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Møller Operators for Scattering on Singular Potentials

J. Kupsch and W. Sandhas
Physikalisches Institut der Universität Bonn

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Abstract. The existence of Møller operators is proved for singular potentials which decrease more rapidly at infinity than the Coulomb potential. The question of their uniqueness is discussed.

1. Introduction

In the formal theory of scattering processes it is of fundamental interest to investigate whether uniquely defined Møller operators exist. Therefore several authors have dealt with this question, especially for the case of potential scattering. Cook [1] was able to show the existence of uniquely defined Møller operators, as long as the potential $V(\boldsymbol{r})$ is square integrable. This proof was extended by Hack [2] to locally square integrable potentials which at infinity decrease faster than const $\cdot\, r^{-1-\varepsilon}$, i.e., more rapidly than the Coulomb potential, and by Kuroda [3] to a class of potentials which includes the cases investigated by Cook and Hack (compare also Jauch and Zinnes [4]). The physically important points of these considerations are explained in the review article of Brenig and Haag [5].

In all the above mentioned proofs it is required that $V(\boldsymbol{r})$ be locally square integrable. For other potentials which do not fulfill this requirement (in the following we will call them "singular"), scattering theory recently has been developed more extensively. Most of these investigations were based on a discussion of the radial Schrödinger equation, i.e., the ordinary methods of stationary scattering theory were used. Although several of the peculiarities connected with singular potentials have been clarified by this procedure, a study from the more transparent viewpoint of formal scattering theory seems desirable. As to the existence of uniquely defined Møller operators some results for spherically symmetric potentials have already been found in this framework. Green and Lanford [6] have shown the existence of Møller operators for potentials which are less singular than $r^{-2+\varepsilon}$ at the origin and Limić [7] got the same result for highly singular potentials that are repulsive at the origin.

In the following we shall give a relatively simple proof for the existence of Møller operators, also valid for highly singular not spherically symmetric potentials. It will be shown that these operators exist under rather weak assumptions (essentially given by condition (2.2) below).

The outline of our proof is the same as that in the article of Brenig and Haag [5] and related to that by Cook [1], Hack [2] and Kuroda [3]. As compared to these papers the following points are different respectively more general in our investigation:

I) It is shown that the criterion used in [5] for the existence of Møller operators can be replaced by a weaker one which allows the treatment of highly singular potentials (cf. Eq. (2.21) and (2.22)).

II) The estimate of free Schrödinger wave packets which is done in [5] by the stationary phase method, is replaced by a rigorous estimate, Eq. (2.10), similar to the kind first used by Ruelle [8] for solutions of the Klein-Gordon equation.

III) The important question whether the Møller operators are unique depends on whether the symmetric differential operator, formally defining the Hamiltonian on a suitable dense domain, has a unique self-adjoint extension. For certain classes of singular potentials the extension is not unique which makes this point rather crucial in our case (the well known difficulties of scattering theory in the case of highly singular attractive potentials originate in this point). Thus we will review the most important results concerning this question in Section 3.

We should mention that shortly before completion of our manuscript, N. Limić [9] published an extension of his above cited proof [7] for the case of not spherically symmetric potentials. Our proof, however, is simpler and uses weaker assumptions for the potential.

2. Proof of existence

In the following we regard a Hamiltonian which is formally given by the symmetric differential operator:

$$H' = -\frac{1}{2m}\nabla^2 + V(\boldsymbol{r})\,. \tag{2.1}$$

The potential $V(\boldsymbol{r})$ is assumed to be a real, Lebesgue-measurable function. The requirement of symmetry of H' imposes a further restriction for $V(\boldsymbol{r})$. Essentially, $V(\boldsymbol{r})$ must be of such a kind that H' is defined on a dense set in the Hilbert space $L^2(R^3)$. (It suffices to require the set of non-locally square integrable points of $V(\boldsymbol{r})$ to be of measure zero.)

