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Mathematical questions of quantum many-body theory

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SEMINAIRE EQUATIONS AUX DERIVEES PARTIELLES   1986 - 1987

MATHEMATICAL QUESTIONS OF

QUANTUM MANY-BODY THEORY.

par I.M. SIGAL

I. INTRODUCTION.

In this talk I present a mathematical discussion of some of the
problems arising in the quantum many-body theory. The fundamental question
I want to adress is :

When and why do many-body systems hold together and when and how do
they disintegrate ?

One of the leading aspects of this review is the interplay between
classical and quantum motions which is a unique feature of many-body
dynamics.

II. HAMILTONIAN.

Consider a quantum N body system in $\mathbb{R}^\nu$. Let E be its configuration
space. This is either a subspace of $\mathbb{R}^{\nu N}$ or $\mathbb{R}^{\nu N}$ itself depending on
whether the center-of-mass motion is removed or not. We equip it with the
inner product

$$< X,Y > \quad = 2 \Sigma m_i X_i Y_i \quad ,$$

depending on the masses $m_i > 0$. The system is entirely described by its
Schrödinger operator (or Hamiltonian)

$$H = - \Delta + V(x) \quad \text{on } L^2(E) \ ,$$

where Δ is the Laplace-Beltrami operator on E and $V(x) = \Sigma_{ij} V_{ij} (x_i - x_j)$,
the sum of pair potentials. For all V's of interest to us H is self-
adjoint.

III. BINDING.

The term binding describes the situation when a collection of particles
forms a stable cluster . In terms of the corresponding Schrödinger operator
this means that the bottom of its spectrum (the ground state energy) is
discrete eigenvalue. Otherwise, the system does not bind.

As an example consider a system consisting of a nucleus of charge

Z and N electrons. The fundamental question from the point of view of structure of matter is : How many electrons can such a nucleus bind ?

A theorem of Zhislin ([Zh]) states that it can bind $N \leqslant Z$ electrons. In other words, atoms and positive ions are stable. The first question we adress is : Can a given nucleus bind an arbitrary number of electrons or is there a critical number after which the systems disintegrates ? The answer to this question is given in Saturation of binding theorem (Ruskai [Ru] , Sigal [Sig1]). There are no arbitrary negative ions in Quantum Mechanics (i.e. atomic binding saturates).More precisely, there is $N_{max}(Z) < \infty$ s.t. a nucleus of charge Z cannot bind more than $N_{max}(Z)$ electrons.

What can we say about $N_{max}(Z)$? The first step is

Theorem (Lieb [Li], Sigal [Sig2] (very large Z))

$$N_{max}(Z) \leqslant 2Z$$

In particular, Lieb's result implies that the double negative ion , H^{--} , of hydrogen (Z=1) is unstable (does not exist). The asymptotical behaviour of $N_{max}(Z)$ was found in the following

Asymptotic bulk neutrality theorem (Lieb, Sigal, Simon and Thirring [LSST]).

$$N_{max}(Z) = Z + o(Z) \tag{1}$$

Thus the large Z-ions are in bulk neutral. Experiments show that $o(Z) \leqslant 3$ for the known elements. This non-periodic fact about the periodic table is sometimes explained to be due to the electrostatic repulsion between electrons (the next charge of ion being negative). This explanation is wrong. Indeed, we have

Strong bosonic binding theorem (Benguria and Lieb [BL]) .

If the electrons were bosons then

$$\varlimsup_{Z \to p} \frac{N_{max}^{bos}(Z)}{Z} > 1.2...$$

Thus without the Pauli principle very negative ions would exist !

Open problem. To give an estimate of the remainder in (1).

Presumably very large Z nuclei can be realized as resonances or in neutron stars. Anyway, it is important to understand what the Schrödinger equation actually predicts. There is no physical argument or conjecture in literature to what this remainder should be. We propose the following

Conjecture. The maximal number of extra electrons a nucleus can bind is determined by the maximal capacity of the outer shell of the corresponding atom. In particular,

$$|N_{max}(Z) - Z| \leqslant const \ Z^{1/3}$$

If the outer shell is empty it presumably can be filled out without destabilizing the systems.

The methods used to prove the results above include the geometrical spectral analysis and potential theory. The former refers to approach based on the relation between the spectrum of H (global property) and the geometry of V and of the configuration space E (local property).

IV. RESONANCES.

The concept of resonance is one of the central concepts in Physics. In the last few years a geometrical theory of resonances has been inter-sively developed for one-body systems ([BC D1,2,BC DS, GS,HeSj, Hi Si,He-Ma Sig6]). Here we report on the work initiating a geometrical theory of resonances in many-body quantum systems.

a. Stark effect. Consider an N electron atom with the Hamiltonian H . Its (energy) spectrum look like

isol.EV's

cont. spec.
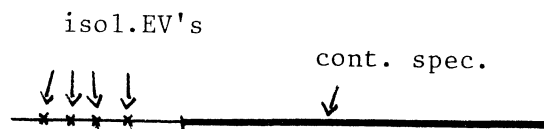
If the atom is now placed in a constant electric field the picture changes dramatically. The new (perturbed) Hamiltonian is

$$H_f = H- f.x \quad ,$$

where f.x is the electric field potential (the vector $f \in \mathbf{R}^{\nu N}$ is related to the electric field strength). The continuous spectrum of H_f fills the

entire axis (see [Tit1-7,AH] for the one particle result, I was unable to locate a many-particle one. Physical intuition suggests that the electric field would tear the electrons off the nucleus and send them to ∞ . In other words H_f would have no eigenvalues. This fact was proven by Titchmarsh [Tit 1-7] for the hydrogen atom and by Avron and Herbst [AH] (see also [HeSi]) for more general one-body systems.

