IL NUOVO CIMENTO Vol. LXI A, N. 4 21 Giugno 1969

A Remark on Bound States in Potential-Scattering Theory.

D. Ruelle (*)
University of California - Irvine

(ricevuto il 25 Novembre 1968)

Summary. – Let $\mathscr{H} = \mathscr{H}_B + \mathscr{H}_C$ be the Hilbert space of an n-particle quantum system, where $\mathscr{H}_B$ is spanned by the bound states and $\mathscr{H}_C$ corresponds to the continuous spectrum of the Hamiltonian. It is shown that the wave functions which are in some sense localized in space and energy form a compact set in $\mathscr{H}$. This is used to prove that a wave packet ψ remains localized at finite distance for all time if $\psi \in \mathscr{H}_B$, and that it disappears at infinity if $\psi \in \mathscr{H}_C$.

1. – Introduction and statement of results.

Let H be the Hamiltonian describing an n-particle system in potential-scattering theory, H acts on a Hilbert space $\mathscr{H} = L^2(R^N)$. We write $\mathscr{H} = \mathscr{H}_B + \mathscr{H}_C$ where $\mathscr{H}_B$ is spanned by the bound states (eigenfunctions of H) and $\mathscr{H}_C$ is the orthogonal complement of $\mathscr{H}_B$. One expects that if $\psi \in \mathscr{H}_B$, the wave function

$$\psi_t = \exp[-iHt]\psi \tag{1}$$

will remain at all times concentrated mostly in some bounded region of R^N. On the other hand if $\psi \in \mathscr{H}_C$, one expects that the probability of finding the system in any fixed bounded region of R^N will vanish for large times. The aim of this note is to give a precise statement and proof of these facts. Remarkably, the proof depends very little on the detailed structure of the interaction; it is in particular valid for the case of potentials which are bounded below,

(*) Permanent address: IHES, 91, Bures-sur-Yvette.

whether or not these potentials vanish at infinity. What is used is the fact (*) that wave functions which are in some sense localized in a bounded region of R^N form a compact set in $\mathscr{H}=L^2(R^N)$ (see Proposition 1 and its corollary in Sect. **3**).

We postpone to Sect. **2** the description of conditions on the interaction, and state immediately our main result.

Theorem. Let H be defined according to A) or B) of Sect. **2**. *Let* $\psi\in\mathscr{H}$.

a) $\psi\in\mathscr{H}_B$ *if and only if for each* $\varepsilon>0$ *there exists an* $R>0$ *such that*

$$\sup_t \int_{|x|\geqslant R} \mathrm{d}x|\psi_t|^2<\varepsilon\,. \tag{2}$$

b) $\psi\in\mathscr{H}_0$ *if and only if, for each* $R>0$,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\int_{|x|\leqslant R}\mathrm{d}x|\psi_t(x)|^2=0\,. \tag{3}$$

2. – Definition of the Hamiltonian.

The Hamiltonian is formally defined by

$$H=-\Delta+V \tag{4}$$

acting on $\mathscr{H}=L^2(R^N)$. Here Δ is the Laplace operator and V is a multiplicative potential. We think of H as describing the system after elimination of the motion of the centre of mass; thus, for n particles in ν dimensions, $N=(n-1)\nu$. We describe two situations where H can be defined naturally as a self-adjoint operator.

A) Let the (real) function V be bounded below. Assume also that there exists a set $S\subset R^N$ such that

a) the complement of S in R^N has Lebesgue measure zero.

b) if $x\in S$, V is square integrable in some neighbourhood of x.

(*) The importance of such a property in relativistic quantum mechanics has been emphasized by HAAG and SWIECA (1). I was encouraged by HAAG to publish the present results, obtained mostly at the end of 1966.

(1) R. HAAG and J. A. SWIECA: *Comm. Math. Phys.*, **1**, 308 (1965).

Let D be the space of functions φ which are twice differentiable, have compact support and satisfy $V\varphi \in L^2(R^N)$. By our assumptions H is naturally defined on D, and D is dense in $\mathscr{H}$. Furthermore, H is bounded below on D and can thus be extended to a self-adjoint operator by the method of FRIEDRICHS (*).

