CLASSICAL ANALOGUES OF THE MOELLER OPERATORS, OF THE PEARSON EXAMPLE
AND OF THE BIRKWANN-KATO INVARIANCE PRINCIPLE

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ABSTRACT

To clarify the physical meaning of the Moeller (wave) operators and their properties, classical Moeller operators (and their modifications for long-range forces) are introduced in close analogy with the quantum operators, like strong limits with respect to the norm \( \| \psi \| = \int |\psi| \rho \mathrm{d} \rho \mathrm{d} q \). The conditions of their existence, unitarity and invariance are considered and shown to be essentially the same as in the quantum case. In particular, a simple exactly solvable example of a non-unitary classical scattering operator (analogue of the Pearson example) is constructed.

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1. - \textbf{INTRODUCTION}

In the time-dependent quantum scattering theory\textsuperscript{1}), an important role is played by the \textit{Moeller} (wave) operators\textsuperscript{*})

\[ W_\pm(H, H_0) = \lim_{\ell \to \pm \infty} e^{i\ell H - i\ell H_0} \]  \hspace{1cm} (1.1)

in terms of which the scattering operator $S$ and the $S$ matrix elements $S_{\alpha\beta}$ are defined as

\[ S = W^*_+ W_-, \hspace{1cm} S_{\alpha\beta} = W^*_+(H, H_\alpha) W_-(H, H_\beta). \]

These operators have a number of properties that we will briefly recall.

The operators $W_\pm$ exist, if the interaction potential $V = H - H_0$ decreases faster than $1/r$ or, being more rigorous, if

\[ \ell \to \pm \infty \quad \| V e^{-i\ell H_0} \psi \| \to 0, \]  \hspace{1cm} (1.2)

where $\ell \to \pm \infty$ and $\psi$ is an element of a set dense in the Hilbert space. In case of long-range forces ($V \sim r^{-\alpha}$, $0 < \alpha < 1$) the limits (1.1) do not exist, but one can define modified \textit{Moeller} operators\textsuperscript{2),3)}

\[ W^h_\pm(H, H_0) = \lim_{\ell \to \pm \infty} e^{i\ell H - i\ell H_0 + i\ell h(p, t)} \]  \hspace{1cm} (1.3)

where the function $h(p, t)$ is chosen in such a way that the limits become meaningful.

The operators $W_\pm$ are isometries

\[ W^*_\pm W_\pm = 1. \]  \hspace{1cm} (1.4)

\textsuperscript{*}) \textit{Notations:} slim is a strong limit, $H, H_0, H_\alpha$ are, respectively, a full, a free and a channel Hamiltonian. The stars mean Hermitian conjugation. Below, the classical quantities will often be denoted identically with their quantum counterparts; the distinction will be clear from the context.
This property implies the relations

\[ \| W_\pm \psi \| = \| \psi \|, \]

(1.5)

\[ W_\pm [A, B] W_\pm^* = [ W_\pm A W_\pm^*, W_\pm B W_\pm^* ], \]

(1.6)

and the unitarity of the scattering operator \( S \), if the ranges \( R_\pm \) of the operators \( W_\pm \) coincide. However, \( R_\pm \) may not coincide with \( \overline{R}_\pm \), and an example is known (the Pearson example [4]), where the evolution operators \( \exp(-i\mathcal{H}t) \), \( \exp(-i\mathcal{H}_0 t) \) are unitary, \( W_\pm \) exist, but \( R_\pm \neq \overline{R}_\pm \) and the operator \( S \) is non-unitary.

The operators \( W_\pm \) have an intertwining property

\[ \mathcal{H} W_\pm = W_\pm \mathcal{H}_0 \]

(1.7)

and an invariance property

\[ W_\pm ( F(\mathcal{H}), F(\mathcal{H}_0) ) = W_\pm ( \mathcal{H}, \mathcal{H}_0 ), \]

(1.8)

where \( F \) is an arbitrary function with a smooth positive derivative [for more details, see Refs. 5, 6]. Property (1.7) is called a Birmann-Kato invariance principle.

These properties proved to be very useful, especially in the relativistic quantum Hamiltonian theory [see Ref. 7] and references therein, where relations (1.7), (1.8) lie in the heart of the proof of the Poincaré invariance of the \( S \) matrix [8].

Unfortunately, the properties of Møller operators are usually derived in a rather formal way that helps little to understand their physical origin [*]. Besides, they are often believed to be of an essentially

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[*] Sometimes, the very idea of an elementary explanation is discouraged. So Kato writes [6], Ch. X, Ph. 7: "The theory centering around the wave operators is peculiar to an infinite dimensional Hilbert space, without having any analogue in the finite-dimensional spaces".
quantum nature. For instance, the necessity of modification (1.3) in case of long-range forces is usually related to a divergence of certain phase shifts, Pearson example involves tunnel effect, etc.

The aim of this paper is to show that the Moeller operators and their properties do have simple and remarkably close classical analogues. Partially, this was already demonstrated in Refs. 9)-12), where the canonical Moeller transformations were introduced as point-to-point limits

$$\omega_{\pm} = \lim_{t \rightarrow \pm} e^{-t} e^0,$$

(1.9)

where $e_t$ and $e^0_t$ denote a full and a free canonical evolution transformation, respectively. The transformations $\omega_{\pm}$ have a clear interpretation and a property analogous to (1.7), but their mathematical similarity with $\omega_{\pm}$ is not as straightforward as one would desire, since the point-to-point convergence is a more delicate process than a strong limit in the Hilbert space. The difference is that the limit (1.9) is sensitive to the existence of exceptional trajectories lying usually on the border-line between the larger classes of trajectories and corresponding to a subset of measure zero of initial values. The limit (1.1), ignoring all subsets of measure zero, is easier to study.

Therefore, in the present paper, we will go a step further and introduce classical Moeller operators in a way very similar to (1.1), namely, as strong limits

$$\omega_{\pm} = \lim_{t \rightarrow \pm} e_t^0 E^{-t} E^0_t,$$

(1.10)

where $E_t$, $E^0_t$ are classical evolution operators defined as linear operators on the space of classical states $P$. This definition makes the formulation and proof of statements rather elementary and has a subsidiary advantage of introducing into the classical case a considerable part of the widely known quantum language.