For atoms and molecules with infinitely heavy nuclei the absence of eigenvalue was shown by Sigal [Sig5].

Open problem. Show that atoms and molecules with finite mass nuclei have no bound states in a constant electric field.

However, the eigenvalues of H do not disappear without trace. As follows from a result of Graffi and Grecchi [GG] and Herbst and Simon [He Si] (see also a beautiful geometric proof by Hunziher [Hn2]) they turn into resonances. The resonance energies is what the physicicts compute by the (divergent) perturbation theory and what accounts for the radiation frequency shifts observed first by Stark. The feature distinguishing the resonances is their life-time or width. For the hydrogen atom the bounds on the width of Stark resonances were given by Oppenheimer [Op] (see e.q. [Lan,LL]). The bounds were riporously justified by Harrel II and Simon [HaSi] who used after Oppenheimer (see also Eppstein [Ep1,2] and Schrödinger [Sch]) separation of variables in hyperbolic coordinates in order to reduce the problem to O.D.E. Here we discuss the bounds of width of Stark resonances for N-electron atoms given by Sigal [Sig8]. This result extends (at least , partially) the classical Oppenheimer formula.

b. Deux chevaux method. To define the resonances we use the method of spectral deformation of Hunziher [Hul] and Sigal [Sig4] (see also Cycon [Cyc] and [BCDS,HiSi]) with a particular choice of a vector field. This method goes back to fundamental works [AC,BC,Sim1,2]. It was dubbed "deux chevaux" by Combes for its simple and unassuming structure. There is another parallel : one can get a lot of milage per gallon using this method. Assume for simplicity that we have N electrons bound to an infinitely heavy nuclei. The configuration space then is $\mathbf{R}^{\nu\,N} (\nu=3)$.
Let

$$v(x) = (w(x_1 \cdot \hat{f}_1)\hat{f}_1 ,\ldots,w(x_N \cdot \hat{f}_N)\hat{f}_N) ,$$

a vector field on $\mathbb{R}^{\nu N}$, with a function w of the form
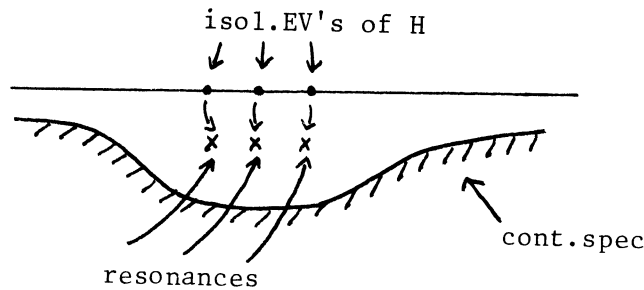
$$\uparrow w$$

$$0\left(\frac{1}{|f|}\right)$$
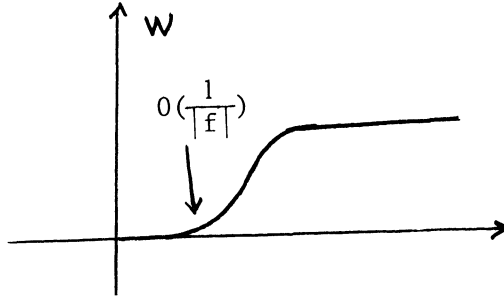
This vector field generates a global flow φ_θ with which we associate
the group of unitary operators

$$U(\theta)i\psi \rightarrow (\mathrm{Jac})^{1/2}\psi_o\varphi_\theta$$

Next, we introduce the family :

$$H_f(\theta) \equiv U(\theta)H_fU(\theta)^{-1}$$

Under certain conditions on v , the flow φ_θ and, consequently, $H_f(\theta)$
have analytic continuations in θ . The spectrum of $H_f(\theta)$ with $\mathrm{Im}\theta > 0$
looks like

isol.EV's of H

resonances   cont.spec

The isolated eigenvalues of $H_f(\theta)$ an independent of v and θ as long as
they stay away from the continuous spectrum. Besides they are not real as
follows from [Sig5]. They are called the resonances of $H_f(\theta)$. The real
and imaginary parts of a resonance are called its energy and width
(= 1/life-time), respectively.