The potential further fulfills the following condition: There exists an $\varepsilon > 0$, and a finite $R \geqq 0$, such that

$$\iiint\limits_{r=R}^{\infty} V^2(\boldsymbol{r})\,(r+1)^{\varepsilon-1}\,d^3\boldsymbol{r} < \infty\,, \quad (|\boldsymbol{r}| = r)\,. \tag{2.2}$$

Without loss of generality we shall assume $\varepsilon \leqq 1$.

The dense domain of H' in $L^2(R^3)$ is chosen to include all test functions [10] of $\mathcal{S}(R^3)$ which vanish for $r < R$. As a real symmetric operator H' has a self-adjoint extension (cf.: e.g. [11] p. 312, [12] p. 361).

In the following H denotes such a self-adjoint, not necessarily unique, extension of H'.

The kinetic energy operator is formally introduced by

$$H_0' = -\frac{1}{2m}\nabla^2, \tag{2.3}$$

where the domain of H_0' can be chosen to include the space $\mathcal{S}(R^3)$. H_0 then denotes the *unique* self-adjoint extension of H_0' [13].

With the help of H and H_0 one can form the unitary operator

$$U(t) = e^{iHt}e^{-iH_0t}, \tag{2.4}$$

which is defined everywhere in $L^2(R^3)$. The strong limits of $U(t)$ are the Møller wave operators (compare, e.g., [5])

$$\Omega_\pm = \lim_{t\to\pm\infty} U(t). \tag{2.5}$$

To prove the existence of $\Omega_\pm$ one has to show the strong convergence of $U(t)$. Because the operators $U(t)$ are uniformly bounded, it suffices to give the proof on a dense set of functions in $L^2(R^3)$. We consider functions $f(\boldsymbol{r})$ of the class $\mathcal{S}(R^3)$. These have the properties:

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\int e^{i\boldsymbol{p}\cdot\boldsymbol{r}}\tilde{f}(\boldsymbol{p})\,d^3\boldsymbol{p} \tag{2.6}$$

and

$$f(\boldsymbol{r},t) = e^{-iH_0t}f(\boldsymbol{r}) = \frac{1}{(2\pi)^{3/2}}\int e^{i\left(\boldsymbol{p}\cdot\boldsymbol{r}-\frac{\boldsymbol{p}^2}{2m}t\right)}\tilde{f}(\boldsymbol{p})\,d^3\boldsymbol{p}, \tag{2.7}$$

with $\tilde{f}(\boldsymbol{p}) \in \mathcal{S}$, $f(\boldsymbol{r},t) \in \mathcal{S}$ and

$$\|f(\boldsymbol{r},t)\|^2 = \int |f(\boldsymbol{r},t)|^2\,d^3\boldsymbol{r} = \text{const}. \tag{2.8}$$

Furthermore, we have from (2.7), for $t \neq 0$,

$$f(\boldsymbol{r},t) = \left(\frac{m}{2\pi i t}\right)^{3/2}\int d^3\boldsymbol{r}'\,e^{i\frac{m}{2t}(\boldsymbol{r}-\boldsymbol{r}')^2}f(\boldsymbol{r}'). \tag{2.9}$$

Equation (2.9) implies the uniform estimate, important for subsequent use:

$$|f(\boldsymbol{r},t)| \leqq C_\alpha\left(\frac{|t|}{r}\right)^\alpha\cdot|t|^{-3/2}, \tag{2.10}$$

which is valid for any $\alpha \geqq 0$ and $|t| \geqq t_0 > 0$ ($C_\alpha = C_\alpha(t_0)$). We shall give a proof of (2.10) at the end of this section (compare also the similar kind of estimate given in [8] for solutions of the Klein-Gordon equation).