Below, after a schematic introduction into a canonical formalism, we will discuss the meaning of the classical Moeller transformations and operators, prove that quantum and classical $\omega_{\pm}$ have almost identical properties and, in particular, construct an exactly solvable classical analogue of the Pearson example.
2. - FORMALISM

We take as a base the usual canonical Hamiltonian formalism that we will briefly recall [for more details, see Refs. 13) and 14], and then recast it into an operator form.

For simplicity of notation, we will mostly limit ourselves to the case of one particle with one-dimensional coordinate \( q \) and momentum \( p \). Denote

\[
\mathcal{F} = \{q, p\}, \quad \mathcal{D} \varepsilon = dq \; dp, \quad \delta (\mathcal{F}) = \delta (q) \delta (p)
\]

and introduce the phase space \( \Phi = \mathbb{R} \times \mathbb{R} \) with points \( \varphi \) and a distance \( \| \varphi \| = |c| \; |p| \). \( \varphi_1 (\varphi) \) will denote a function of \( \varphi \) with values in \( \Phi \).

A state \( \rho (\varphi) \) is an analogue of the quantum density matrix \( \rho (x, y) = \psi (x) \star \psi^*(y) \) is a non-negative generalized function defining a measure \( \rho (\varphi) \) in \( \Phi \). A value \( \rho \) is interpreted as a probability density for the particle to occupy the point \( \varphi \). According to this interpretation, \( \| \rho \| = \int \rho d\varphi \) is a total probability for the particle to be somewhere in \( \Phi \), and a mean value of any dynamical variable \( g_\varphi \) is \( \overline{g} = \int g_\varphi d\varphi \). Clearly, for a physically meaningful state one should have \( \| \rho \| \leq 1 \).

In the particular case, when \( \rho = \delta (\Phi - \varphi) \), the particle occupies the position \( \Phi \). If \( \varphi_1 \) is an invertible function and \( |d\varphi_1 / d\varphi| = 1 \), then \( \rho = \delta (\Phi - \varphi_1 (\varphi)) \) means that the particle occupies the position \( \varphi_1^{-1} (\varphi) \). If the equation \( \delta (\Phi - \varphi_1 (\varphi)) = 0 \) has no real solutions, then \( \rho = 0 \). If this happens, it usually indicates an inconsistency of the problem.

Positions \( \Phi \) are immediately interpretable, so it is useful to introduce a position space \( \Phi \), each point of which is associated with a state \( \rho = \delta (\Phi - \varphi) \). Evidently, a transformation of \( \Phi : K_\varphi = K_\varphi (\varphi) \) where \( K_\varphi (\varphi) \) means a function with values in \( \Phi \), corresponds to an inverse transformation of \( \Phi : K_\varphi^{-1} = K_\varphi^{-1} (\varphi) \). In other respects, \( \Phi \) is very close to the phase space and could be as well called a co-phase space, or phase co-space.

Note that two subsequent transformations of \( \varphi, \Phi, \) and \( \rho \) are combined in different manners

\[
K_2 K_1 \varphi = K_2 (K_1 (\varphi)) = K_1 (K_2 (\varphi)),
\]

(\( \Phi \))
\[ K_2 K_1 \tilde{\varphi} = K_2 K_1^{-1}(\tilde{\varphi}) = K_2^{-1}(K_1^{-1}(\tilde{\varphi})), \]

\[ K_2 K_1 \varphi(\varphi) = K_2 \varphi(K_1(\varphi)) = \varphi(K_1(K_2(\varphi))). \]

The standard way to introduce the canonical formalism is to define the Poisson bracket (PB) of two functions \( A(\varphi), B(\varphi) \) as

\[
[A, B]_{PB} = \left[ \frac{\partial A}{\partial \varphi} \frac{\partial B}{\partial \varphi} - \frac{\partial A}{\partial \varphi'} \frac{\partial B}{\partial \varphi'} \right].
\]

and then to define a canonical transformation (CT) \( \varphi' = K \varphi \) as a one-to-one mapping \( \varphi \rightarrow \varphi' \) conserving PB in the sense

\[
K[A, B]_{PB} = [KA, KB]_{PB}.
\]

Here it is understood that

\[
KA(\varphi) = A(K(\varphi)).
\]

Any infinitesimal CT can be written as

\[
\varphi' = \varphi + \varepsilon [A, \varphi]_{PB} = \{q - \varepsilon A', p + \varepsilon A'\}.
\]

The formal integration of equations \( \varphi' = [A, \varphi]_{PB} \) can be written as an exponent of PB

\[
\varphi' = e^{\varepsilon \{A, \varphi\}_PB}.
\]

The CT of the state, \( \rho = e^{A \rho} \), can be considered as a linear transformation of \( \rho \), and \( e^A \rho \) can be interpreted as a linear operator. To make the formalism of CT closer to the quantum one, we reformulate it in an operator form. First we write PB as

\[\frac{\varepsilon}{\tilde{q}} = \frac{\varepsilon}{\tilde{p}/m}.\]
\[ [\tilde{A}, \tilde{B}]_{PB} = \tilde{A} \tilde{B}, \]

where \( \tilde{A} \) is a differential operator associated with the function \( A \) by

\[
\tilde{A} = A_p \partial_A - A_q \partial_A.
\]

It is easy to check that \( [\tilde{A}, \tilde{B}]_{PB} = C \) implies

\[ [\tilde{A}, \tilde{B}] = \tilde{C}, \]

so PBs of functions correspond to the commutators of associated operators. In terms of operators \( \tilde{A} \) an operator \( E_a \) is an ordinary exponent:

\[ E_a = \exp(a\tilde{A}). \]

Since \( \tilde{A} = [\tilde{A}, \tilde{B}] \), we have

\[ E_a \tilde{B} = E_a \tilde{B} E_{-a}. \]

Every CT can be written as a product of transformations like \( E_a \). So, an operator of a general CT should have the property

\[ K \tilde{B} = K \tilde{B} K^T, \]

(2.3)

where the transposed operator \( K^T \) is defined by the relation \( K^T K = I \) and coincides with \( K^{-1} \) in the case of invertible operators. As a consequence of (2.2), the relation (2.1) turns into a trivial identity

\[ K [\tilde{A}, \tilde{B}] K^T = [K \tilde{A} K^T, K \tilde{B} K^T]. \]

So, the property (2.3) in combination with (2.2) can be taken as a definition of a canonical operator (00).

