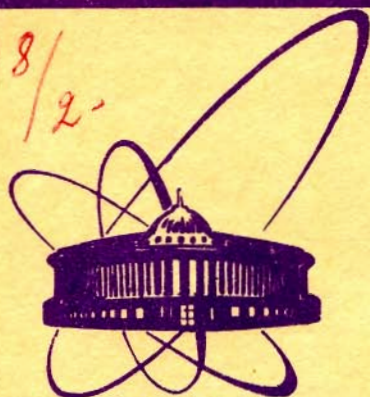


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Квантомеханические псевдогамильтонианы

В рамках теории минимальных унитарных расширений полугрупп сжатий обсуждается вопрос о вложении феноменологического описания квантовомеханической системы посредством несамосопряженного гамильтониана H_p в стандартный формализм квантовой теории. Показано, что эта проблема может быть решена, если принять во внимание приближенный характер феноменологического описания. Смысл этого приближения и понятие псевдогамильтониана строго определены на основе требований применимости теории унитарных расширений и физических принципов. Для абстрактного замкнутого оператора H_p с плотной областью определения приводится необходимое и достаточное условие для того, чтобы он являлся псевдогамильтонианом. Найдены разные достаточные условия для физически интересного случая операторов Шредингера на $L^2(\mathbb{R}^n)$ с комплекснозначным потенциалом.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Сообщение Объединенного института ядерных исследований, Дубна 1979

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Quantum-Mechanical Pseudo-Hamiltonians

The question of incorporating the phenomenological description of a quantum-mechanical system via non-self-adjoint Hamiltonian H_p into the standard formalism of the quantum theory is discussed using the theory of minimal unitary dilations of contractive semigroups. It is shown that this problem can be satisfactorily solved if the approximative character of the phenomenological description is taken into account. The notions of approximative description and of pseudo-Hamiltonian H_p are strictly defined, the definitions being motivated by the requirements of physical adequacy and applicability of the unitary dilations theory. A criterion for an abstract closed densely defined operator H_p to be pseudo-Hamiltonian is formulated. Various sufficient conditions are then obtained for the physically interesting case of Schrödinger operators on $L^2(\mathbb{R}^n)$ with complex potentials.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. Introduction

Quantum-mechanical systems are frequently described phenomenologically using so-called pseudo-Hamiltonians, i.e., non-self-adjoint operators on a state Hilbert space \mathcal{H}_p of the considered system. In most cases one takes $\mathcal{H}_p = L^2(\mathbb{R}^n)$ and $H_p = -\Delta + u$, where u is a complex function (potential). A well-known example of application of pseudo-Hamiltonians is the optical model of the atomic nucleus ^{/1/}, another example represents calculations of the NN bound states with the help of Bryan-Phillips potential ^{/2/} or other model calculations using complex potentials ^{/3/}.

Usually one assumes that the spectrum of H_p reproduces with some accuracy the energy spectrum of the system \mathcal{Y}_p under consideration and that the pure states of \mathcal{Y}_p evolve in time according to the Schrödinger equation

$$i \frac{d\psi}{dt} = H_p \psi .$$

Now, the fact that H_p is not self-adjoint violates the fundamental postulate of the quantum theory concerning the time evolution: the norm of ψ is not generally conserved. Only the case when $\|\psi\|$ does not increase occurs in physical applications; this is expressed mathematically by the dissipativity condition

$$\text{Im}(\psi, H_p \psi) \leq 0 \quad \text{for all } \psi \in D(H_p) . \quad (1)$$

We shall hereafter adopt the common assumption that H_p does not depend on time. Then the time evolution of the system \mathcal{Y}_p is determined by the set $\{V(t) : t \geq 0\} \subset \mathcal{L}(\mathcal{H}_p)$ where

$$V(t) = \exp(-iH_p t) . \quad (2)$$

This further implies that $\{V(t)\}$ has the semigroup property

$$V(t+t') = V(t)V(t') \quad \text{for all } t, t' \geq 0 .$$

Remark: The expression on the right-hand-side of eq.(2) is formal unless H_p is bounded; however, under some additional assumptions specified in sec.2 this expression makes sense also for unbounded H_p , the semigroup property being preserved.

The phenomenological description of a given quantum system \mathcal{S}_p via pseudo-Hamiltonian, whose basic features have been just summarized, is usually incorporated into the standard quantum-theoretical formalism in the following way :

- (i) \mathcal{S}_p is regarded as a non-isolated part of a greater system \mathcal{S} which is fully governed by quantum-mechanical laws ; especially the time evolution is determined by its Hamiltonian H , which is a below-bounded (i.e. $\inf \sigma(H) > -\infty$ where $\sigma(H)$ denotes the spectrum of H) self-adjoint operator on the state Hilbert space \mathcal{H} of \mathcal{S} , $\mathcal{H} \supset \mathcal{H}_p$, which is not reduced by H_p (otherwise \mathcal{S}_p would be isolated),
- (ii) the time evolution of \mathcal{S}_p is uniquely determined by that of \mathcal{S} : if $P \in \mathcal{L}(\mathcal{H})$ is the projection on \mathcal{H}_p , then

$$V(t) = pr_P U(t) \quad \star) \quad , \quad U(t) = \exp(-iHt) \quad .$$

This interpretation causes no troubles as far as one proceeds "from above downwards", i.e., as far as one knows the triplet $\{\mathcal{H}, H, P\}$. Let us stress in this connection one important point which is implied by Williams' theorem /4/: if H is below-bounded and if

$$[P, \exp(-iHt)] \neq 0 \quad \text{for all } t \neq 0 \quad (3)$$

then the set $\{V(t) : t \geq 0\}$, $V(t) = pr_P \exp(-iHt)$, is not a semigroup. Clearly, (3) requires more than the condition " H is not reduced by \mathcal{H}_p "; however, it is very often fulfilled. The same assumption concerning $\sigma(H)$ implies also some other limitations on $\{V(t)\}$ /4-6,9/.