c. Energetically forbidden region and its Riemannian structure. I describe
(in very imprecise terms) the Agmon-type Riemannian metric which plays a
central rôle in our analysis. To explain the meaning of this metric we
begin with the one-body case where the situation is rather simple. In this

case the section of the total potential $V_f(x) = V(x) - f.x$ along the field looks like :
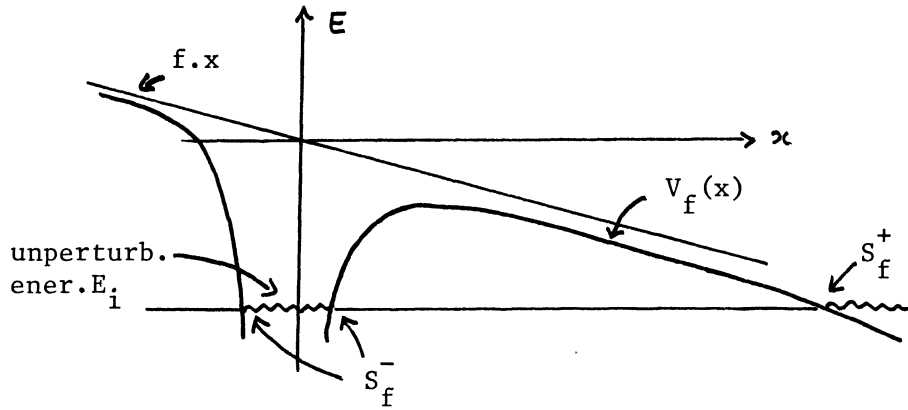
Here E_i is an (unperturbed) eigenvalue of H. The domain between the classical turning surfaces S_f^- and S_f^+ is the classically forbidden region for the energy E_i (the classical conservation of energy law cannot be fulfilled there). It supports the Agmon metric

$$ds^2 = (V_f(x)-E_i)_+ \, dx^2 , \qquad (3)$$

which is the classical Jacobi metric for the instantons (the classical particle in the imaginary time).

In the N-particle can we begin with the geometrical analysis of the configuration space $\mathbb{R}^{\nu N}$. We split the exterior of the ball of radius $|f|^{-\beta}$, where $\beta = 1/1+\mu$, into the regions $\Omega_{a,f}$ labeled by different ordered break-ups $a = \{A,B\}$ of the system $\{1,...,N\}$. In $\Omega_{a,f}$, the subsystem A is the half-space $e.y \leqslant n/|f|^\beta$ while the subsystem B is in $e.y \geqslant n+1/|f|^\beta$ for some $1 \leqslant n \leqslant N$:
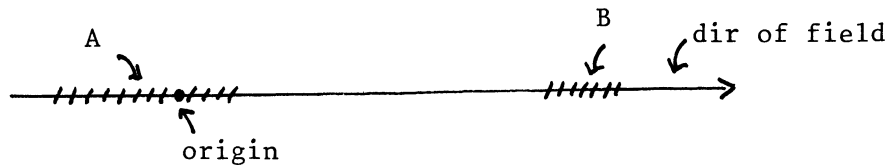
Then the subsystem A is put into it ground state (with the energy E_A) and the subsystem B is allowed to move freely (it is too far from the

origin to be in a bound state). For the latter subsystem we introduce the Agmon metric

$$ds^2 = (V_{B,f}(x) - \mu_A)_+ \, dx^2 \, ,$$

where $V_{B,f}(x)$ is the potential of B , placed in the electric field, $\mu_A = E - E_A$, the energy available to it if $B \neq \emptyset$ and $= E - \min\limits_{A \neq \{1,\ldots,N\}} E_A$ if $B = \emptyset$. Here E is a fixed total energy of the system. Loosely speaking the (energetically) forbidden region is a combination of the classically forbidden region for B in each of these geometric domains :

$$E \, F \, R_f = \bigcup_a \{x \in \Omega_{a,f} | \ V_{B,f}(x) > \mu_A\}$$

d. <u>Width of Stark resonances</u>. I will sketch now the main result of [Sig]. Let E_i be an isolated eigenvalue of H and let $E_i(f)$ be a resonance of H_f (the Stark resonance) born from E_i ($E_i(f) \to E_i$ as $|f| \to 0$). Then the width, $|\text{Im } E_i(f)|$, of this resonance is bounded as

$$|\text{Im } E_i(f)| \leqslant \text{const}|f|^{-1} \exp(-\rho_{i,f} + 0(|f|^{\alpha-1})), \qquad (2)$$

where $2\alpha < 1/1+\mu$, $\rho_{i,f}$ is the length of minimal geodesic between the ball of radius $|f|^{-\beta}$ and the exterior boundary of $E \, F \, R_f$ (the exit surface) in the Riemannian metric described above but for the energy $E = E_i$.