The strong convergence of $U(t)$ is proved if for sufficiently large $|t_1|$ (with $t_2 > t_1 > 0$ respectively $t_2 < t_1 < 0$) the expression

$$\|(U(t_2) - U(t_1))\,f(\boldsymbol{r})\| = \|e^{iHt_2}f(\boldsymbol{r},t_2) - e^{iHt_1}f(\boldsymbol{r},t_1)\| \tag{2.11}$$

becomes arbitrarily small. For the estimate of (2.11) we introduce a function $F(\boldsymbol{r})$ with the properties

$$0 \leqq F(\boldsymbol{r}) \leqq 1 \tag{2.12}$$

$$F(\boldsymbol{r}) = \begin{cases} 0 & \text{for} \quad r \leqq R \\ 1 & \text{for} \quad r \geqq R + \frac{1}{2} \, . \end{cases}$$

Furthermore we assume $(1 - F(\boldsymbol{r})) \in \mathscr{S}(R^3)$, and thus $F(\boldsymbol{r}) \cdot f(\boldsymbol{r}, t)$ belongs to the domain of the originally given operator H'.

It follows

$$\begin{aligned} \|(U(t_2) - U(t_1)) f(\boldsymbol{r})\| \leqq \|e^{iHt_2} F(\boldsymbol{r}) f(\boldsymbol{r}, t_2) - e^{iHt_1} F(\boldsymbol{r}) f(\boldsymbol{r}, t_1)\| + \\ + \|(1 - F(\boldsymbol{r})) f(\boldsymbol{r}, t_2)\| + \|(1 - F(\boldsymbol{r})) f(\boldsymbol{r}, t_1)\| \, . \end{aligned} \tag{2.13}$$

Because of (2.10) the last two terms in (2.13) can be estimated by const $\cdot \, |t_1|^{-3/2}$. Therefore it remains to investigate the expression

$$A(t_2, t_1) = \|e^{iHt_2} F(\boldsymbol{r}) f(\boldsymbol{r}, t_2) - e^{iHt_1} F(\boldsymbol{r}) f(\boldsymbol{r}, t_1)\| \, . \tag{2.14}$$

This can be written in the form

$$A(t_2, t_1) = \left\| \int_{t_1}^{t_2} \frac{d}{dt} (e^{iHt} F(\boldsymbol{r}) f(\boldsymbol{r}, t)) \, dt \right\| \tag{2.15}$$

because the integrand exists (cf. [1], p. 85) and depends continuously on t in the L^2-norm[1].

Now we have

$$A(t_2, t_1) \leqq \left| \int_{t_1}^{t_2} \left\| \frac{d}{dt} (e^{iHt} F(\boldsymbol{r}) f(\boldsymbol{r}, t)) \right\| dt \right| \tag{2.16}$$

and

$$\left\| \frac{d}{dt} (e^{iHt} F(\boldsymbol{r}) f(\boldsymbol{r}, t)) \right\| \leqq \|[H_0, F] f(\boldsymbol{r}, t)\| + \|V(\boldsymbol{r}) F(\boldsymbol{r}) f(\boldsymbol{r}, t)\| \, . \tag{2.17}$$

From (2.9) respectively (2.10) we find

$$\begin{aligned} |[H_0, F] f(\boldsymbol{r}, t)| &= \frac{1}{2m} |f(\boldsymbol{r}, t) \nabla^2 F(\boldsymbol{r}) + 2(\nabla F(\boldsymbol{r})) \cdot (\nabla f(\boldsymbol{r}, t))| \\ &= \begin{cases} \leqq \text{const} \cdot |t|^{-3/2} & \text{for} \quad R \leqq r \leqq R + \frac{1}{2} \\ = 0 \text{ otherwise} \, . \end{cases} \end{aligned} \tag{2.18}$$

This implies

$$\|[H_0, F] f(\boldsymbol{r}, t)\| \leqq \text{const} \cdot |t|^{-3/2} \tag{2.19}$$

and, with (2.17) and (2.16),

$$A(t_2, t_1) \leqq \text{const} \cdot |t_1|^{-1/2} + \left| \int_{t_1}^{t_2} \|V(\boldsymbol{r}) F(\boldsymbol{r}) f(\boldsymbol{r}, t)\| \, dt \right| \, . \tag{2.20}$$

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[1] The continuous t-dependence follows from estimates similar to (2.18) and (2.23) if one takes into consideration that the functions $\nabla f(\boldsymbol{r}, t)$ and $(r + 1)^\alpha f(\boldsymbol{r}, t)$ are continuous in t, uniformly with respect to $\boldsymbol{r}$.

