \frac{k^2}{z'^4}\,\tilde{v} . \tag{2.18}$$

Because of (2.16) we can obtain asymptotic solutions for $z' \to \infty$ $(z \to 0)$, from

$$-\frac{\mathrm{d}^2\tilde{v}_0}{\mathrm{d}z'^2} + g^2 z'^{\alpha-4}\,\tilde{v}_0 = 0 . \tag{2.19}$$

These have the form

$$\tilde{v}_0(z') = \sqrt{z'}\, Z_{1/(\alpha-2)}\left(ig\,\frac{z'^{(\alpha/2)-1}}{\alpha/2 - 1}\right) , \tag{2.20}$$

where Z_ν is a cylinder function of index ν. We define as a fundamental system of the equation

$$\frac{\mathrm{d}^2 w_0}{\mathrm{d}z^2} + \frac{g^2}{z^\alpha}\, w_0 = 0 \tag{2.21}$$

the functions

$$(2.22)\quad \begin{cases} \varphi_0(z, g) = \sqrt{\frac{\pi}{2}}\left(\frac{igz}{\alpha/2-1}\right)^{\frac{1}{2}} H^{(1)}_{1/(\alpha-2)}\left(\frac{igz^{1-(\alpha/2)}}{\alpha/2-1}\right) \exp\left[i\frac{\pi}{2}\left(\frac{\alpha-2}{1}+\frac{1}{2}\right)\right] \xrightarrow[z\to 0]{} \\ \qquad\qquad \xrightarrow[z\to 0]{} z^{\alpha/4}\exp\left[\frac{-g}{\alpha/2-1}z^{1-(\alpha/2)}\right], \\ \varphi_0(z, -g) = \varphi_0(z, g\exp[i\pi]) = \sqrt{\frac{\pi}{2}}\left(\frac{igz}{\alpha/2-1}\right)^{\frac{1}{2}} H^{(2)}_{1/(\alpha-2)}\left(\frac{igz^{1-(\alpha/2)}}{\alpha/2-1}\right)\cdot \\ \qquad\qquad \cdot\exp\left[-i\frac{\pi}{2}\left(\frac{1}{\alpha-2}+\frac{1}{2}\right)\right] \xrightarrow[z\to 0]{} z^{\alpha/4}\exp\left[\frac{g}{\alpha/2-1}z^{1-(\alpha/2)}\right], \\ W(\varphi_0(z, g), \varphi_0(z, -g)) = -2g\,. \end{cases}$$

A solution of the full eq. (2.6) in $L_2(0, a)$ for the potential (2.16) can be obtained from the Volterra integral equation

$$(2.23)\quad \begin{cases} \varphi(z, g, k) = \varphi_0(z, g) - \frac{1}{2g}\int_0^z d\zeta\,\{\varphi_0(z, g)\varphi_0(\zeta, -g) - \varphi_0(z, -g)\varphi_0(\zeta, g)\}\cdot \\ \qquad\qquad\qquad \cdot(k^2 - g^2 V'(\zeta))\varphi(\zeta, g, k)\,. \\ \varphi(z, g, k) = \bar{\varphi}(z, \bar{g}, \bar{k})\,. \end{cases}$$

We clearly have $n_0 = 1$ for a repulsive potential ($g^2 > 0$)and $n_0 = 2$ for an attractive potential ($g^2 < 0$). $n = 1$ is the « limit-point » and $n = 2$ the « limit-circle »-case, first discussed in the famous paper of WEYL [10]. The functions $\varphi(z, \pm g, k)$ may be compared with the solutions

$$(2.24)\quad \begin{cases} \varphi(z, \nu, k) = \Gamma(1+\nu)2^\nu k^{-\nu}\sqrt{z}J_\nu(kz) \xrightarrow[z\to 0]{} z^{\frac{1}{2}}\exp[\nu\ln z]\,, \\ \varphi(z, -\nu, k) = \Gamma(1-\nu)2^\nu k^\nu\sqrt{z}J_{-\nu}(kz) \xrightarrow[z\to 0]{} z^{\frac{1}{2}}\exp[-\nu\ln z]\,, \\ W(\varphi(z, \nu, k), \varphi(z, -\nu, k)) = -2\nu\,, \end{cases}$$

for the potential (2.13) (ν not an integral number).

3. – Self-adjoint extensions.

To construct all self-adjoint extensions of the transformation H, if $n = 1$, we use the method of Stone [8]. According to (2.8) we can decompose the

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[10] H. WEYL: *Math. Ann.*, **68**, 220 (1910).