Note that in the one-particle can described above, $\rho_{i,t}$ is the length of minimal geodesic between classical turning surfaces S_f^- and S_f^+ in the (classical) Agmon Riemannian metric (3) :

classic.
forb. region
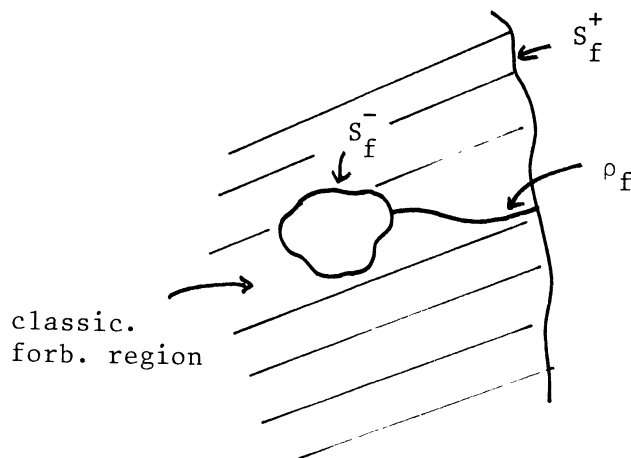
We emphasize that while in the semiclassical theory of resonances in one-body systems (including the one-body stark effect) the leading contribution comes from purely classical, instanton action, in the many-body case this is not true anymore. The quantum data play a crucial rôle in the underlying action. The latter is defined in terms of the eigenvalues of subsystems (ions), geometry of multiparticle configurations and the geometry of potentials.

Open problem. Show non-existence of bound states and existence of resonances and estimate the width of resonances for x-dependent external electric fields.

V. SCATTERING.

Here I will discuss the long-standing problem of asymptotic completeness. It consists of showing that as $t \to \pm \infty$ a many-body system in question disintegrates into independently moving stable subsystems. I will describe the results obtained jointly with A. Soffer and my understanding of the many-body scattering is due, in the large part, to this enjoyful collaboration. Reviews of other works on the subject can be found in [Co, CFKS, En, RS 111, Sig2, TU].

There are two factors determining the character of the scattering process : the range of potentials and the number of particles. As for as scattering is concerned the potentials are divided into the short-range (vanishing at ∞ faster than $|Y|^{-1}$) and long-range (vanishing at ∞ as $|Y|^{-1}$ or slower). When finer points of scattering are considered there is a further subdivision of these classes with the boundaries at $|Y|^{-2}$ for the shortrange and at $|Y|^{-1/2}$ for the long-range cases. As for the number of particles there are two transitions : from 1-2 particles to three particles and from three to four and more particles. The first transition requires the introduction of the geometrical analysis of many-particle configurations while the second, the phase-space (micro-local) analysis (see some discussion in section d).

We consider a general N-body system. Its configuration space in the center of mass frame is

$$X = \{x \in \mathbb{R}^{\nu N} \mid \sum_i m_i x_i = 0\}$$

We assume that the pair potentials are real and obey

$$<Y>^{\mu} \quad (Y.\nabla)^n \; V_{ij}(Y) \quad \text{are} \quad \Delta_Y \text{-compact for } n = 0,1,2 \qquad (4)$$

and with $\mu > 0$. This is, actually, more than is needed for the results below. Under these hypotheses (in fact, $n = 0$ suffices) H is self-adjoint on the Sobolev space $H_2(X)$.

a. <u>Decomposed systems</u>. Let $a = \{C_i\}$ be a partition of the set $\{1,...,N\}$. Such a partition will be called the <u>cluster decomposition</u> and its subsets, the <u>clusters</u>. Denote by I_a the intercluster interaction, i.e. the sum of pair potentials linking different clusters in a. Introduce the truncated Hamiltonians

$$H_a = H - I_a \quad . \qquad (5)$$

They discribe the notion of independent clusters (decomposed systems). Let H^a be the Hamiltonian of the internal motion of the clusters in a . It is obtained from H_a by removing the center-of-man motion of clusters :

$$H_a = H^a \otimes 1\!\!1 \; + \; 1\!\!1 \otimes p_a^2 \quad ,$$

where $p_a = - \nabla$ (grad in the center-of-mass coordinates of clusters), the cluster momentum.

b. <u>Channels</u>. To formulate the problem of asymptotic completeness in mathematical terms we introduce the notion of channels. They describe different scenarios according to which the scattering process can develop. A channel is specified by a pair $\alpha = (a,m)$, where a is cluster decomposition and m designates an eigenfunction of H^a, i.e. the stable motion within each cluster :
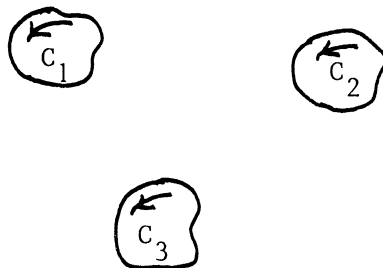
Let φ_α be the channel eigenfunction, i.e. the m-th eigenfunction of H^a (the product of cluster eigenfunctions), and ε_α , the corresponding eigenvalue. The channel Hamiltonian is defined as

$$H_\alpha = \underbrace{\varepsilon_\alpha}_{\substack{\text{energy of intern.} \\ \text{motion}}} + \underbrace{p^2_a}_{\substack{\text{energy of extern.} \\ \text{motion}}}$$

Given a total energy E , a channel α will be called

Open if $E \geqslant \varepsilon_j$, i.e. it is energetically allowed. We say that a is admissible if there is a open channel with a cluster decomposition either a or finer than a .