The next step is to consider states \( \rho(\Phi) \) and their linear combinations \( f(\Phi) \) as elements of a state space \( \mathcal{L} \) defined as a linear space with the norm.
\[ \| f \| = \int |f| \, dy. \]

It implies that two functions \( \rho, \rho_1 \) with the property \( \| \rho - \rho_1 \| = 0 \) represent the same state. Physically, this reflects the fact that no measurement of finite accuracy can distinguish \( \rho \) from \( \rho_1 \), if the functions \( \rho(\phi) \) and \( \rho_1(\phi) \) differ only on a subset of \( \phi \) of measure zero.

For the elements of \( \mathcal{L} \), we will consider only one kind of convergence, namely, the strong convergence \( \lim \rho_t = \rho \) meaning that \( \lim \| \rho_t - \rho \| = 0 \). In case of operators, the expression \( \lim A_t = A \) on a set \( D \subset \mathcal{L} \) will mean that the limit \( \lim A_t \rho = A \rho \) is true for any \( \rho \in D \).

A subset \( D' \) will be called dense in \( D \) (\( D' \subseteq D \)) if for any \( \varepsilon > 0 \) and \( \rho \in D \) one can find \( \rho' \in D' \) such that \( \| \rho' - \rho \| < \varepsilon \). If two operators \( A, A' \) are bounded on \( D \) and coincide on \( D' \subseteq D \), they coincide on \( D \). Since the norm of CEs and of their strong limits is equal to 1, it is usually sufficient to consider them on convenient dense subsets \( D' \). In particular, if \( A_t \) is C0, if the limit \( \lim A_t = A \) is true on \( D' \), and if \( A \) can be defined on \( D \) as a bounded operator, then \( \lim A_t = A \) is true on \( D \).

3. SCATTERING TRANSFORMATIONS AND OPERATORS

To clarify the physical meaning of the Moeller and scattering operators, we consider first the corresponding CEs and the geometrical picture lying behind them.

Let \( H^0, \dot{H}, \) and \( e^{tH^0}, e^{t\dot{H}} \) be two Hamiltonians and two corresponding evolution CEs. The differences of \( e^t \) from \( e^{tH^0} \) which gradually accumulated during the interval \( t = t_2 - t_1 \) can be formally reduced to a single CE \( e^{t_1, t_2} \) inserted in the middle of the evolution \( e^t \) at the moment \( t_1 \).

\(^{+}\) I.e., \( \| A \| < \infty \), \( \| A/\rho \| < \infty \), where \( \| A \|_D = \sup_{D, \rho \neq 0} \| A \rho \| / \| \rho \| \).
\[ e^{ \tau_{t_2-t_1}} = e^{\tau_{t_2-t_1}} e^{\tau_{t_1-t}} e^{\tau_{t_1-t}}. \]

Evidently

\[ e^{\tau_{t_2-t}} = e^{\tau_{t_2-t}} e^{\tau_{t_2-t}} e^{\tau_{t_2-t}} e^{\tau_{t_2-t}}. \]

The limit of this transformation \( s = s', -\omega \) does not depend on \( \tau \) and is a scattering transformation for the Hamiltonian \( H \) with respect to the Hamiltonian \( H_0 \). It is convenient to put \( \tau = 0 \) from the beginning, to denote

\[ \psi_+ (H, H_0) = \psi_+ = e^{-\tau} e^{\tau} \]

and to represent \( s \) as a product \( s = w_t^{\tau_-} w_t^{\tau_+} \) of the transformations

\[ w_t^{\pm} = \text{lim}_{\tau \to \pm \infty} w_t^{\tau} \]

that are classical analogues of Moeller operators and will be referred to as Moeller GPs. These transformations and the limiting procedures involved can be interpreted as follows.

Suppose for simplicity that \( H_0 \) is a Hamiltonian of a free motion:

\[ H_0 = H_0 \left( p^2 \right), \quad d^2 H_0 / dp^2 > 0. \quad (3.1) \]

Let \( t_2 > 0 > t_1 \). Associate with the moment \( t = 0 \) in addition to \( \varphi_0 \), denoting the true position of a particle at \( t = 0 \), the two fictive positions \( \varphi t_1 \) and \( \varphi t_2 \) defined as follows. \( \varphi t_1 \) is the position that would be occupied by the particle if it moved freely from the moment \( t_1 \), till the moment \( t = 0 \). \( \varphi t_2 \) is the position from which the particle moving freely during the time \( t_2 \) would come to the position \( \varphi t_2 \), which is its true position at \( t = t_2 \). In Fig. 1, the corresponding trajectories are given in the position space and in Figs 2, 3, the same is shown in the \( \left( \vec{q}, t \right) \) and \( \left( \vec{p}, t \right) \) planes.
The limiting positions $\tilde{q} = \tilde{q}_-^\infty$ and $\tilde{q}^+ = \tilde{q}_+^\infty$ are analogues of the initial and final scattering states in quantum theory. The transformations $w_\pm$ relate them to $\tilde{q}_0$ and to each other

$$\tilde{q}_0 = w_+ \tilde{q}^+ = s \tilde{q}^-.$$ 

Geometrically, $\tilde{q}^\pm$ look on Figs. 2 and 3 as "aiming" values of the co-ordinates and momenta. Clearly, the existence of $\tilde{q}^\pm$, and hence of $w_\pm$, depends on the existence of the linear asymptotes of the curves on Figs. 2, 3. For the momentum variable, if the existence of $\tilde{p}^\pm$ simply means that $\tilde{H}$ coincide with $H_0$ at large $|t|$. Conditions for the existence of $\tilde{q}^\pm$ are more interesting. The expression

$$\Delta t = (\tilde{q}^+ - \tilde{q}^-) / v,$$

where $v = \partial H_0(\tilde{p}^\pm) / \partial \tilde{p}^\pm$ is an asymptotic speed, is a time advance (or, if $\Delta t < 0$, a time delay) due to the fact that the particle passed through the scattering region. In case of reflection, $\tilde{q} = \frac{1}{2}(\tilde{q}^+ + \tilde{q}^-)$ is the effective position where the turning point would be, if the particle were moving freely before and after the impact. So, if one knows that the centre of scatterer is located at $x_0$, the difference $\tilde{q} - x_0$ contains information about the time advance in this case as well.

In the three-dimensional case, the vectors $\tilde{q}^\pm$, $\tilde{p}^\pm$ give more information about the scatterer, then the usual geometrical treatment of a scattering in terms of an impact parameter and the angle of scattering. Actually, the components of vectors $\tilde{q}^\pm$ parallel to $\tilde{p}^\pm$, that are completely ignored in a geometrical approach, contain information about the time advance.