Proceeding in the reverse direction is not so simple : one must use more complicated mathematics and one meets difficulties in the physical interpretation. As to mathematics, our starting assumption about the semigroup character of $\{V(t)\}$ (supplemented by the requirement that $\{V(t)\}$ is continuous) makes it possible to apply the theory of unitary dilations of contractive semigroups /7/. Then the basic question of existence and uniqueness of the triplet $\{\mathcal{H}, H, P\}$ can be satisfactorily answered (see sec.2). However, using this theory gives rise to a serious prob-

$\star)$ For a given projection $P \in \mathcal{L}(\mathcal{H})$ and any $B \in \mathcal{L}(\mathcal{H})$ one defines $pr_P B = PB \upharpoonright \mathcal{H}_p$. The operator $pr_P B$ is often identified with PBP although the former acts on $P\mathcal{H}$ and the latter on \mathcal{H} .

lem of interpretation : general theorems imply (under some additional assumptions like (3)) that the self-adjoint operator H obtained in this way is not below-bounded and, consequently, H cannot be regarded as Hamiltonian of some quantum system.*)

The main problem of this study is to show that this problem of interpretation can be solved within the framework of the unitary dilations theory ; our starting point is the fact that the phenomenological description of \mathcal{Y}_p is necessarily approximative. Due to this rehabilitation of the unitary dilation procedure we are able to give a correct definition of pseudo-Hamiltonian and to solve the following questions :

- (i) Which are the necessary and sufficient conditions for an operator to be pseudo-Hamiltonian ?
- (ii) How are the properties of a pseudo-Hamiltonian H_p related to the spectral characteristics of the corresponding self-adjoint operator H ?

2. Can the theory of unitary dilations be applied to pseudo-Hamiltonians ?

Let us first remind some facts which have been mentioned in the introduction and will also be used below.

Definition 1 : A one-parameter set of bounded operators $\{V(t) : t \geq 0\}$ on a Hilbert space \mathcal{H} is called continuous contractive semigroup (CCSG) if

- (i) $V(t+t') = V(t)V(t')$ for all $t, t' \geq 0$, $V(0) = I$,
- (ii) $\|V(t)\| \leq 1$ for all $t \geq 0$,
- (iii) $\lim_{t \rightarrow 0^+} V(t)\psi = \psi$ for all $\psi \in \mathcal{H}$.

A linear operator A on \mathcal{H} defined on $D(A) \equiv \{\psi \in \mathcal{H} : \lim_{t \rightarrow 0^+} \frac{1}{t}(I - V(t))\psi \text{ exists}\}$ by $A\psi \equiv \lim_{t \rightarrow 0^+} \frac{1}{t}(I - V(t))\psi$ is called generator of $\{V(t)\}$.

Remarks : 1) These conditions imply continuity of the mapping $V : [0, \infty) \rightarrow \mathcal{L}(\mathcal{H})$ with respect to the strong operator topology.
2) The generator of a CCSG is a closed densely defined operator (/8/, sec.X.8).

*) Hamiltonians which are not below-bounded occur in quantum statistical mechanics in the study of infinite reservoirs /6/. However, it would be clearly not satisfactory from the theoretical point of view if we had to assume the system \mathcal{Y}_p to be always coupled to an infinite reservoir.

Theorem 1 : Let $\{V(t) : t \geq 0\} \subset \mathcal{L}(\mathcal{K}_p)$ be a CCSG . Then there is a Hilbert space $\mathcal{K} \supset \mathcal{K}_p$, a projection P and a self-adjoint operator H on \mathcal{K} such that

$$(i) \quad \mathcal{K}_p = P\mathcal{K} ,$$

$$(ii) \quad V(t) = \text{pr}_p \exp(-iHt) \quad \text{for all } t \geq 0 ,$$

$$(iii) \quad \mathcal{K} = \left(\bigcup_{t \in \mathbb{R}} U(t)\mathcal{K}_p \right)_{\text{lin}} .$$

Moreover, $U(t) = \exp(-iHt)$ is unique up to isomorphism.

Proof of the theorem and some related topics can be found in /7/, secs. I.7,8 . The unitary group $\{U(t) : t \in \mathbb{R}\}$ is called minimal unitary dilation of the CCSG $\{V(t) : t \geq 0\}$.

Theorem 2 : Let $\{U(t) : t \in \mathbb{R}\} \subset \mathcal{L}(\mathcal{K})$ be the minimal unitary dilation of the CCSG $\{V(t) : t \geq 0\} \subset \mathcal{L}(\mathcal{K}_p)$, let further H be the generator of $\{U(t)\}$ and $P\mathcal{K} = \mathcal{K}_p$. If the projection P does not commute with $U(t)$ for any real $t \neq 0$, then the spectrum of H equals the whole \mathbb{R} .

Remark : In Williams paper /4/ this statement is proved under the assumption that "V(t) is non-unitary for each $t > 0$ " instead of that expressed by (3) . It can be shown easily that these conditions are equivalent.

We shall now return to the proper subject of this section : we want to find a way how to overcome the troubles mentioned in the introduction which arise if one tries to interpret a given quantum mechanical system \mathcal{S}_p (described via pseudo-Hamiltonian H_p) as a non-isolated part of some larger system \mathcal{S} that strictly obeys the laws of quantum theory. Let us first of all formulate our basic idea : as the description of \mathcal{S}_p by H_p is phenomenological and consequently approximative, it is reasonable to assume that the system $\mathcal{S} \supset \mathcal{S}_p$ will also be determined only approximatively. We shall further adopt two additional assumptions :

- (A1) the semigroup $\{V(t)\}$ generated by H_p is continuous,
- (A2) the accuracy of the description of the time evolution of \mathcal{S}_p by $\{V(t)\}$ is state-dependent.

Then the above idea can be translated into mathematical language as follows :

To any $\varepsilon > 0$, $\tau > 0$ and any finite subset $M \subset \mathcal{K}_p$ there is

a triplet $\{\mathcal{H}', H', P'\}_{(\varepsilon, \tau, M)}$ such that

$$(R1) \quad \mathcal{K}_p = P' \mathcal{H}' ,$$

$$(R2) \quad H' \text{ is self-adjoint and } \inf \sigma(H') > -\infty ,$$

$$(R3) \quad \|\text{pr}_p \exp(-iH't) - V(t)\psi\| < \varepsilon \quad \text{for all } \psi \in M , t \in [0, \tau] .$$

The \mathcal{H}' and H' are interpreted as the state Hilbert space and Hamiltonian of the system \mathcal{V} , respectively. The following proposition shows that these requirements can be fulfilled if one starts from the triplet $\{\mathcal{H}, H, P\}$ which is assigned to the semi-group $\{V(t) : t \geq 0\}$ by theorem 1. Moreover, it appears that one can choose $\mathcal{H}' = \mathcal{H}$, $P' = P$ for all ε and M and that the H' is some function of the operator H which is close to H in the strong resolvent convergence sense.