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domain D^* in the form

$$D^* = D \oplus D_{+i} \oplus D_{-i}\,, \tag{3.1}$$

where D_{+i} and D_{-i} are the linear manifolds which belong to the eigenvalues $k^2 = +i$ and $k^2 = -i$ of (2.6). Because of $n = 1$ these have dimension one. As we have seen in Sect. **2** every solution of (2.6) is now in $L_2(0, a)$. Hence we may span D_{+i} and D_{-i} by the functions

$$f_{+i} = f\left(z, g, -\exp\left[i\frac{\pi}{4}\right]\right), \qquad f_{-i} = f\left(z, \bar{g}, -\exp\left[i3\frac{\pi}{4}\right]\right) = \overline{f_{+i}}\,, \tag{3.2}$$

defined by (2.11) for a potential of the class (2.10) or by (2.14) for (2.13). We now show that the domain D of H can be characterized as the set of all elements $f \in D^*$ which satisfy

$$[f_{\pm i}, f]_0 = (-\bar{f}_{\pm i} f' + \bar{f}'_{\pm i} f)\,|_{z=0} = 0\,. \tag{3.3}$$

To see this we recall that we have defined D as the set of all $f \in D^*$ such that (2.5) holds for every $g \in D^*$. Every $g \in D^*$ can be written in the form

$$g = g_0 + \alpha_1 f_{+i} + \alpha_2 f_{-i}\,, \qquad g_0 \in D, \tag{3.4}$$

where α_1, α_2 are some complex numbers. Hence (2.5) is equivalent to

$$[f_{+i}, f]_0^\infty = 0\,. \tag{3.5}$$

To reduce (3.5) to the condition (3.3) we use another decomposition of g:

$$g = g'_0 + \beta_1 h_1 + \beta_2 h_2\,, \qquad g'_0 \in D. \tag{3.6}$$

h_1 and h_2 are functions with compact support such that

$$W(h_1, h_2)|_{z=0} \neq 0\,. \tag{3.7}$$

Hence for every g and $f \in D^*$

$$[f, g]^\infty = [f, g'_0]^\infty = [f, g'_0]_0^\infty = 0\,, \tag{3.8}$$

where we have used the fact that D is the closure of the set of functions φ with compact support and $\varphi(0) = 0 = \varphi'(0)$. $f_{\pm i}$ are, of course, elements of D^* and (3.5) implies (3.3).

Because the Hamiltonian is a real transformation, we have to define self-

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adjoint extensions which are real with respect to complex conjugation. To do so we define the function

$$f_\Theta = \frac{1}{2i}\left\{f_{+i}\exp\left[i\frac{\Theta}{2}\right] - f_{-i}\exp\left[-i\frac{\Theta}{2}\right]\right\} \tag{3.9}$$

and the domanin D_Θ as the set of all elements $f \in D^*$ such that

$$[f, f_\Theta]_0 = 0\,. \tag{3.10}$$

The differential operator L with domain D_Θ is a self-adjoint transformation H_Θ in $L_2(0, \infty)$:

$$(g, H_\Theta f) = (H_\Theta g, f)\,, \qquad f, g \in D_\Theta. \tag{3.11}$$

H_Θ is real, because f is a real function. This guarantees that the resolution of the identity is real. As Θ runs from 0 to 2π we get all possible self-adjoint extensions with this property.

Next we determine the solutions $\varphi_\Theta(z, g, k)$ of the differential equation (2.6) which satisfy the boundary condition (3.10). Consider first the potential (2.16). The general solution is

$$\varphi_\Theta(z, g, k) = \varphi(z, g, k) - c\varphi(z, -g, k) \tag{3.12}$$

with some complex number c. The condition

$$[f_\Theta, \varphi_\Theta]_0 = (-f_\Theta \varphi'_\Theta + f'_\Theta \varphi_\Theta)|_{z=0} = W_{z=0}(\varphi_\Theta, f_\Theta) = 0 \tag{3.13}$$

(W_z means the Wronskian evaluated at z) yields

$$c = \frac{W_{z=0}(f_\Theta(z), \varphi(z, g, k))}{W_{z=0}(f_\Theta(z), \varphi(z, -g, k))} = \frac{W_{z=0}(f_\Theta(z), \varphi_0(z, g))}{W_{z=0}(f_\Theta(z), \varphi_0(z, -g))}\,. \tag{3.14}$$

f_Θ is a real function and from (2.22) we see for $g^2 < 0$

$$\varphi_0(z, -g) = \overline{\varphi_0(z, g)}\,. \tag{3.15}$$

Hence $|c| = 1$ and (3.14) may be written as

$$\exp[2i\chi(\Theta)] = \frac{W_{z=0}(f_\Theta(z), \varphi_0(z, g))}{W_{z=0}(f_\Theta(z), \varphi_0(z, -g))}\,. \tag{3.16}$$

By (3.16) a one-to-one correspondence of Θ and χ is set up in the intervals $0 \leqslant \Theta < 2\pi$ and $0 \leqslant \chi < \pi$. The solutions

$$\varphi_\Theta(z, g, k) = \frac{1}{2i}\{\exp[i\chi(\Theta)]\varphi(z, g, k) - \exp[-i\chi(\Theta)]\varphi(z, -g, k)\} \tag{3.17}$$

are real for purely imaginary values of $k = i\varkappa$ ($\varkappa$ real). (3.17) leaves undetermined the phase of the solution for $z \to 0$. This property of the wave-functions has already been discussed by CASE [6].