Classical time advance is an analogue of the phase-shift in the quantum case, or, being more precise, of $(\partial^2 / \partial p^2)(p/m)^{-1}$. The finiteness of $\Delta t$ is a necessary condition for the existence of scattering transformations. For potentials, decreasing with distance as $r^{-1}$ or slower, $\Delta t$ is infinite, so neither $\tilde{q}^\pm$ nor the transformations $w_\pm$, s exist in that case.

Let us now see how the Moeller transformations map the position space $\tilde{q}$ into itself. In the case of the free Hamiltonian (3.1) all the
particles except those having \( \mathbf{p} = 0 \) go to \( \mathbb{R} \) at \( |t| \rightarrow \infty \). Let the set of initial positions \( \mathcal{\Xi}' \) be \( \mathcal{\Xi} \) with the exclusion of the line \( \mathbf{p} = 0 \).

Then the set \( \mathcal{\Xi}' = \mathbf{w}_- \mathcal{\Xi}' \) will contain only the particles that came from \( \mathbb{R} \) and will not contain any "bound" particle whose trajectory does not leave a finite region \( \mathbb{F} \). The typical pattern of trajectories is drawn on Fig. 4. The potential is chosen to be a smooth potential well with two elevations at both edges. In this case the \( \mathcal{\Xi} \) plane is broken into five distinct regions. Regions \( \mathbb{I}_1 \) and \( \mathbb{I}_2 \) contain trajectories of particles that pass through. Regions \( \mathbb{I}_1 \) and \( \mathbb{I}_2 \) contain trajectories of reflected particles, region \( \mathbb{I} \) of "bound" particles.

Points \( X_1, X_2 \) are exceptional. Particles cannot pass through these points since to reach them takes an infinite time. So, if the particles were at the beginning evenly distributed on the border-line of \( \mathbb{I}_1 \), they accumulate after some time above the point \( X_1 \), while the part of the border-line between \( \mathbb{I}_1 \) and \( \mathbb{I}_2 \) adjacent to \( X_1 \) becomes empty of particles, since no fresh supply goes through the point \( X_1 \).

Looking at Fig. 4, one can see that the set \( \mathcal{\Xi} ' \) can include neither \( \mathbb{F} \) with its border-line, nor the border-lines between \( \mathbb{I}_1 \) and \( \mathbb{I}_2 \) and between \( \mathbb{I}_2 \) and \( \mathbb{I}_1 \) (Fig. 5), since it is impossible to get there if the starting point is far away from the origin. \( \mathcal{\Xi} \) has a similar shape (Fig. 6).

The inverse transformation \( w_1^{-1} \) maps \( \mathcal{\Xi} \) into \( \mathcal{\Xi}' \) and is not defined on \( \mathbb{F} \) and some border-lines. It is interesting to see how the transformation \( w_1^{-1} \), being the limit of the transformation \( w_t \), which is defined everywhere, happens to be undefined on \( \mathbb{F} \).

The region \( \mathbb{F}_t \) obtained from \( \mathbb{F} \) by the mapping \( \mathbb{F}_t = w_t^{-1} \mathbb{F} \) at some finite \( t < 0 \), is shown on Fig. 7. Since \( \mathbf{v} = \mathbf{0} \) and the free evolution transformation \( \mathbf{e}_t^0 \) shifts the points \( \mathbf{v} \) proportionally to their velocities \( \mathbf{v}/m \), it follows that at \( t < 0 \) the region \( \mathbb{F}_t \) becomes more and more skew and stretched along the line \( \mathbf{p} = 0 \). At \( t \rightarrow \infty \) \( \mathbb{F}_t \) goes into the line \( \mathbf{p} = 0 \), but it is not a point-to-point mapping because the points \( \mathbf{p}_t = w_t^{-1} \mathbf{p}, \mathbf{p} \in \mathbb{F} \), do not tend to any definite points on the line \( \mathbf{p} = 0 \). So \( w_t^{-1} \) cannot be defined on \( \mathbb{F} \) and \( w_- \) cannot be defined on the line \( \mathbf{p} = 0 \). \( w_+ \) has similar properties.
In case of more dimensions and particles the details of the mappings $w_t$ become very complicated. However, from the operator viewpoint the fine structure of the regions $\delta^+, \delta^-$ becomes unimportant and it is easy to establish the existence of the limits

$$W_t = \lim_{t \to \pm \infty} \mathcal{E}_t^o \mathcal{E}_t^c,$$

where $\mathcal{E}_t^o \rho(q) = \rho(c_t^2 q)$, using almost the same reasoning as in the quantum case.

**Theorem 1** Let $H_0$ have the properties (3.1). If at fixed $p$, large $|q|$, and some $\epsilon > 0$ the potential $V = H - H_0$ satisfies the inequalities

$$|\nabla q V| < |q|^{-\epsilon - 1/2} C(p), \quad |\nabla q V| < |q|^{-\epsilon - 1/2} C(p),$$

then the limits $W_t$ exist.

**Proof**

Let $S \subseteq L$ be a subset of infinitely differentiable functions of finite support. On $S$, $E_t = e^{itH}$. Consider (on $S$) the identity

$$E_t^c E_t^o = 1 + \int_0^t E_{-\tau} \widetilde{V} E_t^o d\tau.$$

The convergence (at $t \to \pm \infty$) of the left-hand side is equivalent to the convergence of an integral in the right-hand side. The strong convergence of the integral implies that

$$J^\pm_t = \| \int_t^\infty E_{-\tau} \widetilde{V} E_t^o \rho d\tau \| < \infty$$

for any $\rho$ from a subset $S' \subseteq S$. Since $\| E_t \| = 1$,

$$J^\pm_t \leq \int_t^\infty \| \widetilde{V} \rho_t \| dt,$$

where

$$\rho_t = E_t \rho = \rho(c_t^2 q - \nabla q t, p), \quad \nabla = \nabla_p H.$$
Let $S'$ be a subset of functions $\varphi$ equal to zero in a small neighbourhood $|v| < \varepsilon_1(\varphi)$ of the line $v = 0$. Denote

\[ \vec{v}_q = \partial_\varphi V, \quad \vec{p}_q = \partial_\varphi \varphi, \quad c_\varphi = \| \vec{p}_q \|, \]

\[ \vec{p}_q, t = \vec{p}_q (q - \nu t, \vec{p}), \quad \vec{V}_p = \partial_\nu V, \ldots \]

\[ c_\varphi = \| A \vec{p}_q \|, \quad (A)_{ij} = \partial_\varphi \varphi_i / \partial_\varphi \varphi_j. \]