Thus we have shown that instead of the criterion usually given for the convergence of $U(t)$,

$$\int_{t_1}^{t_2} \| V(\boldsymbol{r})\, f(\boldsymbol{r}, t)\| \, dt \xrightarrow[(t_1 \to \infty)]{} 0, \quad (t_2 > t_1 > 0) \tag{2.21}$$

(cf. [5] Eq. (1.11a)), it is sufficient to prove the corresponding property with $f(\boldsymbol{r}, t)$ replaced by $F(\boldsymbol{r}) \cdot f(\boldsymbol{r}, t)$, i.e., to prove that

$$\int_{t_1}^{t_2} \| V(\boldsymbol{r})\, F(\boldsymbol{r})\, f(\boldsymbol{r}, t)\| \, dt, \quad (t_2 > t_1 > 0) \tag{2.22}$$

becomes arbitrarily small for sufficiently large t_1. In contrast to (2.21) this criterion allows the treatment of highly singular potentials. To show that it holds for potentials which fulfill the condition (2.2) we regard

$$\begin{aligned} \| V(\boldsymbol{r})\, F(\boldsymbol{r})\, f(\boldsymbol{r}, t)\|^2 &\leqq \iiint_{r=R}^{\infty} V^2(\boldsymbol{r})\, |f(\boldsymbol{r}, t)|^2\, d^3\boldsymbol{r} \\ &= \iiint_{r=R}^{\infty} V^2(\boldsymbol{r})\, (r+1)^{\varepsilon-1}\, |(r+1)^{\frac{1-\varepsilon}{2}} f(\boldsymbol{r}, t)|^2\, d^3\boldsymbol{r}\,. \end{aligned} \tag{2.23}$$

Considering (2.2) and the estimate

$$(r+1)^{\alpha}\, |f(\boldsymbol{r}, t)| \leqq C'_{\alpha} |t|^{\alpha - 3/2} \quad \text{for any} \quad \alpha \geqq 0\,, \tag{2.24}$$

which follows immediately from (2.10), one obtains

$$\| V(\boldsymbol{r})\, F(\boldsymbol{r})\, f(\boldsymbol{r}, t)\|^2 \leqq \text{const} \cdot \frac{1}{|t|^{2+\varepsilon}}\,. \tag{2.25}$$

Thus the integral (2.22) vanishes for $t_1 \to \infty$, i.e., our criterion for convergence is fulfilled.

It remains to show the validity of (2.10). With the help of (2.9) we get, with $|t| \geqq t_0 > 0$ and an integer $n \geqq 0$ (remember $f(\boldsymbol{r}) \in \mathscr{S}$):

$$\begin{aligned} r^{2n} |f(\boldsymbol{r}, t)| &= \left(\frac{m}{2\pi |t|}\right)^{3/2} \left(\frac{t}{m}\right)^{2n} \left| \int d^3\boldsymbol{r}' \,(\nabla_{r'}^{2n} e^{-i\frac{m}{t}\boldsymbol{r}\cdot\boldsymbol{r}'})\, e^{i\frac{m}{2t}\boldsymbol{r}'^2} f(\boldsymbol{r}')\right| \\ &\leqq (2\pi)^{-3/2} \left(\frac{|t|}{m}\right)^{2n-3/2} \int d^3\boldsymbol{r}'\, |\nabla_{r'}^{2n} (e^{i\frac{m}{2t}\boldsymbol{r}'^2} f(\boldsymbol{r}'))| \\ &\leqq C_n |t|^{2n-3/2}\,, \quad C_n = C_n(t_0)\,. \end{aligned} \tag{2.26}$$