The situation is completely the same for the potential (2.13) in the range $\nu^2 < 0$. We just have to substitute ν for g in (31.6). But for $0 < \nu < 1$ we find with (2.24) that

$$\left\{\begin{aligned} c &= \frac{W_{z=0}(f_\Theta(z), \varphi_0(z, \nu))}{W_{z=0}(f_\Theta(z), \varphi_0(z, -\nu))} = 2^{2\nu}\frac{\Gamma(1+\nu)}{\Gamma(1-\nu)}\frac{\cos((\nu\pi/4) + (\Theta'/2))}{\cos((\nu\pi/4) - (\Theta'/2))},\\ \Theta' &= \Theta + \frac{3\pi}{4}\end{aligned}\right. \tag{3.18}$$

is a real number which may have every value between $-\infty$ and $+\infty$. A one-to-one correspondence between Θ in $0 \leqslant \Theta < 2\pi$ and c in $-\infty < c < +\infty$ is given by (3.18). It is possible to define a specific extension by putting $c = 0$. This means that the solutions of the differential eq. (2.6) shall behave like the more regular function $\varphi_0(z, \nu) = z^{\nu+\frac{1}{2}}$ near the origin. We emphasize that such a boundary condition does not make sense for $\nu^2 < 0$ or attractive potentials of the class (2.16). If $\nu = \frac{1}{2}$, the potential (2.13) vanishes and $z = 0$ is a regular boundary point. We may then use a regular boundary condition

$$\varphi(0)\cos\psi - \varphi'(0)\sin\psi = 0\,, \qquad 0 \leqslant \psi < \pi. \tag{3.19}$$

The constant $-c$ is equal to $\operatorname{tg}\psi$:

$$\operatorname{tg}\psi = \left.\frac{\varphi_0(z, \nu = \frac{1}{2}) - c\varphi_0(z, \nu = -\frac{1}{2})}{\varphi_0'(z, \nu = \frac{1}{2}) - c\varphi_0'(z, \nu = -\frac{1}{2})}\right|_{z=0} = -c\,. \tag{3.20}$$

(3.19) defines all self-adjoint extensions, if $z = 0$ is a regular boundary point, *i.e.*, if the integral (2.2) exists.

4. – Spectral representations.

The self-adjoint transformation H ($n = 0$) as each self-adjoint extension H_Θ ($n = 1$) gives rise to a spectral decomposition of the unit operator E in

$L_2(0, \infty)$. An arbitrary function $h \in L_2(0, \infty)$ can be represented in the form

$$(4.1) \qquad h(z) = \int_{-\infty}^{+\infty} \mathrm{d}\varrho(k^2)\tilde{h}(k^2)\varphi(z, g, k) , \qquad \tilde{h}(k^2) = \int_0^\infty \mathrm{d}z\, h(z)\varphi(z, g, k) .$$

Here as in the following we give only the formulae for the transformation H $(n = 0)$. In case of H_Θ, φ_Θ takes the place of φ.

To determine the spectral density $\mathrm{d}\varrho/\mathrm{d}k^2$ we extend the method of Krein [11] to our problem which derives $\mathrm{d}\varrho/\mathrm{d}k^2$ from the resolvent

$$(4.2) \qquad \frac{1}{H - k^2E} \leftrightarrow G(z, \zeta\,|\,g^2, k^2) = \begin{cases} \dfrac{\varphi(z, g, k)f(\zeta, g, -k)}{f(g, -k)} , & z \leqslant \zeta , \\[2ex] \dfrac{\varphi(\zeta, g, k)f(z, g, -k)}{f(g, -k)} . & z > \zeta . \end{cases}$$

$f(g, -k)$ is Jost's function [12]:

$$(4.3) \qquad f(g, -k) = W\big(f(z, g, -k), \varphi(z, g, k)\big) .$$

For two functions h_1, $h_2 \in L_2(0, \infty)$ we have

$$(4.4) \qquad (h_1, h_2) = \int_0^\infty \mathrm{d}z\, \bar{h}_1(z)\, h_2(z) = \int_{-\infty}^{+\infty} \mathrm{d}\varrho(k^2)\bar{\tilde{h}}_1(k^2)\tilde{h}_2(k^2) .$$

This yields

$$(4.5) \qquad \int_0^\infty \mathrm{d}z \int_0^\infty \mathrm{d}\zeta\, G(z, \zeta\,|\,g^2, k^2)\bar{h}(z)h(\zeta) = \int_{-\infty}^{+\infty} \mathrm{d}\varrho(k'^2)\frac{|\tilde{h}(k'^2)|^2}{k'^2 - k^2}$$

for $h_1 = h$ and $h_2 = \big(1/(H - Ek^2)\big)h$. Let $h(z)$ be a function of compact support in a circle of radius δ_a around $z = a$ such that

$$(4.6) \qquad h = q_{\delta_a} , \qquad \int_0^\infty |q_{\delta_a}(z)|^2\, \mathrm{d}z = 1 .$$

([11]) See *e.g.* ref. ([9]).

