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Some Remarks on Singular Attractive Potentials (*).

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Summary. — The difficulties with singular attractive potentials are traced to the fact that they lead to nonself-adjoint Hamiltonians. These are not acceptable in the framework of quantum mechanics.

1. – Introduction.

Singular attractive potentials have been considered for some time in quantum mechanics [1-5], and a closer study revealed that these potentials exhibit properties not shared by nonsingular or less singular potentials like the Coulomb interaction or the harmonic oscillator. It is the intention of this note to shed some light on these problems from a mathematical point of view. Particularly we want to show that even in classical mechanics difficulties are encountered in the naive approach. An argument is then presented which indicates that the Hamiltonian connected with these potentials is not admissible in quantum mechanics, since it is not essentially self-adjoint. Some remarks will also be made concerning the uncritical use of separation of variables in spherical co-ordinates, which explains the spurious second $l = 0$ solutions.

For simplicity we consider only spherically symmetric potentials $V(r)$.

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(1) K. CASE: *Phys. Rev.*, **80**, 797 (1950).
(2) R. M. SPECTOR: *Journ. Math. Phys.*, **5**, 1185 (1965).
(3) R. M. SPECTOR: preprint.
(4) E. VOGT and G. WANNIER: *Phys. Rev.*, **95**, 1190 (1954).
(5) H. ALY and H. MÜLLER: *Journ. Math. Phys.*, **7**, 1 (1966).

We call $V(r)$ singular if $r^{2+\varepsilon}V(r) \to 0$ as $r \to 0$ for some $\varepsilon > 0$ and V bounded and continuous elsewhere.

2. – Classical mechanics.

Solving the equations of the orbits in classical mechanics, one finds that for a given energy all trajectories lead to the origin if the impact parameter b is below a certain critical value b_0 when the potential V is singular attractive. As a particle approaches the origin its trajectory smoothes to some tangent. Physically this means that at the origin the orbit is independent of the energy E and the angular momentum L. As the particle emerges on the other side of the origin it has « forgotten » its former energy and angular momentum because at 0 its orbit was independent of these quantities. The continuation of the orbits through 0 thus poses a problem.

The reason for this difficulty is, that it is generally believed that a classical system of n degrees of freedom is determined by n second-order differential equations with $2n$ initial values. However in this case the origin is a singular point of these equations since infinitely many orbits go through 0 with a given tangent. Actually even a singular circle appears for b_0, but it poses no problem, since it will not contribute to scattering. Thus the integral curves of these equations are strictly only defined from 0 to ∞ or *vice versa* and we need other criteria besides the initial values to continue the integral curves through 0.

In physics these conditions are obviously energy and angular momentum conservation along each orbit. However it should be clear that in the strict differential equation approach to classical mechanics, these conditions have to be given *in addition* to the equations, because though E and L conservation outside 0 are consequences of the symmetries of the differential equations this is not necessarily so at 0. The reason for this is that in the usual derivations of equations in classical mechanics smooth potentials and derivatives are required mathematically. So with some physical goodwill, *i.e.* the postulate of E and L conservation at or around 0, the problem with singular potentials can be made well defined in classical mechanics. In the next Sections we will see that the problems in quantum mechanics are much graver, since the above difficulties remain and new ones appear.

3. – Symmetric operators.

In quantum mechanics the Hamiltonian is defined to be the infinitesimal generator of the dynamical group $\{\mathscr{U}(t)\}$. It is therefore necessary that the Hamiltonian be self-adjoint. However in general the differential operator $\mathscr{H} = -(\hbar^2/2m)\Delta + V(r)$, which we are used to calling the Hamiltonian is only

symmetric. This means ([6,7]) that $\mathscr{H}$ has a dense domain $\theta_{\mathscr{H}}$ and satisfies

$$\langle \mathscr{H} f | g \rangle = \langle f | \mathscr{H} g \rangle \qquad \text{for all } f,\ g \in \theta_{\mathscr{H}}.$$

For differential operators self-adjointness in general is difficult to establish, since it involves questions about the domain. Because of this VON NEUMANN introduced the concept of essentially self-adjoint operators. We call an operator essentially self-adjoint (e.s.) if it has a *unique* self-adjoint extension. Thus we see that the actual Hamiltonian in quantum mechanics is in general not the differential operator $\mathscr{H} = -(\hbar^2/2m)\Delta + V(r)$, but rather a self-adjoint extension $\tilde{\mathscr{H}}$ of this operator. This implies that, in general, a quantum mechanical problem is only well defined if it is given by an e.s. differential operator. This fact has so far attracted only very little attention, because most potentials considered in quantum mechanics lead to e.s. operators ([8,9]). There are however indications that singular attractive potentials do not have this property.