Theorem 3 : Let $\{V(t) : t \geq 0\} \subset \mathcal{U}(\mathcal{H}_p)$ be a CSG and let $\{\mathcal{H}, H, P\}$ be the triplet determining the minimal unitary dilation of $\{V(t)\}$. Then to any $\varepsilon > 0$, $\tau > 0$ and any finite subset $M \subset \mathcal{K}_p$ there exists a sequence $\{f_n\}$ of real Borel functions such that :

- (i) the triplet $\{\mathcal{H}, f_n(H), P\}$ satisfies the conditions (R1)-(R3) for all sufficiently large n ,
- (ii) $f_n(H)$ converges to H in the strong resolvent sense, i.e. $(f_n(H) - zI)^{-1}$ converges strongly to $(H - zI)^{-1}$ for any non-real $z \in \mathbb{C}$.

Proof : Only the non-trivial case $\inf \sigma(H) = -\infty$ has to be considered. Let $\{f_n\}$ be a sequence of real Borel functions such that $\inf f_n = c_n > -\infty$ and $\lim_{n \rightarrow \infty} f_n(x) = x$ for all $x \in \sigma(H)$.

One can take e.g. $f_n(x) = x$ for $x > -n$ and $f_n(x) = 0$ for $x \leq -n$. Then $H_n = f_n(H)$ is a s.a. operator, $\inf \sigma(H_n) \geq c_n$, and further the rules of functional calculus imply strong convergence of $\exp(-iH_n t)$ to $\exp(-iHt)$ for all $t \in \mathbb{R}$. Using the Trotter theorem (/8/, sec.VIII.7) we find out that H_n converges to H in the strong resolvent sense and that the strong convergence of $\exp(-iH_n t)$ to $\exp(-iHt)$ is uniform with respect to t in any finite interval. Thus there is an integer $n(\varepsilon, \tau, M)$ such that

$$\|(\exp(-iH_n t) - \exp(-iHt))\psi\| < \varepsilon$$

for all $\psi \in M$, $0 \leq t \leq \tau$ and $n > n(\varepsilon, \tau, M)$. Then the condition (R3) is satisfied for $H' = H_n$, $n > n(\varepsilon, \tau, M)$. ■

So we are led naturally to the following notion :

Definition 2 : A linear operator H_p on \mathcal{X}_p is called pseudo-Hamiltonian if the operator iH_p generates a CCSG $\{V(t) : t \geq 0\}$. The self-adjoint operator H on $\mathcal{X} \supset \mathcal{X}_p$ generating the minimal unitary dilation of $\{V(t)\}$ is called quasi-Hamiltonian corresponding to H_p .

Summarizing, we can say that the above approach enables to incorporate the phenomenological description of a quantum system \mathcal{Y}_p via pseudo-Hamiltonian into the standard quantum-theoretical formalism in a well-defined approximative manner. Moreover, this incorporation can be performed in the framework of the unitary dilations theory, the "physical" time evolution of \mathcal{Y}_p being arbitrary close to the CCSG generated by H_p and, simultaneously, H being arbitrarily close to the quasi-Hamiltonian corresponding to H_p . That is why it makes sense to consider the questions formulated at the end of section 1.

3. Criteria for pseudo-Hamiltonians

We shall start this section by the "pseudo-Hamiltonian version" of the basic criterion of the contractive semigroup theory. This criterion is advantageous because it is formulated in terms of conditions imposed immediately on the operator H_p . As a corollary, an effective sufficient condition is obtained which is then specified for generalized (non-self-adjoint) Schrödinger operators on $L^2(\mathbb{R}^n)$

$$H_p = -\Delta + u \quad (4)$$

where Δ is the Laplacian and u is some complex potential on $L^2(\mathbb{R}^n)$.

Generators of CCSG on Banach spaces are specified by the fundamental Hille-Yosida theorem (/8/, sec.X.8). However, this theorem involves conditions on the resolvent of the generator, and it is often convenient to replace them by the conditions referring immediately to the generator. This can be done, if one introduces the notion of accretivity; with its help the basic criterion for a closed densely defined operator to be the generator of CCSG can be obtained (/8/, th.X.48). For our purpose it is convenient to reformulate this criterion slightly. Firstly, we shall write it for the operator H_p rather than for the generator A

of $\{V(t)\}$, H_p being related to A by $H_p = -iA$. Secondly, only the special Hilbert space case will be considered. Accretivity of a densely defined linear operator A then simply means that $\text{Re}(\psi, A\psi) \geq 0$ for all $\psi \in D(A)$. The reformulated version of the above-mentioned basic criterion reads :

Theorem 4 : A closed densely defined linear operator H_p on \mathcal{H}_p is a pseudo-Hamiltonian iff the following conditions hold simultaneously :

- (i) $\text{Ran}(H_p - i\lambda I) = \mathcal{H}_p$ for some $\lambda > 0$,
- (ii) $\text{Im}(\psi, H_p \psi) \leq 0$ for all $\psi \in D(H_p)$.

Moreover, if H_p satisfies (i) and (ii), then the whole open upper halfplane belongs to the resolvent set of H_p and

$$(\varphi, (H_p - zI)^{-1} \psi) = i \int_0^{\infty} e^{izt} (\varphi, V(t) \psi) dt$$

for all $\varphi, \psi \in \mathcal{H}_p$ and each $z \in \mathbb{C}$, $\text{Im } z > 0$.

Corollary : Let H_p be a closed densely defined linear operator on \mathcal{H}_p . If the inequalities

$$\text{Im}(\psi, H_p \psi) \leq 0 \quad \text{for all } \psi \in D(H_p), \quad (5a)$$

$$\text{Im}(\varphi, H_p^+ \varphi) \geq 0 \quad \text{for all } \varphi \in D(H_p^+) \quad (5b)$$

hold simultaneously, then H_p is a pseudo-Hamiltonian.