([12]) R. Jost: *Helv. Phys. Acta*, **20**, 256 (1947).

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Making a subtraction at $k^2=i$ we obtain from (4.5)

$$(4.7)\qquad G(a,a|g^2,k^2)=G(a,a|g^2,i)+\lim_{\delta_a\to 0}\left\{\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\varrho(k'^2)}{k'^4+1}|\tilde{q}_{\delta_a}(k'^2)|^2\cdot\frac{1+k^2k'^2}{k'^2-k^2}-i\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\varrho(k'^2)}{k'^4+1}|\tilde{q}_{\delta_a}(k'^2)|^2\right\}.$$

Because

$$(4.8)\qquad \operatorname{Im}G(a,a|g^2,i)=\lim_{\delta_a\to 0}\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\varrho(k'^2)}{k'^4+1}|\tilde{q}(k'^2)|^2,$$

where the integrand is positive, we can interchange limit and integration (Dini's theorem!). Hence

$$(4.9)\qquad \operatorname{Im}G(a,a|g^2,i)=\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\varrho(k'^2)}{k'^4+1}(\varphi(a,g,k'))^2,$$

and

$$(4.10)\qquad G(a,a|g^2,k^2)=\operatorname{Re}G(a,a|g^2,i))+\int\limits_{-\infty}^{+\infty}\frac{\mathrm{d}\varrho(k'^2)}{k'^4+1}\frac{1+k^2k'^2}{k'^2-k^2}(\varphi(a,g,k'))^2,$$

where we have used

$$\lim_{\delta_a\to 0}|\tilde{q}_{\delta_a}(k'^2)|^2=\lim_{\delta_a\to 0}\left|\int\limits_0^\infty \mathrm{d}z\, q_{\delta_a}(z)\varphi(z,g,k')\right|^2=(\varphi(a,g,k'))^2,$$

($\varphi(a,g,k)$ is real for real k). Similarly as in Regge's analysis of complex angular momenta ([13]) it follows from (4.3) and the definitions of the functions $f(z,g,-k)$ and $\varphi(z,g,k)$ that the Jost function $f(g,-k)$ is analytic in the product of the half-planes $\operatorname{Im}k>0$ and $\operatorname{Re}g>0$ with continuous boundary values on $\operatorname{Im}k=0$ and $\operatorname{Re}g=0$. Hence we may infer from (4.10) and (4.2):

$$(4.11)\qquad 2\pi i(\varphi(a,g,k))^2\frac{\mathrm{d}\varrho}{\mathrm{d}k^2}=\lim_{\varepsilon\to 0}\{G(a,a|g^2,k^2+i\varepsilon)-G(a,a|g^2,k^2-i\varepsilon)\}=$$
$$=\varphi(a,g,k)\frac{f(a,g,-k)}{f(g,-k)}-\frac{f(a,g,k)}{f(g,k)}=2ik\frac{(\varphi(a,g,k))^2}{f(g,-k)f(g,k)}.$$

([13]) A. Bottino, A. M. Longoni and T. Regge: *Nuovo Cimento*, **23**, 954 (1962).

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This is the result of Jost and Kohn [14]:

$$\frac{d\varrho}{dk^2} = \frac{k}{\pi}\frac{1}{|f(g,k)|^2}, \qquad k^2 > 0 \tag{4.12}$$

$(f(g,-k) = \overline{f(g,k)})$. For $k^2 < 0$ we get

$$\frac{d\varrho}{dk^2} = \sum_n \frac{1}{N_n^2}\,\delta(k^2+\varkappa_n^2), \qquad k^2 < 0 \tag{4.13}$$

$$N_n^2 = \int_0^\infty dz(\varphi(z,g,i\varkappa_n))^2 = -\frac{1}{4\varkappa_n^2} f(g,i\varkappa_n)\left.\frac{df(g,-i\varkappa)}{d\varkappa}\right|_{\varkappa=\varkappa_n}$$

from the zeros of $f(g,-k)$ in the half-plane $\operatorname{Im} k > 0$.