Let us return to the study of $\mathscr{H} = -(\hbar^2/2m)\Delta + V(r)$. For real potentials $\mathscr{H}$ commutes with the operator of complex conjugation. Therefore $\mathscr{H}$ has a self-adjoint extension $\tilde{\mathscr{H}}$ ([6] p. 1231). However these extensions are, in general, not unique. This lack of uniqueness is expressed by the deficiency index, d.i., (m, m) $m = 0, 1, 2, \ldots, \infty$, m is here the number of parameters or boundary conditions needed in order to determine a self-adjoint extension of $\mathscr{H}$ uniquely. Thus a symmetric operator is only e.s. if and only if its d.i. is $(0, 0)$. In particular we need one parameter to make well defined a quantum mechanical problem with an operator whose d.i. is $(1, 1)$. An example for this is the potential $V = -g/r^2$ for some suitable g. Here it turns out that all bound states depend on one or more parameters ([10]).

4. – Singular attractive potential.

We know from the above that $\mathscr{H} = -(\hbar/2m)\Delta + V$ has a self-adjoint extension $\tilde{\mathscr{H}}$, even if V is singular attractive. Since $\tilde{\mathscr{H}}$ is self-adjoint its spectrum is not empty and there exists at least one eigenfunction of the continuous or discrete spectrum. Since V is spherically symmetric there exists at least one eigenfunction for every l, m. For simplicity we restrict ourselves to $l = 0$, $m = 0$; the other cases are treated similarly since the potential V dominates the angular momentum term $+(l(l+1)/r^2)$ near the origin.

([6]) N. DUNFORD and J. T. SCHWARTZ: *Linear Operators*, vol. **2** (New York, 1963).

([7]) N. I. ACHIESER and I. M. GLASMANN: *Theorie der linearen Operatoren im Hilbert Raum* (Berlin, 1960).

([8]) T. KATO: *Transactions Am. Math. Soc.*, **70**, 195 (1951).

([9]) N. LIMIČ: *Comm. of Math. Phys.*, **1**, 321 (1966).

([10]) P. M. MORSE and H. FESHBACH: *Methods of Theoretical Physics* (New York, 1953).

Assume that $\tilde{\mathscr{H}}\psi(r) = E\psi(r)$. Then we know from Friedrichs' theorem ([11]), that $\mathscr{H}\psi(r) = E\psi(r)$ for all r outside the singularity, *i.e.* for $r > 0$. In other words ψ is a weak solution of the differential equation.

By using the WKB method this implies that $\psi(r) \approx A\psi_+(r) + B\psi_-(r)$ with

$$\psi_\pm(r) \approx \frac{1}{r} V(r)^{-\frac{1}{4}} \exp\left[\pm i \left\{\int_r^{r_0} V(r)^{\frac{1}{2}} \mathrm{d}r\right\}\right]$$

for small r and this holds for any solution $\tilde{\mathscr{H}}\psi(r) = E\psi(r)$. At this stage the δ-function argument is usually introduced ([3]) to show that $\tilde{\mathscr{H}}$ (respectively $\mathscr{H}$) has no solutions, which is absurd in view of the spectral theorem of self-adjoint operators on Hilbert space. The argument is that ψ does not satisfy $\mathscr{H}\psi = E\psi$ strictly but leads to some δ-function term, *i.e.* $\mathscr{H}\psi = E\psi + \delta(r)f(r)\psi$. This argument is fallacious in two respects:

a) The δ-function is neither an element of $\mathscr{L}^2(R^3)$, nor a functional on $\mathscr{L}^2(R^3)$, in fact point evaluation on $\mathscr{L}^2(R^3)$ is senseless.

b) The real Hamiltonian is not $\mathscr{H}$ but $\tilde{\mathscr{H}}$. The difficulty is that most arguments for partial differential equations which are valid on function spaces of differentiable functions cease to be valid in a Hilbert-space theory in this connection.

If $\mathscr{H}$ were e.s. the ratio A/B could be determined uniquely and we would be able to determine a condition that singles out a particular linear combination. The conditions in this case could be given in two forms

a) $\psi(r) \in \mathscr{L}^2(R^3)$ locally.

b) A boundary condition at 0.

The boundary condition has to be given at 0 because the problem is practically insensitive to changes made in the potential for $r \geqslant R_0 > 0$ for some R_0.

But both conditions fail to single out a particular ψ, because if ψ_+ is locally square integrable, then so is ψ_-, and ψ_+ and ψ_- have the same behaviour as $r \to 0$.