For $2n \geqq \alpha$ and $|t| \leqq r$ this implies

$$|f(\boldsymbol{r}, t)| \leqq \left(\frac{r}{|t|}\right)^{2n-\alpha} |f(\boldsymbol{r}, t)| \leqq \left(\frac{|t|}{r}\right)^{\alpha} C_n |t|^{-3/2} \tag{2.27}$$

for $\alpha \geqq 0$ and $|t| \geqq r$ we get from (2.26), with $n = 0$,

$$|f(\boldsymbol{r}, t)| \leqq \left(\frac{|t|}{r}\right)^{\alpha} |f(\boldsymbol{r}, t)| \leqq \left(\frac{|t|}{r}\right)^{\alpha} C_0 |t|^{-3/2}\,, \tag{2.28}$$

and therefore the estimate (2.10) holds, with $C_{\alpha} = \max(C_0, C_n)$.

It should be noted that the assumption for the potential in Kuroda's paper [3][2] is given by (2.2) with $R = 0$ (in this case our proof can be

[2] The potentials considered in Cook's [1] and Hack's [2] papers fulfill this assumption.

simplified by setting $F(\boldsymbol{r}) = 1$). However, we have shown the existence of Møller operators under much less restrictive requirements. Because in our proof R is arbitrary (but finite) the only restriction for $V(\boldsymbol{r})$ in the region $r \leqq R$ is that H' be a real symmetric operator.

3. Uniqueness of $\boldsymbol{H}$

As mentioned in Section 2, the originally given real symmetric operator H' can always be extended to a self-adjoint operator H, such that e^{iHt} and therefore $U(t)$ are defined. The uniqueness of $U(t)$ and hence of $\Omega_{\pm}$ depends on whether the self-adjoint extension of H' is unique. This is the case if and only if the closure $\tilde{H}'$ of H' is self-adjoint (H' is then called essentially self-adjoint [12]).

In the following we review the most important results concerning this question.

a) The case of *square integrable potentials*, i.e., of potentials which fulfill condition (2.2) with $R = 0$ and $\varepsilon = 1$ was investigated by KATO [13]. In KATO's method first H_0' is extended uniquely to a self-adjoint operator H_0 which acts as the multiplication operator $\frac{\boldsymbol{p}^2}{2m}$ in momentum space. It follows that $H_0 + V$ is a self-adjoint operator defined on the domain of H_0. Furthermore $\tilde{H}'$ equals $H_0 + V$, hence H' is essentially self-adjoint. Under the weaker assumption (2.2) with $R = 0$ and $\varepsilon > 0$, a generalization of KATO's proof yields the same result [3].

b) In the case of *singular*, i.e., not locally square integrable potentials this method is not applicable[3]. However, for spherically symmetric potentials some results concerning the question whether unique self-adjoint extensions of H' exist have been achieved by a study of the radial Schrödinger equation, i.e., the extensions of the symmetric operators L_l' ($l = 0, 1, 2, \ldots$) defined in the space $L^2(0, \infty)$ by

$$L_l' \phi(r) = \left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + 2m\,V(r)\right) \phi(r) \tag{3.1}$$

have been investigated. The domain D' of L_l' is restricted to functions $\phi(r)$ that vanish in an individual neighborhood of the point zero and for sufficiently large r (compare the definition of the operator L_0' given in [14] p. 173).

For potentials which fulfill the condition

$$\int_0^{R_1} |V(r)|\, r\, dr < \infty, \quad 0 < R_1 < \infty \tag{3.2}$$

and are locally integrable in the interval $R_1 \leqq r < \infty$ the operator L_0' is

[3] The important point in KATO's proof that $V(\boldsymbol{r})$ is defined on the complete domain of H_0' does not hold if $V(\boldsymbol{r})$ is not locally square integrable.