B) Let $\nu \leqslant 3$ and V be a sum of pair potentials $\Phi_{ij}(x_j - x_i)$ such that $\Phi_{ij} \in L^2(R^\nu) + L^\infty(R^\nu)$. In that case a theorem of KATO (**) asserts that if φ belongs to the domain D of the Laplace operator, then $V\varphi \in L^2(R^N)$, and that (4) defines H as a self-adjoint operator on D. Furthermore, if $a > 0$, there exists $b > 0$ such that for all $\varphi \in D$.

$$\|V\varphi\| \leqslant a\|\Delta\varphi\| + b\|\varphi\| . \tag{5}$$

3. – Proofs.

In all the propositions below, it is assumed that H is defined according to A) or B) of Sect. **2**. Let $E(\lambda)$ be the spectral projection of H corresponding to the interval $(-\infty, \lambda]$; we denote again by $E(\lambda)$ the range of $E(\lambda)$.

Lemma. Given $\varepsilon > 0$, $R > 0$ and λ_0 there exists a finite-dimensional subspace F of $\mathscr{H}$ such that, for all $\psi \in E(\lambda_0)$,

$$\|\psi_F\| > \left[\int\limits_{|x|<R} \mathrm{d}x |\psi(x)|^2\right]^{\frac{1}{2}} - \varepsilon\|\psi\| , \tag{6}$$

where ψ_F is the component of ψ along F.

Let first H be defined according to A); since V is bounded below, there exists $\bar{\lambda}$ such that, for all $\psi \in E(\lambda_0)$,

$$(\psi, -\Delta\psi) \leqslant \bar{\lambda}\|\psi\|^2 . \tag{7}$$

If H is defined according to (B) we have, using (5)

$$\|\Delta\psi\| \leqslant \|H\psi\| + \|V\psi\| \leqslant \|H\psi\| + a\|\Delta\psi\| + b\|\psi\| .$$

(*) See RIESZ and NAGY (2) Sect. **124**.

(2) F. RIESZ and B. SZ.-NAGY: *Leçons d'Analyse Fonctionelle*, Académie des Sciences de Hongrie, 1955.

(**) For this and extensions to k-body potentials and $\nu > 3$, see KATO (3,4) and NELSON (5).

(3) T. KATO: *Trans. Am. Math. Soc.*, **70**, 195 (1951).

(4) T. KATO: *Perturbation Theory of Linear Operators* (Berlin, 1966).

(5) E. NELSON: *Journ. Math. Phys.*, **5**, 332 (1964).

Hence, taking $a<1$,

$$(\psi, -\Delta\psi)\leqslant \|\psi\|\,\|\Delta\psi\|\leqslant\|\psi\|(1-a)^{-1}[\|H\psi\|+b\|\psi\|]$$

and (7) holds again.

Let χ be the characteristic function of the set $\left\{x\in R^N: \sum_{i=1}^{N}|x^i|^2<R^2\right\}$, then

$$(\psi,\chi\psi)=\int_{|x|<R} dx|\psi(x)|^2 . \tag{8}$$

Consider now the Hamiltonian

$$\tilde{H}=-\Delta-\lambda\chi , \tag{9}$$

with $\lambda\geqslant 2\varepsilon^{-2}\bar{\lambda}$; we have by (7) and (8)

$$(\psi,\tilde{H}\psi)\leqslant \tfrac{1}{2}\lambda\varepsilon^2\|\psi\|^2-\lambda\int_{|x|<R} dx|\psi(x)|^2 . \tag{10}$$

The part of the spectrum of $\tilde{H}$ below $-\frac{1}{2}\lambda\varepsilon^2$ consists of a finite number of eigenvalues (*); let F be the space spanned by the corresponding eigenfunctions, then

$$(\psi,\tilde{H}\psi)\geqslant-\tfrac{1}{2}\lambda\varepsilon^2\|\psi\|^2-\lambda\|\psi_F\|^2 . \tag{11}$$

Comparison of (10) and (11) yields

$$\|\psi_F\|^2\geqslant\int_{|x|<R} dx|\psi(x)|^2-\varepsilon^2\|\psi\|^2 , \tag{12}$$

from which (6) follows.