Proof : The above inequalities yield for any $\lambda > 0$

$$\|(H_p - i\lambda I) \psi\| \geq \lambda \|\psi\| \quad \text{for all } \psi \in D(H_p),$$

$$\|(H_p^+ + i\lambda I) \varphi\| \geq \lambda \|\varphi\| \quad \text{for all } \varphi \in D(H_p^+).$$

The first of these relations implies that $\text{Ran}(H_p - i\lambda I)$ is closed and the second one shows that $\ker(H_p^+ + i\lambda I) = \{0\}$; hence

$$\text{Ran}(H_p - i\lambda I) = \overline{\text{Ran}(H_p - i\lambda I)} = \ker(H_p^+ + i\lambda I)^\perp = \mathcal{H}_p;$$

and the theorem can be applied. ■

We shall further examine how the conditions (5a,b) can be applied to the class of operators specified by eq.(4). The formal differential operation

$$-\Delta = - \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$$

is replaced in the standard way by the operator T on $L^2(\mathbb{R}^n)$:

$$T = F^{-1} S F$$

where F is the Fourier-Plancherel operator on $L^2(\mathbb{R}^n)$ and S is the self-adjoint operator of multiplication by $s : s(x_1, \dots, x_n) = \sum_{j=1}^n x_j^2$. Consequently, the free Hamiltonian T is self-adjoint. The set $C_0^\infty(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$ of C^∞ -functions with compact support is a core of T and $T\varphi = -\Delta\varphi$ for each $\varphi \in C_0^\infty(\mathbb{R}^n)$ (/8/, th. IX.27).

Secondly, we must specify the complex potential. Let u be a complex Borel function on \mathbb{R}^n . We denote by U the corresponding operator of multiplication by u , thus U is a densely defined operator on $L^2(\mathbb{R}^n)$, its adjoint U^+ being the operator of multiplication by \bar{u} . We must allow u to assume infinite values on some Borel set M_u^∞ ; otherwise singular potentials would be excluded. However, we shall limit ourselves to such functions for which M_u^∞ is a zero set with respect to the Lebesgue measure m on \mathbb{R}^n (excluding thus, e.g., the hard-core potentials). Such functions will be called almost regular. Let us mention the following useful equivalence:

A complex Borel function u on \mathbb{R}^n is almost regular iff to any non-zero Borel subset $M \subset \mathbb{R}^n$ there exists a non-zero compact Borel subset $M_c \subset M$ such that

$$\int_{M_c} |u|^2 dm < \infty \quad (6)$$

The proof can be easily performed using the decomposition

$$M = (M \cap M_u) \cup M_u^{\text{fin}}, \quad M_u^{\text{fin}} = \bigcup_{n=1}^{\infty} M_u^{(n)}, \quad M_u^{(n)} = \{x \in M : |u(x)| < n\}$$

and the fact that m is a regular and σ -finite measure.

The class of generalized Schrödinger operators (GSO) will be now specified as follows:

Definition 3: Let u be an almost regular complex Borel function on \mathbb{R}^n and let $H_0 = T + U$, $D(H_0) \equiv D = D(T) \cap D(U)$, be densely defined. Then the closure of H_0 is called the GSO (corresponding to u).

Remarks: 1) The closure \bar{H}_0 always exists: as $H_0^+ \supset T + U^+$ and $D(U^+) = D(U)$, it holds $D(H_0^+) \supset D$, i.e. H_0^+ is densely defined.

2) If H is a GSO, $H = \overline{T + U}$, then $H^+ = (T + U)^{+++} \supset T + U^+$, i.e.

$$H^+ \supset \overline{T + U^+} \quad (7)$$

The special case when equality holds in (7) will be considered below.

3) The above restriction to almost regular Borel functions has

the following important consequence : to any non-zero Borel set $M \subset \mathbb{R}^n$ there exists a compact Borel subset M_c , $0 < m(M_c) < \infty$, such that the set $C_0^\infty(M_c)$ of C^∞ -functions with support in M_c lies in $D(T+U)$. This is due to the obvious inclusion $C_0^\infty(M_c) \subset D(T)$ and to eq.(6) which implies $C_0^\infty(M_c) \subset D(U)$.

Theorem 5 : Let H be a GSO on $L^2(\mathbb{R}^n)$, $H = \overline{T+U}$. Then the condition

$$w(x) \equiv \operatorname{Im} u(x) \leq 0 \quad \text{a.e. in } \mathbb{R}^n \quad (8)$$

is necessary for H to be a pseudo-Hamiltonian. Moreover, if H^+ is the GSO corresponding to \bar{u} , i.e. if equality holds in (7), then the condition is also sufficient.

Proof : 1) Suppose the Borel set $M_+ = \{x \in \mathbb{R}^n : w(x) > 0\}$ to be non-zero. As u is almost regular, there exists a non-zero compact Borel set $N_+ \subset M_+$ such that (6) holds for $M_c = N_+$. Thus $C_0^\infty(N_+)$ is in $D(H)$ (see remark 3 above) and any non-zero $\varphi \in C_0^\infty(N_+)$ satisfies

$$\operatorname{Im}(\varphi, H\varphi) = \operatorname{Im}(\varphi, (T+U)\varphi) = (\varphi, W\varphi) = \int_{N_+} |\varphi|^2 w \, dm > 0.$$

Then theorem 4 implies that H is not a pseudo-Hamiltonian.

2) As the operator of multiplication by \bar{u} equals U^+ and $D(U) = D(U^+)$, we see that the domain of $H_\star = T+U^+$ is D . Using eq.(8) we obtain for each $\varphi \in D$

$$\operatorname{Im}(\varphi, H_0\varphi) = -\operatorname{Im}(\varphi, H_\star\varphi) = (\varphi, W\varphi) \leq 0.$$

In view of the condition $\bar{H}_0 = H$ and the assumption $\bar{H}_\star = H^+$ we further find out that H satisfies the inequalities (5a,b) and hence H is a pseudo-Hamiltonian. ■

The above sufficient condition is not very convenient for applications since difficulties may arise when verifying that equality holds in (7). It would be therefore desirable to exhibit explicitly some classes of complex potentials which give rise to pseudo-Hamiltonians. One can use methods of perturbation theory, especially the following statement of Kato-Rellich type (8, sec. X.8):

Lemma : Let H be a densely defined closable operator such that \bar{H} is a pseudo-Hamiltonian. If B is a closed accretive operator, $D(B) \supset D(H)$, and if there exist non-negative constants $a, b, a < 1$, such that

$$\|B\varphi\| \leq a\|H\varphi\| + b\|\varphi\| \quad \text{for all } \varphi \in D(H)$$

then $D(\bar{H}) \subset D(B)$ and the operator $\bar{H} - iB$ on $D(\bar{H})$ is a closed pseudo-Hamiltonian.