not essentially self-adjoint (compare [6], [15]). This result is valid also for spherically symmetric potentials which are restricted by the conditions given in Section 3a) because (3.2) holds for these potentials. We would like to stress that there is no contradiction to KATO's proof. Since the functions of D' all vanish in a neighborhood of the point zero, the operator L_0' in comparison to the originally given operator H', has been contracted so strongly that it can no longer be extended in a unique manner. However, the unique extension of H' given by $\tilde{H}'$, can also be deduced from L_0' by choosing among all possible extensions of L_0' the one which fulfills the boundary condition that its proper and improper eigenfunctions are $0(r)$ as $r \to 0$. Using this boundary condition also in the case of singular potentials satisfying (3.2) and[4]

$$\int_{R_1}^{\infty} |V(r)|\, dr < \infty , \tag{3.3}$$

it is possible to select one extension to be physically meaningful (cf. [6], [7]). The operators L_l' are essentially self-adjoint for $l \neq 0$. In this way Møller operators can be defined uniquely, too.

Highly singular potentials with the restrictions:

$$V(r) = \frac{g^2}{r^{\alpha}} + V_0(r) \quad \text{for} \quad 0 < r \leqq R_1 \tag{3.4}$$

$$\int_{R_1}^{\infty} |V(r)|\, r\, dr < \infty \tag{3.5}$$

with $\alpha \geqq 2$ and

$$\int_{0}^{R_1} |V_0(r)|\, r\, dr < \infty \tag{3.6}$$

have been studied by MEETZ [15] (compare also [7]). For $\alpha > 2$ it was shown[5] that L_l' and thus H' are essentially self-adjoint[6] only in the case of $g^2 > 0$, i.e., if the highly singular part of the potential is repulsive (for $g^2 < 0$ the operators L_l' are not essentially self-adjoint and no extension can be selected as the physically meaningful one by the methods given in [6] and [15]).

We note that the assumption (3.5) can be replaced by (3.3) or by

$$\int_{R_1}^{\infty} V^2(r)\, dr < \infty \tag{3.7}$$

without any change of the results mentioned above. This follows if (3.3) is valid under consideration of [14], p. 203, Satz 4[7] and if (3.7) is valid with the help of [14], p. 305, Satz 7.

[4] Eq. (3.3), as well as (3.7), is valid for potentials $V(r)$ which fulfill (2.2) with $R \leqq R_1$.

[5] Concerning the peculiarities in the special case $\alpha = 2$ compare [15].

[6] If a contraction of H' is essentially self-adjoint the same result holds for H' itself (cf. [13]).

[7] The necessary condition of this theorem is not fulfilled.

If the potential $V(\boldsymbol{r})$ is of the form

$$V(\boldsymbol{r}) = V_1(r) + V_2(\boldsymbol{r}) \tag{3.8}$$

where $V_2(\boldsymbol{r})$ is a bounded, but not necessarily spherically symmetric function, it suffices to investigate the operator

$$H_1' = -\frac{1}{2m} \nabla^2 + V_1(r) \tag{3.9}$$

by the methods given above. Because $\tilde{H}_1'$ and $\tilde{H}_1' + V_2(\boldsymbol{r})$ have the same deficiency-index (cf. [14], p. 150), the statements concerning the unique self-adjoint extension are equivalent for the two operators.

Thus uniquely defined Møller operators exist, e.g., for potentials which fulfill the restrictions

$$V(\boldsymbol{r}) = \frac{g^2}{r^\alpha} + V_2(\boldsymbol{r}), \quad \text{for} \quad 0 < r < R_1 \tag{3.10}$$

and

$$|V(\boldsymbol{r})| \leqq \frac{\text{const}}{r^{1+\beta}}, \quad \text{for} \quad R_1 \leqq r < \infty \tag{3.11}$$

with

$$g^2 > 0, \ \alpha > 2, \ \beta > 0 \quad \text{and} \quad |V_2(\boldsymbol{r})| \leqq \text{const}.$$

Finally it should be noted that recently N. LIMIĆ proved the essential self-adjointness of H' for a more general class of (at the origin) highly singular repulsive potentials [16].

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