c. Asymptotic completeness. Short range potentials. There are different equivalent definitions of the N-body asymptotic completeness (AC). We present the one given in [SigSof1] : For any $\psi \in L^2(X)$ and any $\varepsilon > 0$ there are L^2-functions $\psi^{\pm}_{\alpha,\varepsilon}$ of the cluster center-of-mass coordinates so that

$$\lim_{t \to \pm\infty} \| \psi_t - \sum_{\text{open } \alpha} \varphi_\alpha \otimes e^{-iH_\alpha t} \psi^{\pm}_{\alpha,\varepsilon} \| \leqslant \varepsilon \ , \tag{6}$$

where $\psi_t = e^{-iHt}\psi$, the total evolution (the solution of the time-dependent Schrödinger equation with the initial condition ψ). The terms $\varphi_\alpha \otimes e^{-iH_\alpha t}\psi^{\pm}_{\alpha,\varepsilon}$ describe the propagation of free stable clusters. The ε accounts for the fact that some of the clusters may have zero relative velocities and their drifting apart is due to the spreading of wave-packets (diffusion) rather than propagation.

Theorem. (Sigal and Soffer [Sig Sof 1]) Assume the pair potentials obey (4) with $\mu > 1$. Then the corresponding system is asymptotically complete.

d. Asymptotic clustering. First we reduce the AC problem to proving the following geometrical statement (recall that we are dealing with the short-range systems). Let $E \in \mathbb{R}$. There is an interval Δ around E so that for any $\psi \in \text{Ran } E_\Delta(H)$ there are $\psi^{\pm}_a$ so that

$$\| \psi_t - \Sigma \, e^{-iH_a t} \, \psi_a^\pm \| \to 0 \quad \text{as } t \to \underline{+} \infty , \tag{7}$$

where the sum extends over the a's with at least two clusters.

This statement will be called the <u>asymptotic clustering at the energy</u> E .

<u>Proposition</u>. Assume a system under consideration is asymptotically clustering for any $E \neq \epsilon_\alpha$ for all α . Then it is asymptotically complete.

<u>Idea of the proof</u>. Separates the discrete part of H^a and use the continuity of the rest : in the obvious notations

$$e^{-iH_a t} u = \Sigma_\alpha e^{-iH_\alpha t} P_a u$$
$$+ \, e^{-iH_a t} P_a^{cont} u$$

In the last term we cut off a small neighbourhood of the H^a-thresholds and throw it into the ϵ-basket of (6). Then we apply the H^a-asymptotic clustering to the rest. We continue this process till we wind up with only stable clusters. $\square$

The proof above follows the development of the actual physical process. First, if the system is not at a threshold energy it disintegrates into a number of independent subsystems. Those of the subsystems which are in bound states are stable. The others, provided their energies are not threshold , break down further into smaller subsystems. Those with threshold energies disintegrate due to the diffusion.

<u>Theorem</u>. (Sigal and Soffer [Sig Sof 1]). Assume the pair potentials obey (4) with $\mu > 1$. Then the system is asymptotically clustering for all continuous non-threshold energies.

Thus this theorem and the proposition above imply the asymptotic completeness theorem. We emphasize here that the asymptotic clustering is a statement about the propagation. The argument taking care of diffusion is trivial in the case of short-range systems : it is just the strong continuity of the spectral projections $E_\Omega(H^a)$ on the orthogonal complements of the point spectrum subspaces.

Below we outline the idea of the proof of the asymptotic clustering theorem. We break the proof into three major steps. But first we need one more definition.

e.<u>Interaction planes</u>. The crucial feature of many-body Hamiltonians is that their potentials do not vanish at infinity. Indeed, define the subspaces

$$X_a = \{x \in X \mid x_i = x_j \quad \text{if } i.j \in \text{same cluster of a}\}$$

These are configuration spaces for the cluster centers-of-mass. For $a = \{(1)...(N)\}$, $X_a = X$ and we exclude this case from consideration. Clearly, $V(x)$ does not, in general, vanish if $x \to \infty$ along one of the X_a' s. We call X_a the interaction planes. We denote by x_a and ξ_a the projections of $x \in X$ and $\xi \in X'$ onto X_a and its dual X_a' , respectively.

We draw the "traces" of these planes on the unit sphere in the configuration space X for three and four particles :