An explicit expression for $\tilde{V}_p \tilde{t}$ in terms of these derivatives leads to the inequality

\[ \| \tilde{V}_p \tilde{t} \| \leq \| \vec{V}_p \cdot \vec{p}_q, \tilde{t} \| + \| \vec{V}_q \cdot \vec{p}_p, \tilde{t} \| + \| \vec{t} \tilde{V}_q \cdot A \vec{p}_q, \tilde{t} \|. \]

The estimation of the right-hand side terms at large $|t|$ using the equality

\[ \| a E^0 \delta \| = \| (E^0 - a) \delta \| \]

finiteness of $\rho$ and conditions (3.3) gives

\[ \| \vec{V}_p \cdot \vec{p}_q, \tilde{t} \| < c_\varphi C_\rho (P_1^2) |t \epsilon_1, (\rho)|^{-1-\varepsilon}, \]

\[ \| \vec{V}_q \cdot \vec{p}_p, \tilde{t} \| < c_\rho C (P_2^2) |t \epsilon_1, (\rho)|^{-2-\varepsilon}, \]

\[ \| \vec{t} \tilde{V}_q \cdot A \vec{p}_q, \tilde{t} \| < |t| c_\varphi C (P_3^2) |t \epsilon_1, (\rho)|^{-2-\varepsilon}, \]

where $P_1$, $P_2$, $P_3$ are some points in the support of $\rho(q, \vec{p})$. So $\| \tilde{V}_p \| \sim \sim |t|^{-1-\varepsilon}$ which entails the existence of $\tilde{\varepsilon}_1^2$ and $W_t$ on $S'$. Since $S'$

is dense in $S$ and $L$, and $W_t$ are bounded, the limits (3.2) exist on $L$.

We shall call isometries the operators $A$ on $L$ with the property

\[ \| A \varphi \| = \| \varphi \| \] and those with the property $A^* = A^{-1}$, unitary operators. With this terminology, the operators $W_t = E_{-t} R_t^2$ are unitary and their strong limits $\hat{W}_t$ if they exist, are isometries. $\hat{W}_t$ map $L$ into subspaces $R_t$. 

of states $\rho(\varphi)$ equal to zero inside the region $\mathbb{R}_+ = \phi_+ \setminus \phi_-$ ($\phi_+$ are obtained from $\phi_+$ by a trivial mapping $\varphi \rightarrow \varphi$). The transposed operators $W_\pm$ are also defined on all $\phi_+$ but transform the states $\rho$ from the subspaces $\mathbb{S}_\pm = \phi_\pm$ into zero.

If $R_+ = R_-$, then the scattering operator $S = W_+^\dagger W_-$ is unitary. In the case presented in Figs. 5 and 6 the inner parts of the regions $\mathbb{R}_4$ coincide, so $R_+ = R_-$ and $\mathbb{S}_+ = \mathbb{S}_-$ and $S$ is unitary. The example when $R_+ \not= R_-$ and $S$ is not unitary is discussed in the next section.

4. - ANALOGUE OF THE PEARSON EXAMPLE

Here we return again to the one-dimensional case. In Fig. 4, there are two points $X_1$, $X_2$ through which the particles cannot pass and nearby which they accumulate. The accumulation happens if the potential $V(q)$ has a smooth summit and the particle has the initial energy $E$ exactly equal to the height of the summit (Fig. 8). Then the particle speed $v(q) = \frac{\partial}{\partial p} H(p, q)|_{p=P(q)}$, where $p(q)$ is determined by the equation $E = H(p, q)$, is proportional to $q_0 - q$ near the position of summit $q_0$, and the integral

$$T = \int_{q_0}^{q} \frac{dq}{v(q)}$$

that gives the time spent on the interval from $q$ to $q_0$, diverges. That means that the point $q_0$ is never reached.

A potential $V(q)$ may have only a countable number of smooth summits, each corresponding to an accumulation point in the position space and to a trajectory starting from that point and excluded from the regions $\phi_\pm$. These points and trajectories form evidently a set of measure zero, so the ranges $R_\pm$ of the operators $W_\pm$ are not affected by the exclusion of this set from the regions $\phi_\pm$, and the equality $R_+ = R_-$ and the unitarity of $S$ remain true for any $V(q)$.

But, if a potential is velocity-dependent, $V = V(q, p)$, then it is possible, using the dependence on $p$, to adjust the height of its summit to the energy of the particle in such a way that the condition near the summit $v \sim q - q_0$ will be satisfied for a continuous range of initial energies. So the particles with the energies in this range will neither pass through, nor be reflected.
In the example

\[ H_0 = \frac{p^2}{2}, \quad V = -\frac{p^2}{2\cosh^2 q}, \quad H = \frac{p^2}{2} \frac{\sinh^2 q}{\cosh^2 q} \]

the potential has a smooth summit at \( q_0 = 0 \) and the condition that \( v \sim q \) near \( q = 0 \) is fulfilled for any initial energy \( E > 0 \). Indeed, the equation \( E = H(q, p(q)) \) near \( q = 0 \) gives

\[ |p| = |\cosh q| \frac{\sqrt{2E}}{|q|} \approx \frac{1}{|q|}, \quad |v(q)| = |p \cdot \frac{q^2}{2} q| = |\frac{q}{2} \sqrt{2E}| \sim |q|. \]

So, all the particles coming from \( \pm \infty \) neither pass through the point \( q = 0 \), nor are reflected, and are thus accumulated near the origin.

The exact expression for the evolution \( \beta \) in the \( \overline{\beta} \) space is

\[ E_{\pm} \overline{\beta} = \left\{ \tilde{q}_{\pm}, \tilde{p}_{\pm} \right\} = \left\{ \text{arsh} \left( e^{\mp t} \frac{q}{2} \right), e^{\pm \frac{t}{2} \left( e^{\pm t} \frac{q}{2} \right)^2} \right\}, \]

where \( \kappa = \frac{\pi}{2} \frac{\tilde{q}}{2}, \kappa^2 = 2H \). The trajectories can be classified into four different families each occupying one quarter of the \( \overline{\beta} \) plane (Fig. 9).