Let us consider the possible cases for the potential (2.13) as examples. In the range $\nu > 1$ we have $n = 0$. The spectral density can be evaluated with the functions (2.14) and (2.24):

$$\nu > 1: \quad \frac{d\varrho}{dk^2} = \frac{k}{\pi}\frac{1}{|f(\nu,k)|^2} = \frac{1}{2\cdot 4^\nu \Gamma^2(1+\nu)k^{-2\nu}}; \qquad k^2 > 0\,. \tag{4.14}$$

The corresponding decomposition of E leads to the Hankel transformation

$$\nu > 1: \quad h(z) = \frac{1}{2}\int_0^\infty dk'^2 \sqrt{z}\,J_\nu(k'z)\int_0^\infty dz'\sqrt{z'}\,J_\nu(k'z')h(z')\,. \tag{4.15}$$

For ν-values between 0 and 1 we define a self-adjoint extension by

$$\varphi_\Theta(z,\nu,k) = \varphi(z,\nu,k) - c\,\varphi(z,-\nu,k)\,, \tag{4.16}$$

where c is a real number. We find

$$\left\{\begin{aligned} |f_\Theta(\nu,k)|^2 &= \frac{2k}{\pi}\,4^\nu\Gamma^2(1+\nu)k^{-2\nu}\{1-2c'k^{2\nu}\cos\nu\pi + c'^2k^{4\nu}\},\\ c' &= \frac{2^{-\nu}\Gamma(1-\nu)}{2^\nu\Gamma(1+\nu)}\,c\,. \end{aligned}\right. \tag{4.17}$$

[14] R. Jost and W. Kohn: *Kgl. Dan. Viden. Sels., Mat.-Fys. Medd.*, **27**, no. 9 (1953).

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The resolution of the identity is

$$(4.18)\qquad \begin{matrix} 0<\nu<1\,; \\ c'>0\,, \end{matrix}\qquad h(z)=\frac{1}{2}\int_0^\infty \mathrm{d}k'^2\,\frac{1}{(1-2c'\,k'^{2\nu}\cos\nu\pi+c'^2k'^{4\nu})}\cdot$$

$$\cdot\sqrt{z}\,\big(J_\nu(k'z)-c'\,k'^{2\nu}\,J_{-\nu}(k'z)\big)\int_0^\infty \mathrm{d}z^2\sqrt{z'}\,\big(J_\nu\,(k'z')-c'\,J_{-\nu}(k'z')\big)\,h(z')\,.$$

The Jost function

$$(4.19)\qquad f_\Theta(\nu,-k)=\sqrt{\frac{\pi k}{2}\,\frac{2}{\pi i}}\exp\left[i\frac{\pi}{4}\right]2^\nu\Gamma(1+\nu)\,\cdot$$

$$\cdot\left\{k^{-\nu}\exp\left[i\frac{\pi}{2}\nu\right]-c'\,k^\nu\exp\left[-i\frac{\pi}{2}\nu\right]\right\}$$

has a zero in the upper half-plane at

$$(4.20)\qquad \varkappa=\left(\frac{1}{c'}\right)^{1/2\nu},$$

if $c'>0$. This obscure « bound state » does not occur for the physically reasonable boundary condition $c=0$. The example (4.18) can be found in Titchmarsh's book [15].

Last we consider the attractive range $\nu^2<0$ ($\nu=i\gamma$, γ real). The Jost function of the self-adjoint extension

$$(4.21)\qquad \varphi_\Theta(z,i\gamma,k)=\frac{1}{2i}\{\exp\left[i\chi(\theta)\right]\varphi(z,i\gamma,k)-\exp\left[-i\chi(\Theta)\right]\varphi(z,-i\gamma,k)\}$$

is

$$(4.22)\qquad f_\Theta(i\gamma,-k)=W(f(z,i\gamma,-k),\varphi_\Theta(z,i\gamma,k))=$$

$$=\exp\left[-i\frac{\pi}{4}\right]\sqrt{\frac{k\pi}{2}\,\frac{2}{\pi}}\,|\Gamma(1+i\gamma)|\,\cdot$$

$$\cdot\left\{\exp\left[-\frac{\pi}{2}\gamma\right]\exp\left[i(\chi'-\gamma\ln k)\right]-\exp\left[\frac{\pi}{2}\gamma\right]\exp\left[-i(\chi'-\gamma\ln k)\right]\right\},$$

where

$$(4.23)\qquad \chi'=\chi+\varphi(\gamma)+\gamma\ln 2\,,\qquad \Gamma(1+i\gamma)=|\Gamma(1+i\gamma)|\exp\left[i\,\varphi(\gamma)\right].$$

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(15) E. C. TITCHMARSH: *Eigenfunction Expansions Associated with Second-Order Differential Equations* (Oxford, 1946).

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It has zeros in the upper half-plane at

$$(4.24)\qquad \varkappa_n^2 = \exp\left[\frac{2\chi'}{\gamma}\right]\exp\left[\frac{2n\pi}{\gamma}\right], \qquad n = 0, \pm 1, \pm 2, \ldots,$$

accumlating at $k^2 = 0$ and $k^2 = \infty$. These bound states have already been obtained by CASE [6]. Each spectral point is shifted to the next one, if χ' runs from 0 to π, *i.e.*, all extensions are passed. The point spectra for $\chi' = 0$ and $\chi' = \pi$ are identical, because there are two accumulation points. (4.22) yields the spectral density

$$(4.25)\qquad \frac{d\varrho}{dk^2} = \begin{cases} \dfrac{k}{\pi}\dfrac{1}{|f_\Theta|^2} = \dfrac{1}{2|\Gamma(1+i\gamma)|^2 4\{\cosh^2(\pi\gamma/2) - \cos^2(\chi' - \gamma \ln k)\}}, & k^2 > 0, \\ \displaystyle\sum_{n=-\infty}^{+\infty} \frac{2\varkappa_n^2}{\gamma^2}\,\delta(k^2 + \varkappa_n^2). & k^2 < 0. \end{cases}$$