N = 3   N = 4
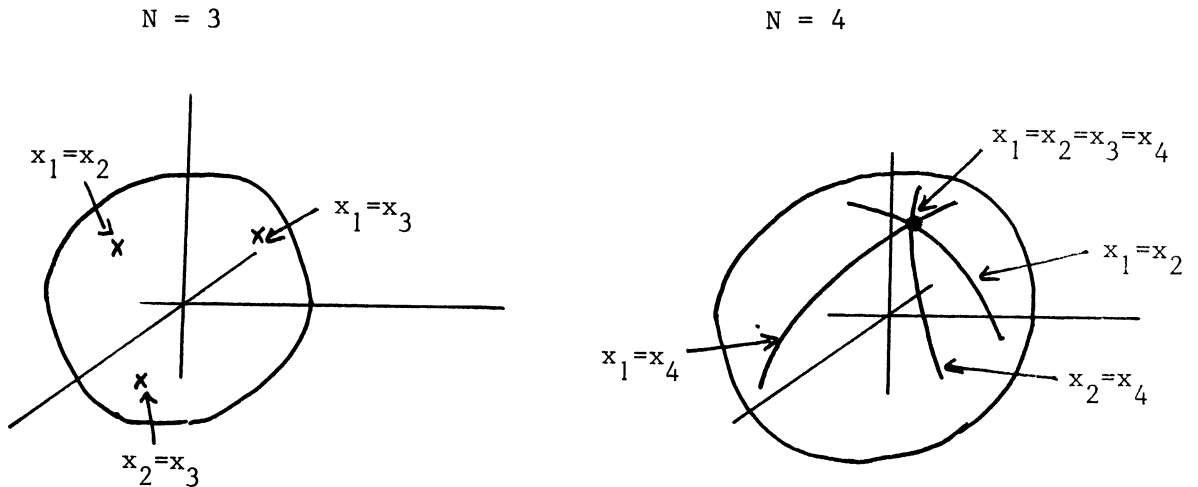
This shows the crucial difference between 3 and $N \geqslant 4$ body systems. In the three body case the interaction planes, X_a , do not intersect (except at the origin), while in the $N \geqslant 4$ body case all these planes are connected. It allows to separate channels in the three body case geometrically and reduce the problem to the free propagation estimates (away from the inter-action planes).

f. <u>Propagation set</u>. The asymptotic completeness can be given the following geometrical interpretation. As $t \to \pm \infty$, the total evolution approaches a superposition of a free (classical) motion along one of the X_a's and a bounded (quantum) motion in the perpendicular direction :

X_a

classical motion along X_a

quantum motion in perp. direction
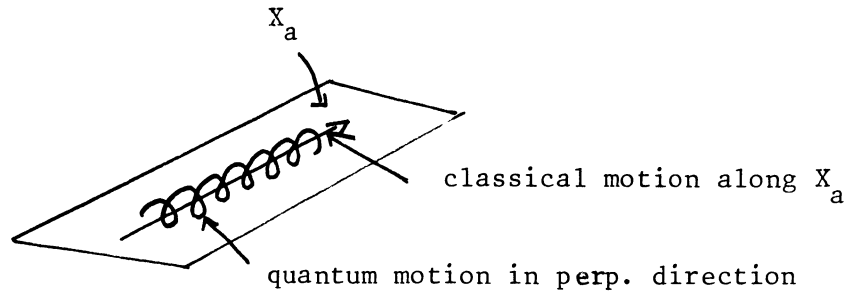
Here we assume that the initial energy E is non-threshold (i.e. $\neq \varepsilon_\alpha$ for all α_s') and we ignore the diffusion part of the motion.

The set of "classical" trajectories in the phase-space $X \times X'$ corresponding to the motion described above is

$$PS_E = \underset{\text{admissible } a}{U} \{ (x,\xi) \in \Gamma_a \times \Sigma_{a,E} \big| X \| \nabla |\xi_a|^2 \} \ ,$$

where $\Gamma_a = X_a \setminus \underset{c \text{ coarser than } a}{U} X_c$ and $\Sigma_{a,E}$ is the energy shell

$$\Sigma_{a,E} = \underset{b \text{ finer than } a}{U} \{\xi \in X' \big| \ |\xi_a| = \sqrt{E - \varepsilon_\beta}\}$$

Remark. Since PS_E is a candidate for a propagation set, $\Sigma_{a,E}$ cannot be replaced by the channel energy shell $H_\alpha(\xi_a) = E$. This is, again, due to a possible motion of stable clusters with zero relative velocities. Such a motion is not propagative.

The fact that the kinetic energy is of the form $|\xi|^2$ is crucial here. It allows us to define the velocities $\nabla |\xi a|^2$ of separated but not necessarily stable clusters.

We mention two properties of the set above :

(a) PS_E is not classical, i.e. it cannot be determined in terms of the corresponding classical Hamiltonian $|\xi|^2 + V(x)$ only.

(b) The a-components, π_α , of PS_E do not, in general intersect.

g. **Propagation estimates.** Let E be a non-threshold point of continuum.

We show that there is an interval Δ around E so that the evolution ψ_t
starting at $\psi \in$ Ran E_Δ(H) "vanishes" as $t \to +\infty$ away from (a conical neigh-
bourhood) of the set PS. An analogous statement holds also for $t \to -\infty$.

Loosely speaking , it can happen that a system can start (at t = 0 or
the distant past) at some component, π_α , but then it winds up in the
remote future on a collection of other components
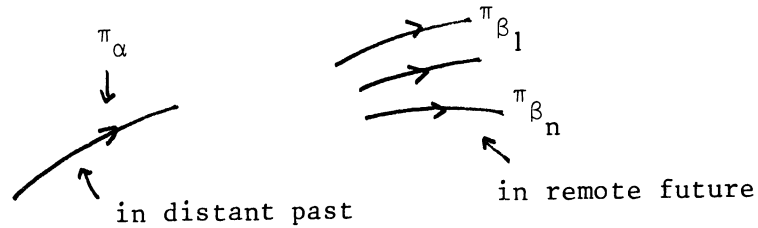
These facts translated into the framework of propagation of singularities
would mean that the characteris tics are not classical but defined in part by
the pseudodifferential operator itself and the singularities jump from
on characteristic to another (in general disjoint) characteristic.