Proposition 1. *Let the real function δ on* R *tend to zero at $+\infty$ and*

$$S=\{\psi\in\mathscr{H}: \|\psi-E(\lambda)\psi\|\leqslant\delta(\lambda)\|\psi\| \text{ for all } \lambda\} . \tag{13}$$

Given $\varepsilon>0$ and $R>0$ there exists a finite-dimensional subspace F of $\mathscr{H}$ such

---

(*) A proof of this fact could be obtained by direct computation; another proof, due to LANFORD, is presented in the Appendix (Proposition 2). An extension to multiparticle Hamiltonian has been obtained by HUNZIKER ([6]).

([6]) W. HUNZIKER: *Helv. Phys. Acta*, **39**, 451 (1966).

that, for all $\psi \in S$,

$$\|\psi_F\| \geqslant \left[\int\limits_{|x|<R} dx |\psi(x)|^2\right]^{\frac{1}{2}} - \varepsilon \|\psi\| . \tag{14}$$

We choose λ_0 such that $\delta(\lambda_0) \leqslant \frac{1}{3}\varepsilon$. According to the lemma there exists a finite-dimensional subspace F of $\mathscr{H}$ such that, for all $\psi \in \mathscr{H}$,

$$\begin{aligned}\|(E(\lambda_0)\psi)_F\| &\geqslant \left[\int\limits_{|x|<R} dx |(E(\lambda_0)\psi)(x)|^2\right]^{\frac{1}{2}} - \frac{1}{3}\varepsilon\|E(\lambda_0)\psi\| \geqslant \\ &\geqslant \left[\int\limits_{|x|<R} dx |(E(\lambda_0)\psi)(x)|^2\right]^{\frac{1}{2}} - \frac{1}{3}\varepsilon\|\psi\| .\end{aligned} \tag{15}$$

For $\psi \in S$, we have

$$\|(E(\lambda_0)\psi)_F\| - \|\psi_F\| \leqslant \|(\psi - E(\lambda_0)\psi)_F\| \leqslant \|\psi - E(\lambda_0)\psi\| \leqslant \tfrac{1}{3}\varepsilon\|\psi\| ,$$

$$\begin{aligned}&\left[\int\limits_{|x|<R} dx |(E(\lambda_0)\psi)(x)|^2\right]^{\frac{1}{2}} - \left[\int\limits_{|x|<R} dx |\psi(x)|^2\right]^{\frac{1}{2}} \geqslant \\ &\qquad \geqslant -\left[\int\limits_{|x|<R} dx |\psi(x) - (E(\lambda_0)\psi)(x)|^2\right]^{\frac{1}{2}} \geqslant -\|\psi - E(\lambda_0)\psi\| \geqslant -\frac{1}{3}\varepsilon\|\psi\| .\end{aligned}$$

Inserting these inequalities into (15) yields (14).

Corollary. Let S *be given by* (14) *and*

$$T = \left\{\psi \in \mathscr{H} : \left[\int\limits_{|x|>R} dx |\psi(x)|^2\right]^{\frac{1}{2}} \leqslant \eta(R) \text{ for all } R \geqslant 0\right\} , \tag{16}$$

where the real function η *tends to zero at* $+\infty$. *The set* $S \cap T$ *has compact closure in* $\mathscr{H}$.

Notice first that $\psi \in T$ implies $\|\psi\| \leqslant \eta(0)$, therefore $S \cap T$ is bounded, the compactness follows from (14) and (16).

Proposition 2. *Let* $\varepsilon > 0$ *and* $\psi \in \mathscr{H}$; *let* ψ_t *be defined by* (1).

a) Given $R > 0$ *there exists a finite-dimensional subspace* F *of* $\mathscr{H}$ *such that for all* t

$$\|\psi_{tF}\| \geqslant \left[\int\limits_{|x|<R} dx |\psi_t(x)|^2\right]^{\frac{1}{2}} - \varepsilon . \tag{17}$$

b) Given a finite-dimensional subspace F *of* $\mathscr{H}$ *there exists* $R > 0$ *such that for all* t

$$\left[\int\limits_{|x|<R} dx |\psi_t(x)|^2\right]^{\frac{1}{2}} \geqslant \|\psi_{tF}\| - \varepsilon . \tag{18}$$

a) We may assume $\|\psi\| = 1$. If $\delta(\lambda) = \|\psi - E(\lambda)\psi\|$, the set $\{\psi_t : t \in R\}$ is contained in the set S defined by (13), and (17) follows from Proposition 1.