It is invariant under the transformation $\chi' \to \chi' + m\pi$ (m an integral number). The S-matrix element is

$$(4.26)\qquad S_\Theta(\nu, k) = \frac{f_\Theta(\nu, k)}{f_\Theta(\nu, -k)} =$$
$$= i\,\frac{\exp[\gamma(\pi/2)]\exp[i(\chi' - \gamma \ln k)] - \exp[-\gamma(\pi/2)]\exp[-i(\chi' - \gamma \ln k)]}{\exp[-\gamma(\pi/2)]\exp[i(\chi' - \gamma \ln k)] - \exp[\gamma(\pi/2)]\exp[-i(\chi' - \gamma \ln k)]}\qquad \operatorname{Im} k > 0.$$

Thus far we have considered the spectral representation of the resolvent

$$(4.27)\qquad \frac{1}{H - k^2 E} = \frac{1}{-d^2/dz^2 + g^2 V - k^2}$$

in the complex k^2-plane ($\operatorname{Im} k > 0$) for real values of g^2. In a similar way we can arrive at a spectral representation in the complex g^2-plane for $k^2 < 0$ which displays the analyticity properties in g^2. The representation is related to a resolution of the identity in the space $L_2^V(0, \infty)$ which is the set of all functions $v(z)$ such that

$$(4.28)\qquad \int_0^\infty dz\, V(z)\,|v(z)|^2 < \infty.$$

(Recall $V(z) > 0$.) Every $v \in L_2^V(0, \infty)$ can be represented in the form

$$(4.29)\qquad v(z) = \int_{-\infty}^{+\infty} d\sigma(g^2)\,\tilde{v}(g^2)\,f(z, g, i\varkappa), \qquad \tilde{v}(g^2) = \int_0^\infty dz\; v(z)\,V(z)\,f(z, g, i\varkappa).$$

Proceeding as in the k^2-plane we obtain

$$G(a, a\,|\,g^2, -\varkappa^2) = \operatorname{Re} G(a, a\,|\,i, -\varkappa^2) + \int_{-\infty}^{+\infty} \frac{d\sigma(g'^2)}{g'^4+1}\,\frac{1+g^2g'^2}{g^2-g'^2}\,(f(a, g', i\varkappa))^2 . \tag{4.30}$$

Because of (2.11) the functions $f(z, g', i\varkappa)$ are real for all $g^2 \gtrless 0$. The l.h.s. of (4.30) is analytic in the half-plane $\operatorname{Re} g > 0$. Hence the spectrum extends only from $-\infty$ to 0 and we can determine the continuous part of the spectral density from the discontinuity across the cut:

$$\frac{d\sigma}{dg^2} = \frac{-ig}{\pi}\,\frac{1}{|f(g, i\varkappa)|^2} + \sum_n \frac{1}{N_n'^2}\,\delta(g^2+g_n^2)\,, \qquad g^2<0\,, \tag{4.31}$$

$$N_n'^2 = \int_0^\infty dz\, V(z)\, f^2(z, g_n, i\varkappa)\,. \tag{4.32}$$

The discrete points $g_n^2 < 0$ are the necessary coupling constants for the existence of bound states with energy $-\varkappa^2$. The resolvent can be represented by the integral:

$$G(z, \zeta\,|\,g^2, -\varkappa^2)) = \operatorname{Re} G(z, \zeta\,|\,i, -\varkappa^2) + \int_{-\infty}^{0} \frac{d\sigma(g'^2)}{g'^4+1}\,\frac{1+g^2g'^2}{g^2-g'^2}\, f(z, g', i\varkappa)\, f(\zeta, g', i\varkappa)\,. \tag{4.33}$$

The existence of (4.33) follows from

$$\operatorname{Im} G(a, a\,|\,i, -\varkappa^2) = \int_{-\infty}^{0} \frac{d\sigma(g'^2)}{g'^4+1}\,(f(a, g', i\varkappa))^2\,. \tag{4.34}$$

If the potential has the property

$$\int_0^\infty dz\, zV(z) < \infty\,, \tag{4.35}$$

then there are only discrete spectral points accumulating at $-\infty$ [16]. For $k^2>0$ the g_n^2 become clearly complex. An illustration of this situation is given by Regge's analysis of complex angular momenta [13] which is related to the

(16) K. MEETZ: *Journ. Math. Phys.*, **3**, 690 (1962).