The application of this lemma to a GSO of the type $H = \bar{H}_0$, $H_0 = T + V + iW$ depends on the way in which H_0 is divided into unperturbed part and perturbation. We shall firstly consider the case when W , the absorptive part of the complex potential, is regarded as a perturbation :

Theorem 6 : Let H on $L^2(\mathbb{R}^n)$ corresponding to $u = v + iw$ and let the inequality (8) hold. If the operator $H_1 \equiv (T+V) \upharpoonright D$ is e.s.a. and if the inequality

$$\|W\psi\| \leq a\|H_1\psi\| + b\|\psi\| \quad (9)$$

is valid for all $\psi \in D$ and some non-negative a, b , $a < 1$, then H is a pseudo-Hamiltonian and moreover, it holds

$$H = \bar{H}_1 + iW, \quad D(H) = D(\bar{H}_1).$$

Proof : As W and \bar{H}_1 are self-adjoint and $-W$ is accretive, we find out, applying the lemma, that $H' = \bar{H}_1 + iW$, $D(H') = D(\bar{H}_1)$, is a closed densely defined pseudo-Hamiltonian. The obvious inclusion $H_0 = H_1 + iW \subset \bar{H}_1 + iW = H'$ yields $H \equiv \bar{H}_0 \subset H'$. On the other hand, the inequality (9) implies

$$\|H_0\psi\| \leq (a+1)\|H_1\psi\| + b\|\psi\| \quad \text{for all } \psi \in D,$$

and from this estimate one easily gets $D(\bar{H}_1) \subset D(\bar{H}_0)$. Hence it holds $H = H' = \bar{H}_1 + iW$. i.e., H is a pseudo-Hamiltonian. ■

As the inequality (9) is automatically fulfilled if W is a bounded operator, the following simplified version of theorem 6 holds:

Corollary : Let H be a GSO on $L^2(\mathbb{R}^n)$ corresponding to $u = v + iw$ with $w \in L^\infty(\mathbb{R}^n)$ and non-positive a.e. in \mathbb{R}^n . If $H_1 \equiv T + V$ is e.s.a., then H is a pseudo-Hamiltonian and $H = \bar{H}_1 + iW$.

The next theorem (which is analogous to the well-known sufficient condition for self-adjointness of Schrödinger operators - cf. /8/, th.X.15) concerns the situation where the whole complex potential U is regarded as a perturbation of T . Let us first consider the important special case $n \leq 3$.

Theorem 7 : Let H be a GSO on $L^2(\mathbb{R}^n)$, $n \leq 3$, corresponding to $u = v + iw$ where w obeys (8). If there exist Borel functions

u_1, u_2 such that $u = u_1 + u_2$, $u_1 \in L^2(\mathbb{R}^n)$, $u_2 \in L^\infty(\mathbb{R}^n)$ \star , then H is a pseudo-Hamiltonian and it holds

$$H = T + U, \quad D(H) = D(T).$$

Proof is based on the following properties of the free Hamiltonian T on $L^2(\mathbb{R}^n)$, $n \leq 3$ (cf. /8/, th. IX.28): $D(T) \subset L^\infty(\mathbb{R}^n)$ and to any $a > 0$ there exists $b > 0$ such that

$$\|\varphi\|_\infty \leq a\|T\varphi\| + b\|\varphi\| \quad \text{for all } \varphi \in D(T) \quad \star\star \quad (+)$$

where $\|\varphi\|_\infty \equiv \sup_{x \in \mathbb{R}^n} \text{ess } |\varphi(x)|$ is the L^∞ -norm of φ . Now, the decomposition $u = u_1 + u_2$ yields for each $\psi \in L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$

$$\|U\psi\| \leq \|U_1\psi\| + \|U_2\psi\| \leq \|u_1\| \|\psi\|_\infty + \|u_2\|_\infty \|\psi\|. \quad (++)$$

This relation shows that $L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n) \subset D(U)$, in particular $C_0^\infty(\mathbb{R}^n) \subset D(U)$. Combining it with (+) we get

$$\|U\psi\| \leq a\|u_1\| \|T\psi\| + (b\|u_1\| + \|u_2\|_\infty) \|\psi\| \quad \text{for all } \psi \in C_0^\infty(\mathbb{R}^n);$$

the same holds if U is replaced by the accretive operator iU . If we choose a so that $a\|u_1\| < 1$, we see that the operators $T \upharpoonright C_0^\infty(\mathbb{R}^n)$ and iU fulfill the assumptions of the lemma; hence $D(T) \subset D(U)$ and $T + U$ is a closed pseudo-Hamiltonian, i.e. it holds $H = T + U$, $D(H) = D(T)$. \blacksquare

Remark: Validity of this theorem can be extended to the case $n > 3$ if some additional requirements are imposed on U . We shall mention the physically interesting "Z-particle" case: $n = 3Z$, $Z = 2, 3, \dots$. For convenience radius vectors

$$\vec{x}_k = (x_{3k-2}, x_{3k-1}, x_{3k}) \quad , \quad 1 \leq k \leq Z$$

will be used instead of $3Z$ coordinates x_k . The (simplest possible) Z-particle extension of the theorem now reads:

Let $U = \sum_{k=1}^Z U_k$, where $(U_k \psi)(\vec{x}_1, \dots, \vec{x}_Z) = u_k(\vec{x}_k)(\vec{x}_1, \dots, \vec{x}_Z)$ and each u_k is a complex Borel function from $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ such that $\text{Im } u_k(x) \leq 0$ a.e. in \mathbb{R}^3 . Then $D(T) \subset D(U)$ and the operator $T + U$ is a pseudo-Hamiltonian.

\star) This condition is sometimes written as $u \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)$. The functions u_1, u_2 are, of course, generally different from v, w .

$\star\star$) This statement does not hold for $n > 3$ and this is the reason for the above restriction on n . However, under some additional conditions on u this restriction can be dropped (see remark below).