b) Let $(\psi^\alpha)_{1\leqslant\alpha\leqslant m}$ be an orthonormal basis of F. We choose an orthonormal system $(\tilde\psi^\alpha)_{1\leqslant\alpha\leqslant m}$ in $L^2(R^N)$ formed by functions with compact support such that $\|\psi^\alpha - \tilde\psi^\alpha\| \leqslant [m\|\psi\|^2]^{-1}\varepsilon^2$. Taking R such that the supports of the $\tilde\psi^\alpha$ are contained in $\{x : |x| < R\}$, we have

$$\|\psi_{tF}\|^2 - \varepsilon^2 = \sum_\alpha |(\psi^\alpha, \psi_t)|^2 - \varepsilon^2 \leqslant \sum_\alpha |(\tilde\psi^\alpha, \psi_t)|^2 =$$

$$= \sum_\alpha \left| \int_{|x|<R} \mathrm{d}x\, \tilde\psi^\alpha(x)^* \psi_t(x) \right|^2 \leqslant \int_{|x|<R} \mathrm{d}x |\psi_t(x)|^2 ,$$

which proves (18).

Proposition 3. *Let* $\psi \in \mathscr{H}$.

a) $\psi \in \mathscr{H}_B$ *if and only if the set* $\{\psi_t : t \in R\}$ *has compact closure in* $\mathscr{H}$.

b) $\psi \in \mathscr{H}_C$ *if and only if for every* $\varphi \in \mathscr{H}$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T \mathrm{d}t |(\varphi, \psi_t)|^2 = 0 . \tag{19}$$

For a proof of these statements see JACOBS [7] Sect. **8**.

We come now to the proof of the theorem stated in Sect. **1**. According to Proposition 3 *a*), $\psi \in \mathscr{H}_B$ if and only if, for all $\varepsilon > 0$, there is a finite-dimensional subspace F of $\mathscr{H}$ such that, for all t,

$$\|\psi_{tF}\| \geqslant \|\psi_t\| - \varepsilon . \tag{20}$$

By Proposition 2, this holds if and only if, for all $\varepsilon > 0$, there exists $R > 0$ such that, for all t,

$$\left[\int_{|x|<R} \mathrm{d}x |\psi_t(x)|^2 \right]^{\frac{1}{2}} \geqslant \|\psi_t\| - \varepsilon ,$$

or equivalently

$$\int_{|x|<R} \mathrm{d}x |\psi_t(x)|^2 \geqslant \|\psi_t\|^2 - \varepsilon . \tag{21}$$

This proves part *a*) of the theorem.

According to Proposition 3 *b*), $\psi \in \mathscr{H}_C$ if and only if, for every finite-

[7] K. JACOBS: *Lecture Notes on Ergodic Theory*, Aarhus Universitet, Aarhus, 1963.

dimensional subspace F of $\mathscr{H}$,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{d}t\,\|\psi_{tF}\|^2 = 0\,. \tag{22}$$

By Proposition 2, this holds if and only if (3) holds for every $R > 0$, proving part b) of the theorem.

Appendix (by O. Lanford)

Proposition 1. *Let H_0 be a positive self-adjoint operator, V a symmetric operator; suppose that, for some $\lambda_0 > 0$, $V(\lambda_0 + H_0)^{-1}$ is an (everywhere defined) compact operator with norm strictly less than one. Then $H_0 + V$ is self-adjoint and its negative part is compact.*

It suffices to show that, for all $\lambda \geqslant \lambda_0$, $(\lambda + H_0 + V)^{-1}$ is everywhere defined and bounded, and that the negative part of $1/\lambda - (\lambda + H_0 + V)^{-1}$ is compact. For this, it suffices to show that

$$(\lambda + H_0 + V)^{-1} = (\lambda + H_0)^{-1} + T\,,$$

where T is compact. (Suppose $\Phi_1, \Phi_2, \ldots$ is an infinite sequence of mutually orthogonal normalized vectors; then

$$\limsup_n \big((\lambda + H_0 + V)^{-1}\Phi_n, \Phi_n\big) \leqslant \limsup_n \big((\lambda + H_0)^{-1}\Phi_n, \Phi_n\big) + \limsup_n \|T\Phi_n\| \leqslant 1/\lambda,$$

since $\|T\Phi_n\| \to 0$.)