To prove the propagation estimates we construct pseudodifferential
operators whose commutators with H restricted to an energy shell with a
non-threshold E are microlocally positive. Observe that the Poisson
brackets of the corresponding symbols are not positive in the basic cases.
Of course, one cannot expect to obtain non-classical propagation estimates
on the classical level. Our method is a logical step in the development of
the positive commutators method. It departs from the method of energetically
local commutators of Mourre [Mo] which, in turn, is a far reaching extension
of the method of (globally) positive commutators of Kato [Ka2] and Lavine
[La1-6] . Note here the crucial difference with the method of positive
commutators of Hörmander [Hö] in propagation of singularities. There all
the basic estimates are done on the classical, symbolic level and the
quantization comes in as a smoothing correction. Of course, the singularities
in this theory propagate along the classical trajectories (characteristics)
defined entirely in terms of the principal symbol. (Another distinction which
appears already in the one-body case is that the scattering theory requires
not only micro-local but also global estimates on the evolution.)

h. <u>Decoupling of channels</u>. Let E be a non-threshold energy. We construct a collection $\{j_{a,E}(x,p_a)\}$ of bounded pseudo-differential operators (we do not specify here the class) satisfying

(i) It is a phase-space partition of unity in the sense

$$\| \Sigma \; j_{a,E}(x,p_a) \; u-u \| \leqslant C \| <x>^{-\varepsilon} u \|$$

with $\varepsilon > 0$

(ii) On supp $j_{a,E}(x,\xi_a)$ the distance between the clusters in a grows proportionally to the distance to the origin.

(iii) supp$(\nabla_x j_{a,E}(x,\xi_a))$ (the "boundary" of $j_{a,E}(x,\xi_a)$) is away from PS_E .

Due to property (ii) each $j_{a,E}$ lives on the family of channels with the same geometry. Property (iii) shows that this partition separates the channels.

i. <u>Microlocal wave operators</u>. We claim that on supp $j_{a,E}$ the full dynamics behaves as the truncated dynamics of independent clusters. To demonstrate this we introduce the micro-local Deift-Simon wave operators

$$W^{\pm}_{a,E} = \text{s-} \lim_{t\to\pm\infty} e^{iH_a t} \; j_{a,E}(x,p) e^{-iHt} \quad \text{on Ran } E_\Delta(H), \qquad (8)$$

where Δ is a small interval containing E , if the limits exist. (Deift and Simon [DS] have introduced such operators for cut-off functions on the configuration space X alone).

The first step in the proof of existence of $W^{\pm}_{a,E}$ follows the Cook-Kato argument (see e.g. [Ka1, CFKS]). Namely, let $W_a(t)$ denote the operator function standing after the sign of limit on the r.h.s. of (8). Writing it as an integral of derivative (Fundamental theorem of calculus) yields

$$W_a(\psi) = j_{a,E} + i \int_o^t e^{iH_a s} K e^{-iHs} ds , \qquad (9)$$

where $K = H_a j_{a,E} - j_{a,E} H$. Next, using the Cauchy criterion we reduce the problem of existence of the strong limit (8) to the problem of strong convergence of the integral on the r.h.s. of (9) on Ran $E_\Delta(H)$. To analyse the later problem we write

$$K = [H_a, j_{a,E}] - j_{a,E} I_a \qquad (10)$$

(here we used (5)). Due to condition (4) on the potentials and property (ii) of $j_{a,E}$ we have

$$j_{a,E} I_a = O(|x|^{-\mu})$$

Due to a result of Perry, Sigal and Simon [PSS] (see also Mourre [Mo]) this term leads to a convergent contribution to the integral, provided $\mu > 1$. (This is the only place where $\mu > 1$ is required). Next, since

$$[H_a, j_{a,E}] = [-\Delta, j_{a,E}]$$

$$= - 2 \nabla_x j_{a,E} \cdot \nabla - \Delta_x j_{a,E}$$

and due to property (ii) of $j_{a,E}$, the second term on the r.h.s. of (10) lives away from PS_E and therefore leads due to the propagation estimates to a convergent contribution as well. This completes the outline of the proof of existence of (8).

Next, an elementary argument shows that the existence of $W_{a,E}^{\pm}$ for some E implies the asymptotic clustering for the some E . Indeed, let $\psi \in \mathrm{Ran}\ E_\Delta(H)$. We have

$$\psi_t = \Sigma\ j_{a,E}(x,p)\psi_t + O(|x|^{-\epsilon})\psi_t$$

$$= \Sigma\ e^{-iH_a t}\ W_{a,E}^{\pm}\psi + R^{\pm}(t)\ ,$$

where

$$R(t) = \Sigma\ e^{-iH_a t}\ (W_a(\psi) - W_{a,E}^{\pm})\psi$$

$$+ O(|x|^{-\epsilon})\psi_t$$

Due to the existence of $W_{a,E}^{\pm}$ and the absolute continuity of H (which is one of the results of [PSS]),

$$\| R^{\pm}(t) \| \to 0 \qquad \text{as } t \to \pm \infty\ ,$$

provided E is non-threshold. This proves the asymptotic clustering (and also provide the expressions for the amplitudes $\psi_a^{\pm}$ in (7)).