Validity of this statement is, in fact, due to the following inequality (cf./8/, th.X.16) :

$$\|U\psi\| \leq \alpha \|T\psi\| + \beta \|\psi\|, \quad \psi \in C_0^\infty(\mathbb{R}^{3Z}), \quad 0 < \alpha < 1, \quad \beta > 0.$$

As $u(\vec{x}_1, \dots, \vec{x}_Z) = \sum_{k=1}^Z u_k(\vec{x}_k)$ is a Borel function and the conditions imposed on $\text{Im } u_k$ imply $\text{Im } u \leq 0$ a.e. in \mathbb{R}^{3Z} , we see that the operator iU is closed and accretive. The statement then follows from the lemma. Some more complicated cases including two-particle forces can be handled in the analogous way (cf./13/).

4. Eigenvalues of pseudo-Hamiltonians

As mentioned above, the dynamics and energy spectrum of a non-isolated quantum system \mathcal{H}_p can be approximately described by means of a suitably chosen pseudo-Hamiltonian H_p . As H_p is not self-adjoint, it can be very complicated to find its relevant characteristics (spectrum, etc.). On the other hand, the quasi-Hamiltonian H is uniquely assigned to H_p and self-adjoint, the determination of its spectral characteristics being a standard quantum-mechanical problem. In this section we shall study relations between spectral properties of H and eigenvalues of H_p .

Let us first examine possible relations between H_p and the operator $\text{pr}_P H$. With the help of defs. 1, 2 one obtains easily

$$H_p \varphi = PH\varphi = \text{pr}_P H\varphi \quad \text{for all } \varphi \in D(H_p) \cap D(H).$$

Value of this relation, however, is rather low since it provides no information about the set $D(H_p) \cap D(H)$. It is even possible that this set contains the zero vector only so that the operators H_p and $\text{pr}_P H$ can be quite different :

Example : Let \mathcal{H}_p be the one-dimensional subspace of $L^2(\mathbb{R})$ spanned by the unit vector $\psi_0 : \psi_0(x) = (y/\pi)^{1/2} (x^2 + y^2)^{-1/2}$, $y > 0$. Clearly, the set $\{V(t) = \exp(-yt)I_p : t \geq 0\} \subset \mathcal{L}(\mathcal{H}_p)$ is a CGSG. One easily verifies that it holds for each $t \geq 0$

$$V(t) = \text{pr}_P(\exp(-iQt))$$

where Q is the self-adjoint operator of multiplication by x on $L^2(\mathbb{R})$. Further the unitary group $\{U(t) = \exp(-iQt) : t \in \mathbb{R}\} \subset \mathcal{L}(\mathcal{H})$ is the minimal unitary dilation of $\{V(t)\}$. In order to verify the minimality condition (iii) of theorem 1 which reads

$$\overline{\left(\bigcup_{t \in \mathbb{R}} \exp(-iQt)\psi_0 \right)_{\text{lin}}} = L^2(\mathbb{R})$$

one has to show that there are no non-zero vectors in $L^2(\mathbb{R})$ orthogonal to $M = \bigcup_{t \in \mathbb{R}} \exp(-iQt) \psi_0$. Let $\varphi \in M^\perp$, then the Fourier transform of φ , $\varphi(x) = \psi(x) \psi_0(x)$ equals identically zero so that $\varphi(x) = 0$ a.e. in \mathbb{R} . Now, $\psi_0(x) > 0$ for all $x \in \mathbb{R}$, thus $\psi = 0$. As $D(H_p) = \mathcal{H}_p$ and $\psi_0 \notin D(Q)$, we have $D(H_p) \cap D(Q) = \{0\}$.

We see therefore that the projection of H is of no use. This is mainly due to the fact that H is in general unbounded and consequently its domain is not the whole \mathcal{H} . This suggests that we should consider bounded functions of H instead of H itself. It is known^{9/} that the operator set $\{F_t : t \in \mathbb{R}\}$ related to the spectral family $\{E_t : t \in \mathbb{R}\}$ of H by $F_t = \text{pr}_p E_t$ can be successfully applied for studying various properties of the semi-group $\{V(t)\}$. We shall examine another family of bounded functions of H : the resolvent.

Theorem 8: Let H_p be a pseudo-Hamiltonian on \mathcal{H}_p , H the corresponding quasi-Hamiltonian on \mathcal{H} , $\mathcal{H}_p = P\mathcal{H}$. We denote by $R_p(z)$ and $R(z)$ the resolvents of H_p and H , respectively, and by $E(\cdot)$ the spectral measure of H , then it holds

$$R_p(z) = \text{pr}_p R(z) \quad \text{for all } z \in \mathbb{C}, \text{ Im } z > 0, \quad (10)$$

$$(\varphi, E([\alpha, \beta])\psi) + (\varphi, E((\alpha, \beta))\psi) = \frac{2}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{\alpha}^{\beta} (\varphi, \text{Im } R_p(s+i\varepsilon)\psi) ds \quad (11)$$

for any $\varphi, \psi \in \mathcal{H}_p$ and all $\alpha, \beta \in \mathbb{R}$, $\alpha < \beta$.

Proof: According to theorem 4, the $R_p(z)$ exists for all $z \in \mathbb{C}$, $\text{Im } z > 0$, and it holds for any $\varphi, \psi \in \mathcal{H}_p$

$$\begin{aligned} (\varphi, R_p(z)\psi) &= i \int_0^{\infty} e^{izt} (\varphi, V(t)\psi) dt = i \int_0^{\infty} e^{izt} (\varphi, U(t)\psi) dt = \\ &= (\varphi, R(z)\psi) \end{aligned} \quad (\star)$$

The last equality follows again from theorem 4 or it can be obtained directly using the functional calculus and Fubini's theorem. As φ and ψ are arbitrary vectors of \mathcal{H}_p , the relation (\star) is equivalent to eq.(10).