Now

$$(\lambda + H_0 + V)^{-1} = (\lambda + H_0)^{-1}\big(1 + V(\lambda + H_0)^{-1}\big)^{-1} =$$

$$= (\lambda + H_0)^{-1} - (\lambda + H_0)^{-1}\sum_{n=0}^{\infty}\big(-V(\lambda + H_0)^{-1}\big)^n V(\lambda + H_0)^{-1}\,.$$

By hypothesis, $V(\lambda_0 + H_0)^{-1}$ is a compact operator of norm strictly less than one; the same is true of $V(\lambda + H_0)^{-1}$ because

$$V(\lambda + H_0)^{-1} = V(\lambda_0 + H_0)^{-1}(\lambda_0 + H_0)(\lambda + H_0)^{-1}$$

and

$$\|(\lambda_0 + H_0)(\lambda + H_0)^{-1}\| \leqslant 1\,.$$

Hence, $(\lambda + H_0 + V)^{-1} - (\lambda + H_0)^{-1}$ is compact, and the proposition is proved.

Proposition 2. *Let f be a bounded real-valued square-integrable function on R^N; then the operator $-\Delta + f$ on $L^2(\mathsf{R}^N)$ has compact negative part.*

By Proposition 1, it will suffice to find $\lambda > 0$ such that $f(\lambda - \Delta)^{-1}$ is a compact operator of norm strictly less than one. Since $\|f\cdot(\lambda - \Delta)^{-1}\| \leqslant \|f\|_\infty \cdot 1/\lambda$, it suffices to show that

$$f\cdot(\lambda - \Delta)^{-1}$$

is compact for all $\lambda > 0$. Since

$$f\cdot(\lambda - \Delta)^{-1}$$

is a norm limit of operators of the form

$$f\cdot(\lambda - \Delta)^{-1}\boldsymbol{P}_K\,,$$

where $\boldsymbol{P}_K$ is the spectral projection for Δ onto a compact interval K, it suffices to prove that $f\cdot(\lambda - \Delta)^{-1}\boldsymbol{P}_K$ is compact. If χ_K is the characteristic function of the interval K, then $f\cdot(\lambda - \Delta)^{-1}\boldsymbol{P}_K$ may be realized as an integral operator R^N with kernel

$$\tilde{f}(k' - k)\,\frac{1}{\lambda + k^2}\,\chi_K(-k^2)\,.$$

The kernel is square-integrable; therefore, $f\cdot(\lambda - \Delta)^{-1}\boldsymbol{P}_K$ is a Hilbert-Schmidt operator and so in particular is compact.

Remark. For $N = 1, 2, 3$ the operator $f\cdot(\lambda - \Delta)^{-1}$ is already Hilbert-Schmidt, and its Hilbert-Schmidt norm goes to zero as $\lambda \to \infty$; therefore the condition that f be bounded is superfluous.

RIASSUNTO (*)

Sia $\mathscr{H} = \mathscr{H}_B + \mathscr{H}_C$ lo spazio hilbertiano di un sistema quantistico di n particelle, in cui $\mathscr{H}_B$ è coperto dagli stati legati e $\mathscr{H}_C$ corrisponde allo spettro continuo dell'hamiltoniana. Si dimostra che le funzioni d'onda che sono in un certo senso localizzate nello spazio e nell'energia formano un insieme compatto in $\mathscr{H}$. Da ciò si dimostra che un pacchetto d'onde ψ rimane localizzato ad una distanza finita in tutti gli istanti se $\psi \in \mathscr{H}_B$, e che scompare all'infinito se $\psi \in \mathscr{H}_C$.

(*) *Traduzione a cura della Redazione.*

Замечания о связанных состояниях в потенциальной теории рассеяния.

Резюме автором не представлено.