The Moller KT can be found explicitly and are

\[ \omega_{\pm} \overline{\beta} = \left\{ \pm \text{sign} \tilde{p}, \text{arsh} \left( \frac{1}{2} \left( e^{\pm \frac{\tilde{q}}{2} \text{sign} \tilde{p}} \right) \right), \overline{p} \left( 1 + q e^{\pm 2 \frac{\tilde{q}}{2} \text{sign} \tilde{p}} \right)^{1/2} \right\}. \]

The regions \( \frac{1}{2} \overline{\beta} = w_{\pm} \overline{\beta} \) occupy each two quarters of the \( \overline{\beta} \) plane, as shown by Fig. 10, and do not intersect.

Figure 11 shows how the transformation \( w_{\pm} = E_{\pm} E_0 \) that maps all \( \overline{\beta} \) upon all \( \overline{\beta} \), in the limit \( t \to \pm \infty \) concentrates all the transformed points \( w_{\pm} \overline{\beta} \) in a part of \( \overline{\beta} \). On this figure, the trajectories corresponding to two successive transformations \( E_{\pm} \) and \( E_{-\pm} \), entering \( w_{\pm} \), are drawn for reasonably large \( t \to \infty \). It can be seen that, no matter where they start, they stop in \( \overline{\beta} \), if \( t \) is large enough.
The ranges \( R_\pm \) of the operators \( W_\pm \) include, evidently, only the states \( \rho \) that have support only in the corresponding regions \( \phi_\pm \). Thus, \( W_\pm^T R_\pm = 0 \), \( W_\pm^T R_\mp = 0 \), and the scattering operator vanishes \( S = W_+^T W_- = 0 \).

It is instructive to see what happens if the coupling constant that can be introduced into \( H \) as a multiplier before \( V \) is made a little smaller or greater than one.

In case of \( H = H_0 + (1 - \epsilon)V \), the speed at the point \( \bar{q} = 0 \) is always non-zero, so every particle approaching this point just passes through it in a finite time, everything is completely normal and \( S \) is unitary.

In case of \( H = H_0 + (1 + \epsilon)V \), there are in \( \phi \) two points \( \bar{q}_\pm \equiv \sqrt{\epsilon} \), where the speed is zero. The particles that approach these points reach them in a finite time, since their speed in the vicinity of these points is proportional to \( \sqrt{|\bar{q}_\pm|} \), as is usual for turning points. But the points \( \bar{q}_\pm \) are not regular turning points because when the particle reaches \( \bar{q}_\pm \) the momentum \( \vec{p} \) becomes infinite and the particle becomes lost from the position space \( \phi \) when \( |\vec{p}| = \infty \) the state vanishes: \( \rho = 0 \) (\( \vec{p} = \bar{q}_\pm \)). Figure 12 shows that there is no possibility to continue the trajectories through the points \( \bar{q}_\pm \). Consequently, the evolution operator \( E_t \) is defined on a region \( \phi_t \) that shrinks with \( t \), and the corresponding evolution operator \( E_t \) in \( \mathcal{L} \) is not unitary.

We see that the discussed example is unstable to the infinitesimal variation of the coupling constant. The case when the operator \( E_t \) is unitary but \( R_\pm \neq R_\mp \) lies on the border-line between the ordinary case and the case of non-unitary \( E_t \). The quantum example of Pearson has exactly the same instability.

Comparing quantum and classical cases, it should be remembered that the velocity dependent classical potentials correspond to non-local interactions in the quantum formalism. The Pearson example is local, but it is easy to construct many non-local variations of this example that are based upon the same principle as the given classical example. In many of them the wave packet approaching the point \( q_0 \) will be partly reflecting, partly compressing near this point.
5. **LONG-RANGE FORCES**

In Refs. (10)-12), the classical scattering by long-range forces was considered in the frame of the point-to-point convergence. Here, much simpler treatment in terms of strong limits in \( L \) will be given. But first we shall discuss the geometrical and physical pictures that lie behind the modified definition of the Moeller operators in the case of slowly decreasing potentials.

If the interaction is short-range, the trajectory \( \Phi_t \) in the \( (t, \Phi) \) space has (straight) asymptotes passing through the hyperplane \( t = 0 \) at points \( \Phi_\infty \). The Moeller CTs relating \( \Phi_t \) with \( \Phi_0 \) make sense only if the points \( \Phi_\infty \) exist. However, if the interaction potential decreases with distance as \( r^{-1} \) or slower, the line \( \{t, \Phi_t\} \) has no asymptotes in the \( (t, \Phi) \) space. Physically that means that the advance (or delay) time of a scattered particle is infinite.

To avoid this difficulty, the advance time has to be either ignored, or redefined. The most evident way to ignore the time advance is to project trajectories upon the \( \Phi \) space and consider only the static, geometrical picture of scattering. The projected trajectories have asymptotes for a large class of long-range potentials (see conditions of the theorem below). The intersection of these asymptotes with the hyperplane \( \Phi_z = 0 \) gives two \((3+2)\) dimensional points \( \Phi_{T_\pm} = (\Phi_{\pm}, \Phi_z) \). These points (together with the knowledge of \( H_0 \)) define the asymptotes completely and thus contain all static information about the scattering. In particular, the relation between \( \Phi_{T-} \) and \( \Phi_{T+} \) specifies the effective position of the scattering centre.

Let \( \Phi'_0 \) be a point of a trajectory belonging to the hyperplane \( \Phi_z = 0 \). Then the six-dimensional points \( \Phi'_T = (\Phi_{T'}, 0) \) and \( \Phi'_0 \) can be related by some transformations having roughly the same meaning as the Moeller ones. The choice of the hyperplane \( \Phi_z = 0 \) is clearly arbitrary, and any other points \( \Phi_\pm \) and \( \Phi_0 \) belonging to the asymptotes and to the trajectory give the same information about the scattering.

This geometrical picture can be related with a canonical formalism as follows. The existence of the asymptotes in the \( \Phi \) space implies that, when \( t \to \infty \) or \( t \to -\infty \), a point moving along the asymptotes with a
certain variable velocity may approach infinitely close to the particle flying along the true trajectory. The straight non-uniform motion of a point corresponds to CT or CO of the form

$$E^F(t) = \exp \left[ t \tilde{H}_0 + \tilde{F}(\vec{p}, t) \right].$$

So, if the function \( F \) regulating the velocity of the point on the asymptote makes the velocity close enough to the velocity on a nearby piece of a trajectory, the limits

$$W^F_\pm = \lim_{t \to \pm \infty} E_{-t} E^F(t)$$

should exist and may be used as a definition of modified Moeller operators for the case of long-range forces.