In order to prove (11) we use the Stone's formula (see [8/, th.VII.13 and sec.VIII.3): if H is self-adjoint operator on \mathcal{H} then for any $\varphi, \psi \in \mathcal{H}$ and all $\alpha, \beta \in \mathbb{R}$, $\alpha < \beta$ the relation

$$(\varphi, E([\alpha, \beta])\psi) + (\varphi, E((\alpha, \beta))\psi) = \frac{2}{\pi} \lim_{\varepsilon \rightarrow 0^+} \int_{\alpha}^{\beta} (\varphi, \text{Im } R(s+i\varepsilon)\psi) ds \quad (\star\star)$$

holds. In particular, if $\varphi, \psi \in \mathcal{H}_p$ the relation (\star) may be applied, then $(\star\star)$ becomes eq.(11). ■

Remark : Eq.(11) represents itself a generalization of the result obtained by Horwitz et al.^{/10/} for a strongly contractive semi-group (or strict CCSG in terminology of ref.6, i.e., $s\text{-}\lim_{t \rightarrow \infty} V(t) = 0$) on a finite-dimensional \mathcal{X}_p .

Corollary : Let $\lambda_0 = m - i\gamma$ be an eigenvalue of H_p and let $\psi_0 \in \mathcal{X}_p$ be the corresponding normalized eigenvector.

(a) If $\gamma = 0$, then $\psi_0 \in D(H)$ and $H\psi_0 = \lambda_0\psi_0$.

(b) If $\gamma > 0$, then $\psi_0 \notin D(H)$ and $\sigma(H) = \mathbb{R}$; moreover, ψ_0 belongs to the subspace \mathcal{X}_{ac} referring to the absolutely continuous spectrum of H . *

Proof : For any $z \in \mathbb{C}$, $\text{Im } z > 0$, we have $R_p(z)\psi_0 = (\lambda_0 - z)^{-1}\psi_0$. If one puts $\varphi = \psi = \psi_0$ in (11), the integration can be performed which yields

$$(\psi_0, E([\alpha, \beta])\psi_0) + (\psi_0, E((\alpha, \beta))\psi_0) = \frac{2}{\pi} \lim_{\varepsilon \rightarrow 0^+} (\arctg \frac{\beta - m}{\varepsilon + \gamma} - \arctg \frac{\alpha - m}{\varepsilon + \gamma}).$$

For $\gamma = 0$ we put $\alpha = m = \lambda_0$, then

$$(\psi_0, E([\lambda_0, \beta])\psi_0) + (\psi_0, E((\lambda_0, \beta))\psi_0) = 1, \quad \beta > \lambda_0.$$

Let $\{\beta_n\}_{n=1}^{\infty} \subset \mathbb{R}$ be a decreasing sequence, $\beta_n \rightarrow \lambda_0$; one can always choose it so that $(\psi_0, E(\{\beta_n\})\psi_0) = 0$ for all n . Then

$$\begin{aligned} & (\psi_0, E([\lambda_0, \beta_n])\psi_0) + (\psi_0, E((\lambda_0, \beta_n))\psi_0) = \\ & = (\psi_0, E(\{\lambda_0\})\psi_0) + 2(\psi_0, (E_{\beta_n} - E_{\lambda_0})\psi_0), \end{aligned}$$

and since the mapping $t \mapsto E_t$, $E_t = E((-\infty, t])$, $t \in \mathbb{R}$, is strongly continuous on the right, we get, taking the limit, $1 = (\psi_0, E(\{\lambda_0\})\psi_0)$. This proves (a). If $\gamma > 0$ we have for any $\alpha, \beta \in \mathbb{R}$, $\alpha < \beta$:

$$(\psi_0, E([\alpha, \beta])\psi_0) + (\psi_0, E((\alpha, \beta))\psi_0) = \frac{2}{\pi} (\arctg \frac{\beta - m}{\gamma} - \arctg \frac{\alpha - m}{\gamma}). \quad (+)$$

By the same argument as in the previous case we find

$$(\psi_0, E(\{t\})\psi_0) = 0 \quad \text{for all } t \in \mathbb{R}$$

which means that the function $f : f(t) = (\psi_0, E_t\psi_0)$ is continuous. Then the left-hand side of (+) becomes $2(\psi_0, (E_{\beta} - E_{\alpha})\psi_0)$ so that taking the limit $\alpha \rightarrow -\infty$ we find

$$f(\beta) = (\psi_0, E_{\beta}\psi_0) = \frac{1}{\pi} \arctg \frac{\beta - m}{\gamma} + \frac{1}{2}.$$

Hence it holds $E((\beta - \varepsilon, \beta + \varepsilon))\psi_0 \neq 0$ for any $\beta \in \mathbb{R}$, $\varepsilon > 0$, i.e.

*) The case $\gamma < 0$ is excluded by the dissipativity condition (see theorem 4).

$\mathcal{D}(H) = \mathbb{R}$. In addition, the right-hand side of the last relation is absolutely continuous with respect to β , thus $\psi_0 \in \mathcal{H}_{ac}$. Finally, the integral

$$\int_{\mathbb{R}} t^2 d(\psi_0, E_t \psi_0) = \int_{\mathbb{R}} t^2 \frac{f}{F} \frac{dt}{(t-m)^2 + \gamma^2}$$

diverges so that $\psi_0 \notin D(H)$.

Concluding this section we shall examine what the above statements tell us about the set $\mathcal{D}_{\mathbb{R}}(H_p)$ of real eigenvalues of H_p . Let $\lambda \in \mathcal{D}_{\mathbb{R}}(H_p)$; the corresponding eigenspace will be denoted as $\mathcal{G}_p(\lambda)$ and the projection on it by $E_p(\lambda)$. Analogously the set of all eigenvalues of H will be denoted by $\mathcal{D}(H)$ and the eigenspace belonging to a given $\lambda \in \mathcal{D}(H)$ by $\mathcal{G}(\lambda)$. In this notation the above corollary reads

$$\begin{aligned} \mathcal{D}_{\mathbb{R}}(H_p) &\subset \mathcal{D}(H) \quad , \\ \mathcal{G}_p(\lambda) &\subset \mathcal{G}(\lambda) \quad \text{for any } \lambda \in \mathcal{D}_{\mathbb{R}}(H_p) . \end{aligned} \quad (12)$$

If $\lambda \in \mathcal{D}_{\mathbb{R}}(H_p)$ then the first of these relations implies $U(t)\psi = \exp(-i\lambda t)\psi$ for all $t \in \mathbb{R}$ and any $\psi \in \mathcal{G}_p(\lambda)$, i.e. $V(t)\psi = PU(t)\psi = \exp(-i\lambda t)\psi$ and $V^+(t)\psi = PU^+(t)\psi = PU(-t)\psi = \exp(i\lambda t)\psi$. Thus the semigroup $\{V(t) : t \geq 0\}$ is reduced by $\mathcal{G}_p(\lambda)$. Using def. 1 one finds easily that the operator H_p itself is reduced by $\mathcal{G}_p(\lambda)$. We see therefore that it is sufficient to study the restriction $H_p^{(r)}$ of H_p onto the orthogonal complement $\sum_{\lambda \in \mathcal{D}_{\mathbb{R}}(H_p)} \oplus \mathcal{G}_p(\lambda)$ provided the set $\mathcal{D}_{\mathbb{R}}(H_p)$ is known (notice that the subspaces in the direct sum are mutually orthogonal since each $\psi \in \mathcal{G}_p(\lambda)$ is an eigenvector of the self-adjoint operator H belonging to the eigenvalue λ of H).