Requiring orthogonality for all solutions we find ([1]) that

$$\psi(r) \approx \frac{1}{r} V(r)^{-\frac{1}{4}} \cos\left\{\int_r^{r_0} V(r)^{\frac{1}{2}} \mathrm{d}r + \alpha\right\},$$

where α is an arbitrary parameter, which is not determined by $\mathscr{H}$.

([11]) K. O. FRIEDRICHS: *Am. Journ. Math.*, **61**. 523 (1939).

Since for every l and m we have to determine the parameter α_{lm}, we see that the differential operator $\mathscr{H}$ is not only not e.s. but even has d.i. (∞, ∞).

The arbitrary phases α_{lm} were first introduced by CASE [1] in the case $l = m = 0$.

In general therefore the operator $\mathscr{H} = -(\hbar^2/2m)\Delta + V(r)$ with $V(r)$ singular attractive is not admissible in quantum mechanics since it is not e.s. and only yields a well-defined problem in quantum mechanics if we are given the phases α_{lm} or some physical model which determines these parameters. It should be remarked here that the various methods of analytic continuations are just particular ways to fix these constants α_{lm}. Physically this is probably not a very compelling procedure. The determination of the α_{lm} by cut-off has the disadvantage that all results will strongly depend on the cut-off.

The fact that $\mathscr{H}$ has d.i. (∞, ∞) shows that $\mathscr{H}$ also has nonself-adjoint extensions and would for example allow inelastic scattering. Most of the peculiar problems with singular attractive potentials can be traced to the great variety of possible extensions. These difficulties make the study of singular attractive potentials rather academic. However our discussion shows that before trying to solve a quantum mechanical problem it is important to establish the essential self adjointness of the operators.

5. – Separation in spherical co-ordinates.

Another problem which has puzzled physicists for some time is the appearance of spurious $l = 0$ solutions of the Schrödinger equation for not too singular potentials, particularly the hydrogen atom. Indeed let V be such that $r^{2-\varepsilon}V(r) \to 0$ as $r \to 0$ for some $\varepsilon > 0$, then we know that the two solutions ψ_1, ψ_2 of the radial Schrödinger equation behave as [12] $\psi_1 \sim r^{-l-1}, \psi_2 \sim r^l$ as $r \to 0$. For $l \geqslant 1$, ψ_1 is not square integrable, hence can be discarded. For $l = 0$ the radial Schrödinger equation however gives two possible solutions and the above argument fails. Many explanations have been given in order to show that ψ_1 is not admissible. The most prominent ones are:

i) ψ_1 is more singular than ψ_2,

and

ii) δ-function argument.

Both arguments are however not acceptable in a Hilbert-space theory, which is the framework of quantum mechanics. To state this dilemma in more rigorous terms, we have [8]:

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[12] A. MESSIAH: *Quantum Mechanics*, vol. **1** (Amsterdam, 1958).

Theorem. The Schrödinger Hamiltonian $\mathscr{H} = -(\hbar^2/2m)\Delta + V(r)$ with $V(r)$ such that $\int_0^R r^2|V(r)|^2 \mathrm{d}^3r < \infty$ for some $R > 0$ and $|V(r)| < \infty$ for $r > R$ is essentially self-adjoint and the eigenfunctions are bounded.

But the radial Schrödinger equation is not e.s. for $l = 0$. In fact one can show:

Theorem. The differential operator $\mathscr{H}_r = -(\hbar^2/2m)(\mathrm{d}^2/\mathrm{d}r^2) + V(r)$ with V as above and attractive has d.i. $(1, 1)$ on $\mathscr{L}^2([0, \infty])$.

The reason for this is, that through the separation in spherical co-ordinates we introduce an additional boundary point 0, for which we need an additional boundary condition in order to make the problem self-adjoint. This boundary condition has to be obtained from the full Schrödinger equation. From Kato's theorem it is the requirement that the ψ bounded at 0.

For the singular attractive case however this fails since both functions behave essentially in the same manner at 0. We therefore had to conclude that in this case the Hamiltonian has d.i. (∞, ∞).

We have seen above that the uncritical use of the separation of variables in spherical co-ordinates introduces difficulties through spurious solutions. Obviously we would expect similar results for the separation of variables in other co-ordinates as soon as we introduce new boundary points.

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RIASSUNTO (*)

Si rintraccia l'origine delle difficoltà che si incontrano con i potenziali attrattivi singolari nel fatto che essi portano ad hamiltoniane non autoaggiunte. Queste non sono accettabili nello schema della meccanica quantistica.

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Некоторые замечания о сингулярных потенциалах притяжения.

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