Evidently, the replacement of \( F \) by \( F' = F + f(\vec{p}, t) \), where \( f \) is an arbitrary function having limits at \( t \to \pm \infty \), does not influence the existence of limits (5.1) and is equivalent to a different choice of points \( \vec{q}_1, \vec{q}_0 \) for a given point \( \vec{q}_m \). A certain \( F' \) will lead to CO \( W^F_\pm \) relating the points \( \vec{q}_1, \vec{q}_0 \) lying in the hyperplane \( \vec{q}_2 = 0 \), but it is usually difficult to find that specific \( F' \). So, the modified Moeller operators are commonly defined with the help of the simplest function \( F \) assuring their existence.

Now we go to the formal analysis of the existence of the limits (5.1). Suppose that \( H_0 = H_0(\vec{p}) \) and denote

$$F_\xi = \partial_\xi F, \quad F_\vec{p} = \partial_\vec{p} F, \quad F_{\xi \vec{p}} = \partial_{\xi \vec{p}} F, \quad F_\vec{p} \vec{p} = \Delta_\vec{p} F,$$

$$V_\xi = \partial_\xi V, \quad V_\vec{p} = \partial_\vec{p} V, \quad \vec{p}_q = \partial_\vec{p} \vec{q}, \quad \vec{p}_\vec{p} = \partial_\vec{p} \vec{p},$$

$$\vec{v} = \partial_\vec{p} H_0, \quad \gamma = \Delta_\vec{p} H_0, \quad q = |\vec{q}|,$$
\[ \vec{q}_{t} = \vec{q} + t \vec{v} + \vec{F}_{p} = \exp (\pm t \vec{H} \pm \vec{F}) \vec{q}, \]

\[ A^{t} = A (\vec{q}_{t}, \vec{p}, t), \]

\[ \vec{g} (\vec{q}, \vec{p}, t) = -\vec{F}_{t_{p}} + (t \vec{\gamma} + F_{pp}) \vec{V}_{q}^{t} + \vec{V}_{p}^{t}. \]

**Theorem 2** Let at large \( q \) and for some \( \omega > 0 \)

\[ |V| < C (\vec{p}) q^{-\omega} \]

and at \( \vec{p} \neq 0 \)

\[ J = \int_{t}^{\infty} \text{sign} t |\vec{g} (\vec{q}, \vec{p}, t)| dt < \infty. \]  

(5.2)

Then \( N_{t} \) exist.

**Proof**

Proceeding as in the proof of Theorem 1, we will suppose that \( \rho \in S' \) and show that the function \( N_{t} = \| \partial_{t} N_{t} \| \), where \( N_{t} = \epsilon_{-t} \exp (t), \)

decreases with \( |t| \) sufficiently fast so that the integral

\[ \int_{t} N_{t} dt \] converges. Since

\[ N_{t} = \| (-\vec{V}_{q} \cdot \vec{\partial}_{p} + \vec{V}_{p} \cdot \vec{\partial}_{q} - \vec{F}_{t_{p}} \cdot \vec{\partial}_{q}) \vec{\rho}^{t} \| = \]

\[ = \| -\vec{V}_{q} \cdot [-\vec{\gamma} (t \vec{\gamma} + F_{pp}) \vec{\rho}^{t} + \vec{\rho}^{t} + (\vec{V}_{p} - \vec{F}_{t_{p}}) \cdot \vec{\rho}^{t} \| \]

and

\[ \| A \vec{\rho}^{t} \| = \| A^{t} \vec{\rho} \|, \]

we have

\[ N_{t} = \| \left[ (t \vec{\gamma} + F_{pp}) \vec{V}_{q}^{t} + \vec{V}_{p}^{t} - \vec{F}_{t_{p}} \right] \vec{\rho}^{t} - \vec{V}_{q}^{t} \cdot \vec{\rho}^{t} \| \].
The function $\Psi_q^{t-}$ decreases faster than $t^{-1-\alpha}$. So the existence of $M$ depends only on the asymptotic behaviour of the function in the square brackets which at large $|t|$ and $\phi \in \text{supp } \rho$ is the same as the behaviour of $g(0, p, t)$. Thus, the existence of $J$ entails the existence of $M$. The same argument as in Theorem 1 shows that $\Psi_{q}^{F}$ exists as well.

The simplest way to find the function $F$ or the operator $F = \int_{p}^{\infty} \delta_{q}^{n} \, \text{sign } t \left[ -g^{n} + (t \gamma + F_{p}^{n-1}) \nabla_{q} (q^{n-1}, p, \gamma_{n-1}, \gamma_{n}) \right]$, (5.3)

where $q_{\gamma}^{n-1} = tV + \int_{t}^{\infty} g_{\gamma}^{n-1} \, dt$ and $g_{\gamma}^{n}(\alpha, t)$ are arbitrary functions satisfying the condition $\int_{t}^{\infty} g_{\gamma}^{n} \, dt < \infty$ and chosen from considerations of convenience.

In case

$H_{0} = \frac{p_{\gamma}^{2}}{2m}$, \quad $V = q^{-\alpha}$, \quad $F^{\gamma} = 0$ \quad $\gamma' = 0$, \quad (5.3) gives

$\Psi^{\gamma} = \begin{cases} \int_{t}^{\infty} & \text{at } \alpha = 1, \\ |t|^{-\alpha} & \text{at } \alpha < 1. \end{cases}$

$F^{\gamma}(\alpha)$ satisfies (5.2) at $\alpha > \frac{1}{2}$, so at $\alpha > \frac{1}{2}$ one iteration is sufficient. At $\alpha \leq \frac{1}{2}$, higher iterations of (5.3) are needed.