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potential (2.13). In this case the spectral integral extends only from $-\infty$ to $g^2 = -\frac{1}{4}$ ($\nu = 0$). Hence the resolvent can be expanded into powers of g^2 in the region $|g^2| < \frac{1}{4}$ for $k^2 < 0$. From the experience with potentials of the class (4.35) ([16]) we believe that this is also true for $k^2 > 0$.

5. – Cut-off limits.

Having discussed the mathematical problems connected with singular potentials in some detail we are left with the question of physical interpretation. In principle these potentials have to be rejected, if they do imply a Hamiltonian not bounded below, but one may regard them as mathematical idealizations. However, this does make sense only, if a specific self-adjoint extension can be selected according to physical arguments. We shall show now that the usually adopted cut-off procedure does not offer a possibility to do so.

We define the « regularized » potential

$$V_R(z) = \begin{cases} V(z) & b \leqslant z\,, \\ V(b) & 0 \leqslant z < b\,, \end{cases} \tag{5.1}$$

where $V(z)$ is a singular potential of the class (2.13) or (2.16). We could just as well have chosen another function $V_R(z)$ which is regular at the origin and tends to $V(z)$ in the limit of some cut-off parameter. The conclusions to be drawn do not depend on the method of « regularization ». Now consider $z = b$ as a regular boundary point. Then a boundary condition of the form (3.19)

$$w(b) \cos \psi(b) - w'(b) \sin \psi(b) = 0 \tag{5.2}$$

defines some self-adjoint extension of the differential operator L in the interval (b, ∞). The solution of the differential eq. (2.6) under the boundary condition (5.2) is

$$\varphi_b(z, g, k) = \varphi(z, g, k) - t(b)\, \varphi(z, -g, k)\,, \qquad z \geqslant b, \tag{5.3}$$

with

$$t(b) = \frac{\varphi(b, g, k) \cos \psi(b) - \varphi'(b, g, k) \sin \psi(b)}{\varphi(b, -g, k) \cos \psi(b) - \varphi'(b, -g, k) \sin \psi(b)}\,. \tag{5.4}$$

In the interval $0 \leqslant z < b$ we have the solution

$$w(z) = \sin z\sqrt{k^2 - g^2 V(b)} \tag{5.5}$$

under the regular boundary condition $w(0)=0$. Hence

$$\operatorname{cotg}\psi(b)=\sqrt{k^2-g^2V(b)}\,\operatorname{cotg}\sqrt{k^2-g^2V(b)}\,b\ . \tag{5.6}$$

The question is: does $t(b)$ tend to a definite limit for $b\to 0$, if we insert (5.6) into (5.4)?

Consider first the potential (2.13) with the fundamental system (2.24):

$$g^2V(b)=\frac{\nu^2-\frac14}{b^2}\,;\qquad \begin{cases}\varphi(b,\nu,k)\to b^{\nu+\frac12}\\ \varphi(b,-\nu,k)\to b^{-\nu+\frac12}\end{cases}\qquad b\to 0\ . \tag{5.7}$$

This yields:

$$t(b)\to b^{2\nu}\,\frac{\sqrt{\frac14-\nu^2}\cos\sqrt{\frac14-\nu^2}-(\nu+\frac12)\sin\sqrt{\frac14-\nu^2}}{\sqrt{\frac14-\nu^2}\cos\sqrt{\frac14-\nu^2}-(-\nu+\frac12)\sin\sqrt{\frac14-\nu^2}}\ . \tag{5.8}$$

Hence $t(b)\to 0$ for $b\to 0$, if $\nu>0$ (the system (2.24) cannot be used for integral values of ν) and the regularization selects the solution $\varphi(z,\nu,k)$. While this is to be expected for $\nu>1$ because then $\varphi(z,\nu,k)$ is the only solution in $L_2(0,a)$, a specific self-adjoint extension corresponding to the value $c=0$ (see (3.14)) is defined in the range $0<\nu<1$. However, for $\nu^2<0$ $(\nu=i\gamma)$ we find

$$t(b)\to\exp[2i\gamma\ln b-2i\delta(\gamma)]\,,\quad \exp[-2i\delta(\gamma)]= \tag{5.9}$$

$$=\frac{\sqrt{\frac14+\gamma^2}\cos\sqrt{\frac14+\gamma^2}-(i\gamma+\frac12)\sin\sqrt{\frac14+\gamma^2}}{\sqrt{\frac14+\gamma^2}\cos\sqrt{\frac14+\gamma^2}-(-i\gamma+\frac12)\sin\sqrt{\frac14+\gamma^2}}$$

and all we can say is $|t(b)|=1$. No definite extension of the form (3.10) can be obtained by regularization.