In some cases the semigroup $\{V(t)\}$ itself guarantees that $\mathcal{D}_{\mathbb{R}}(H_p) = \emptyset$, i.e. $H_p = H_p^{(r)}$. This occurs e.g. if $w\text{-}\lim_{t \rightarrow \infty} V(t) = 0$, then the spectrum of H is continuous^{5,6,10/}; thus H_p cannot have any real eigenvalues since H has none. However, in general the set $\mathcal{D}_{\mathbb{R}}(H_p)$ is non-empty. We limit ourselves here to the discussion how it can be determined provided that one knows all the eigenvalues of H together with the corresponding eigenspaces. In view of the relations (12) we need conditions ensuring that a given $\lambda \in \mathcal{D}(H)$ lies (or does not lie) in $\mathcal{D}_{\mathbb{R}}(H_p)$. The following simple criterion holds :

Theorem 9 : An eigenvalue λ of H lies in $\mathcal{D}_{\mathbb{R}}(H_p)$ iff

$$\mathcal{G}(\lambda) \cap \mathcal{X}_p \neq \{0\} . \quad (13)$$

Moreover, it holds $\mathcal{G}(\lambda) \cap \mathcal{X}_p = \mathcal{G}_p(\lambda)$.

Proof : Suppose (13) to be fulfilled, then for any non-zero $\psi \in \mathcal{G}(\lambda) \cap \mathcal{X}_p$ one has $U(t)\psi = \exp(-i\lambda t)\psi$, which implies

$$\frac{1}{t}(\psi - V(t)\psi) = \frac{1}{t}P(I - U(t))\psi \xrightarrow{t \rightarrow 0^+} -i\lambda\psi .$$

Hence $\psi \in D(H_p)$ and $H_p\psi = \lambda\psi$, i.e. $\lambda \in \mathcal{D}_R(H_p)$ and $\mathcal{G}(\lambda) \cap \mathcal{X}_p \subset \mathcal{G}_p(\lambda)$. The opposite inclusion and the implication $\lambda \in \mathcal{D}_R(H_p) \Rightarrow \Rightarrow (13)$ follow from the relations (12). ■

Remark : For any $\lambda \in \mathcal{D}(H)$ it holds

$$\mathcal{G}(\lambda) \cap \mathcal{X}_p^\perp = \{0\} ,$$

i.e. H has no eigenvector orthogonal to \mathcal{X}_p . This is a simple consequence of the minimality condition (iii) of theorem 1 : let $H\psi = \lambda\psi$ and $(\varphi, \psi) = 0$ for all $\varphi \in \mathcal{X}_p$. Then

$$(U(t)\varphi, \psi) = e^{i\lambda t}(U(t)\varphi, U(t)\psi) = e^{i\lambda t}(\varphi, \psi) = 0$$

for all $\varphi \in \mathcal{X}_p$ and any $t \in \mathbb{R}$, then by the minimality condition $(\bigcup_{t \in \mathbb{R}} U(t)\mathcal{X}_p)^\perp = \{0\}$ so that $\psi = 0$.

The condition (13) can be formulated in terms of operators $F(M) = \text{pr}_P E(M)$, M being any Borel set in \mathbb{R} (cf./9/). As λ is an eigenvalue of H , the projection $E(\lambda) = E(\{\lambda\})$ onto $\mathcal{G}(\lambda)$ is non-zero. Let $G(\lambda)$ be the projection onto $\mathcal{G}(\lambda) \cap \mathcal{X}_p$, then it holds /11/

$$G(\lambda) = s\text{-}\lim_{n \rightarrow \infty} G_n , \quad G_n = (PE(\lambda))^n . \quad (14)$$

In view of the obvious relation $\mathcal{G}(\lambda) \cap \mathcal{X}_p \subset \mathcal{X}_p = P\mathcal{X}$ we have $PG(\lambda) = G(\lambda)P = G(\lambda)$ so that $G(\lambda)$ is reduced by \mathcal{X}_p , the part of it lying in \mathcal{X}_p being zero. Hence the condition (13) is equivalent to $\text{pr}_P G(\lambda) \neq 0$. Now, the relation (14) implies that for any $\psi \in \mathcal{X}_p$ it holds $\text{pr}_P G_n \psi \rightarrow \text{pr}_P G(\lambda)\psi$, and further $\text{pr}_P G_n \psi = (PE(\lambda))^n \psi = (\text{pr}_P E(\lambda))^n \psi = F(\{\lambda\})^n \psi$. We have thus proved :

Corollary : An eigenvalue λ of H does not lie in $\mathcal{D}_R(H_p)$ iff $s\text{-}\lim_{n \rightarrow \infty} F(\{\lambda\})^n = 0$.

5. Concluding remarks

a) We have presented one possible way of incorporating the phenomenological description of a given non-isolated quantum-me-

chanical system into the standard formalism of the quantum theory. There are two essential steps in our approach : (i) the assumption that the phenomenological description is approximative in a strictly defined sense, (ii) application of the theory of unitary dilations of contractive semigroups. The following interesting question arises : can these steps be traced out in derivations of concrete optical potentials from microscopic models in nuclear physics ?

b) Spectral properties of a class of Schrödinger operators with complex potentials on $L^2(0, \infty)$ were investigated by Ljance using methods of the theory of linear differential operators^{/12/}. These results could provide useful information about spectral properties of some spherically symmetric pseudo-Hamiltonians on $L^2(\mathbb{R}^3)$ after performing the partial wave decomposition. The information we could get in this way about H_p would probably be more complete than that obtained indirectly, via quasi-Hamiltonian, as described in sec.4 .

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