Comparing with the quantum case 2), 3), one can see that the results are essentially the same.
6. - INVARIANCE PRINCIPLE

Equality (1.8) says that in the quantum case the Hamiltonians \( H \) and \( F(H) \), where \( F = f > 0 \), lead to the same scattering. The classical analogue of this statement is almost trivial. Compare evolution transformations

\[
E_t = e^{t \widehat{H}}, \quad E_t' = e^{t \widehat{F(H)}} = e^{t f(H) \widehat{H}}.
\]

Since \( H \) is an integral of motion both for \( E_t \) and \( E'_t \), the trajectories \( \sigma_t = E_t \sigma \) and \( \sigma'_t = E'_t \sigma \) in the \((t, \sigma)\) space differ only by an energy-dependent scaling factor \( f = f(H(\sigma)) \) at the variable \( t \). If \( \sigma_t \) has asymptotes, \( \sigma'_t \) has them as well, and the points \( \sigma_t, \sigma'_t \) where these trajectories and their asymptotes pass through the hyperplane \( t = 0 \) are evidently the same in both cases. So scattering is physically the same in both cases and one can expect that

\[
W_+ = W_+ \quad \equiv \quad W_+ (F(H), F(H_0)). \tag{6.1}
\]

However, the formal proof of (6.1) needs some caution, since the limits \( W_+ \), \( W'_+ \) are more delicate than the geometrical picture discussed above and may fail to exist even if the trajectories \( \sigma_t, \sigma'_t \) do have asymptotes in \((t, \sigma)\) space.

One source of trouble is trivial and can be easily eliminated. In classical theory, potentials are usually defined up to an inessential constant \( C \). Since \( H_0 + C = \tilde{H}_0 \), the expression \( e^{-t \tilde{H}} e^{t \tilde{H}_0} \) is not sensitive to the replacement of \( H_0 \) by \( H_0 + C \). Unfortunately, the expressions \( f(H_0) \) and \( e^{-t \tilde{F}(H)} e^{t \tilde{F}(H_0)} \) are sensitive to such a shift of \( H_0 \). So, (6.1) may make sense only if the "inessential" constant \( C \) is properly fixed. Usually, it is tacitly assumed that at infinity \( H \) coincides with \( H_0 \) and \( C = 0 \). In a more general case, if the potential depends on the sign of \( \sigma \), it may happen that at \( t \to \infty \) and at \( t \to -\infty \) different constants \( C_\pm \) should be taken. Hamiltonians \( H_\pm = H_0 + C_\pm \) can be fixed by the requirement \( H \tilde{W}_\pm = \tilde{W} \tilde{H}_\pm \), or by the equivalent relation

\[
*) \text{In a quantum case this corresponds to interactions with a rather exotic long-range non-locality.}
\]
\[
\lim_{t \to \pm \infty} (H - H_{\pm}) e^{t \tilde{H}_0} = 0.
\]

Then (6.1) can be replaced by

\[
W_+ = W_+ \equiv W_+ \left( F(H), F(H_{\pm}) \right).
\]

(6.2)

Another source of trouble is that the difference \( V_+ = F(H) - F(H_{\pm}) \) playing the role of a potential strongly depends on momentum. For such potentials, two successive transformations \( \exp[-t F(H)] \) and \( \exp[t F(H_{\pm})] \) that enter \( W_+ \), correspond to trajectories that are not tangent at the point \( \tilde{\varphi}_t = \exp[t F(H_{\pm})] \), where they meet. If the angle between the trajectories at that point decreases as \( t^{-1} \), the limits \( W_+ \) may exist, but the points \( \tilde{\varphi}_t = W_+ \tilde{\varphi} \) may lie outside the asymptotes to the trajectory \( \tilde{\varphi}_t = \exp[t F(H)] \). To exclude such cases we will make an assumption that \( W_+ \) decreases sufficiently fast at large distances.

**Theorem 3** Let the limits

\[
\lim_{t \to \pm \infty} t \left[ \frac{d}{dt} \left( H \left( e^{-\frac{t}{\gamma}} \tilde{H}_0 \right) \right) - \frac{d}{dt} \left( H_{\pm} \right) \right] = 0 \quad (6.3)
\]

be true for almost all \( \varphi \in \Phi \). Then, if \( W_+ \) exist, \( W_+ \) exist as well and the equality (6.2) holds.

**Proof**

Denote \( \rho_t = e^{t \tilde{H}_0} \rho \). Then

\[
W_+ \rho = \lim_{t \to \infty} e^{-t} \tilde{F}(H) \rho = \lim_{t \to \infty} e^{-t} F(H) \rho + \lim_{t \to \infty} e^{-t} F(H_{\pm}) \Delta \rho,
\]

where

\[
\Delta \rho = \rho \int_t \frac{df(H_{\pm})}{f(H)} - \rho \int_t \frac{df(H)}{f(H)}
\]

and \( \rho \int_t df(H) \) means \( \rho \left|_{r = t} \right. df(H) \).
The existence of \( W_+ \) in the sense of strong limits implies that almost everywhere
\[
\lim_{\tau \to \infty} e^{\tau \tilde{\mathcal{H}}} \int_{\tau}^\infty \rho \, d\tau = W_+ \rho,
\]
and vice versa. Since almost everywhere
\[
\lim_{t \to \infty} e^{-t \tilde{\mathcal{F}}(H)} \int_{0}^{t} \mathcal{F}(H) \, dt = \left( \lim_{\tau \to \infty} e^{\tau \tilde{\mathcal{H}}} \right) = W_+ \rho,
\]
once has
\[
\lim_{t \to \infty} e^{-t \tilde{\mathcal{F}}(H)} \int_{0}^{t} \mathcal{F}(H) \, dt = W_+ \rho.
\]
Consider now \( \Delta \rho \). Denoting \( f_+ = \mathcal{F}(H_+(\chi)) \) and substituting \( \varphi = \chi - t f_+ \), we obtain \( H_+(\varphi) = H_+(\chi) \), \( \rho(\varphi) = \rho_-(f_+ + \varphi) \) and
\[
\Delta \rho = \mathcal{F}(\chi) - \mathcal{F} \left[ f_+ (H_+(\chi - t f_+)) - \mathcal{F} \right] (\chi).
\]
Due to (6.3) \( \Delta \rho \) tends almost everywhere to zero as \( t \to \infty \), and therefore \( \lim \Delta \rho = 0, \lim e^{-t \tilde{\mathcal{F}}(H)} \Delta \rho = 0 \). So, \( W_+ \rho = W_+ \varphi \). The limit at \( t = \infty \) is similar to the limit at \( t = \infty \).

The potentials that may violate (6.3) are long-range ones. So, for all ordinary potentials (6.2) is true and the Birman-Kato invariance principle is valid in classical mechanics as well.

ACKNOWLEDGEMENTS

The author is grateful to W. Chirring and W. U. Amrein for helpful discussions.
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