A similar analysis for the potential (2.16) with the fundamental system (2.23)

$$V(b)=\frac{1}{b^\alpha}+V'(b)\,;\qquad \begin{cases}\varphi(b,g,k)\longrightarrow b^{\alpha/4}\exp\left[\frac{-g}{q}\,b^{-q}\right]\\ \varphi(b,-g,k)\xrightarrow[b\to 0]{} b^{\alpha/4}\exp\left[\frac{g}{q}\,b^{-q}\right]\end{cases},\qquad q=\frac{\alpha}{2}-1 \tag{5.10}$$

results in

$$t(b)\xrightarrow[b\to 0]{}\exp\left[-\frac{2g}{q}\,b^{-q}\right]\frac{\cos(\sqrt{-g^2}\,b^{-q})\sqrt{-g^2}-g\sin(\sqrt{-g^2}\,b^{-q})}{\cos(\sqrt{-g^2}\,b^{-q})\sqrt{-g^2}+g\sin(\sqrt{-g^2}\,b^{-q})}\ . \tag{5.11}$$

The regularization selects the solution $\varphi(z,g,k)$ in $L_2(0,a)$ for $g^2>0$ and does not lead to some definite self-adjoint extension for $g^2<0$, because

$$t(b)\to\exp\left[-\frac{2i\beta}{q}\,b^{-q}-2i\beta b^{-q}\right],\qquad g=i\beta\ . \tag{5.12}$$

We arrive at the disappointing conclusion that either the regularization is not necessary, because the transformation H is already self-adjoint ($n=0$), or it does not result in a definite extension $H_\Theta(n=1)$ with the only exception of the potential (2.12) in the range $0<\nu<1$.

6. – Conclusion.

The potentials which we have discussed are examples of the more general class:

$$V(z)=\frac{g^2}{z^\alpha}+\widetilde{V}(z)\,, \tag{6.1}$$

where

$$\int_0^b \mathrm{d}z\, z\,|\widetilde{V}(z)|<\infty \qquad \text{and} \qquad \alpha\geqslant 2.$$

The sign of the regular potential $\widetilde{V}(z)$ may be arbitrary. As we have seen the case $\alpha=2$ has to be considered separately. We may then put $g^2=\nu^2-\frac{1}{4}$ and have to distinguish three ranges of ν^2-values:

1) $\nu^2\geqslant 1$. The potential is « strongly » repulsive near the origin. The transformation H is self-adjoint ($n=0$). Every sequence of regularized transformations tends to H in the limit of the cut-off parameter.

2) $0\leqslant\nu^2<1$. The potential is « weakly » repulsive ($\frac{1}{4}<\nu^2<1$) or « weakly » attractive ($0\leqslant\nu^2<\frac{1}{4}$) near the origin. There exists a class of self-adjoint extensions $H_\Theta\,(n=1)$. A regularization method selects the extension belonging to the boundary condition $\varphi_\Theta(z)\sim z^{\nu+\frac{1}{2}}$ for $z\to 0$.

3) $\nu^2<0$. The potential is « strongly » attractive near the origin. Again we have a class of self-adjoint extensions $H_\Theta\,(n=1)$. But a regularization does not lead to a definite extension.

The generalization to higher angular momenta ($l>0$) is obvious. We just have to substitute $\nu^2-l(l+1)$ for ν^2.

If $\alpha>2$, only two ranges of coupling constant values g^2 have to be distinguished:

1) $g^2>0$. The potential is repulsive near the origin. Every regularization method results in the self-adjoint transformation H ($n=0$).

2) $g^2 < 0$. The potential is attractive near the origin. There is a class of self-adjoint extensions H_Θ $(n=1)$. It is not possible to select a definite one by a regularization method.

If we wish to consider higher angular momenta $(l > 0)$, we may treat the centrifugal term $-l(l+1)/z^2$ as a perturbation and absorb it in the integrand of the Volterra eqs. (2.11) and (2.23).

The general theory can of course also be extended to superpositions of potentials of the class (6.1), *e.g.*:

$$V(z) = \sum_{i=1}^{r} \frac{g_i^2}{z^{\alpha_i}} + \tilde{V}(z)\,, \qquad \alpha_i \geqslant 2\,. \tag{6.2}$$

In analogy to (2.21) we may then use

$$\frac{\mathrm{d}^2 w_0}{\mathrm{d}z^2} + \left(\sum_{i=1}^{r}{}' \frac{g_i^2}{z^{\alpha_i}}\right) w_0(z) = 0 \tag{6.3}$$

as the unperturbed equation for the definition of the solutions $\varphi(z)$, where in the sum $\sum'$ all terms with $\alpha_i = 2$ have been dropped, because they can be treated as a perturbation.

RIASSUNTO (*)

Si studiano gli aspetti matematici dei potenziali singolari nella meccanica quantistica non relativistica in funzione delle trasformazioni autoaggiunte riferite a operatori differenziali singolari nello spazio $L_2(0, \infty)$. Il contenuto fisico è espresso dalla decomposizione spettrale e per potenziali attrattivi si trova che è determinato solo sino ad un parametro che definisce una particolare estensione. In generale, con un procedimento di taglio non è possibile determinare un'estensione specifica.

(*) *Traduzione a cura della Redazione.*