j. <u>Long-range potentials</u>. If the pair potentials are long-range (i.e. $\mu \leqslant 1$ in (4)), even as clusters depart from each other the intercluster interaction cannot be discarded entirely. Let $\theta_\delta(s)$ be a smooth function, $= 0$ for $s < \delta$ and $= 1$ for $s > 2\delta$. Denote

$$K_\alpha(x_a, \xi_a, t) = H_\alpha(\xi_a) + I_{a,t}(x_a) \quad , \tag{11}$$

where $I_{a,t}(x_a) = I_a(x_a) \theta_\delta(\frac{|x_a|}{t})$ (the low velocity is cut-off) with $I_a(x_a)$, the restriction of $I_a(x)$ to X_a. We pick δ depending on the total energy E (fixed in advance), say $\delta = \frac{1}{2}(E-\varepsilon_\alpha)$. Let $S_\alpha(\xi_a, t)$ be a solution to the Hamiltonian-Jacobi equation

$$\frac{\partial S_\alpha}{\partial t} = K_\alpha(\frac{\partial S_\alpha}{\partial \xi_a} , \xi_a, t),$$

obeying $S_\alpha|_{t=0} = 0$ or a sufficiently high (depending on μ) iteration of this equation. We formulate the asymptotic completeness for the long-range scattering as follows : For any $\psi \in L^2(X)$ and any $\varepsilon > 0$ there are $\psi_{\alpha,\varepsilon}^\pm \in L^2(X_a)$ so that

$$\lim_{t \to \pm\infty} \| \psi_t - \Sigma \varphi_\alpha \otimes e^{-iS_\alpha(p_a, t)} \psi_{\alpha,s}^\pm \| < \varepsilon$$

To justify this definition we have to assume that the bound states φ_α $\varphi_\alpha \in L^2(X \otimes X_a, <x^a>^\varepsilon dx^a)$ with $\varepsilon > 0$. Namely, this allow us to set $x^a = 0$ in the last term in (11). Here x^a is the projection of x into $X \ominus X_a$.

If $\mu > 1/2$ in (4) then the leading term in the expansion

$$\frac{\partial S_\alpha}{\partial t} = \nabla H_\alpha(\xi_a)t + O(t^{1-\mu})$$

suffices for the definition of asymptotic completeness. Moreover, due to the specific form of the kinetic energy term in H (in other words since the center-of-mass motion separates) we have that

$$\nabla H_\alpha(\xi_a) = 2\xi_a \quad ,$$

which is independent of dynamics (i.e. the bound states).
This allows to formulate the asymptotic clustering in this case. Define

$$H_a(t) = H_a + I_{a,t}(x^a, 2p_a t)$$

Let $U_a(t)$ be the evolution generated by $H_a(t)$:

$$i \frac{dU_a(t)}{d} = H_a(t)U_a(t) \quad \text{and} \quad U_a(0) = \text{id}$$

We define the asymptotic clustering at one energy E similarly to the short-range case but with (7) replaced by

$$\| \psi_t - \Sigma \, U_a(t)\psi_a^{\pm} \| \to 0 \quad \text{as } t \to \pm \infty$$

Open problem. Formulate the asymptotic clustering for the very long-range systems (i.e. $\mu \leqslant 1/2$).

Theorem. (Sigal and Soffer [SigSof2]) let the pair potentials obey (4) with $\mu = 1$ (i.e. the potentials are Coulomb-type). Then system in question is asymptotically clustering at any non-threshold energy.

Open problem. Prove the asymptotic clustering at non-threshold energies for long-range systems with $\mu > 1/2$ and $N \geqslant 4$.

k. Sharp propagation estimates. The propagation estimates discussed in sections f and g hold for pair potentials of arbitrary decay. However, they are not sufficient to prove the asymptotic clustering for long-range systems. First of all the propagation set must be specified more precisely. We suggest the following definition :

$$PS_E^{LR} = \underset{\alpha \text{ open}}{U} \{ (x,\xi) \in \Gamma_a \times \Sigma_{\alpha,E} \, \Big| \, x = \frac{\partial S_\alpha}{\partial \xi_a} \}$$

In other words, the asymptotic free evolution is modified and the coefficient of proportionality between the position and velocity(the time)is introduced. More importantly, the estimates defining the propagation set must be strengthened. More precisely, we must show that ψ_t "vanishes" outside a parabolic conical neighbourhood of PS_E^{LR} . For a two-cluster a we have to show that ψ_t "vanishes" on the domain

$$|x^a| < \varepsilon^t \quad \text{and} \quad \Big| x_a - \frac{\partial S_\alpha}{\partial \xi_a} \Big| > t^\gamma$$

with $\gamma < \mu \leqslant 1$. (Remember that $|x|$ and $\left|\dfrac{\partial S_\alpha}{\partial \xi_a}\right| \sim t$.)

$$x = \frac{\partial S_\alpha}{\partial \xi_a}$$

$$O(t^\gamma)$$
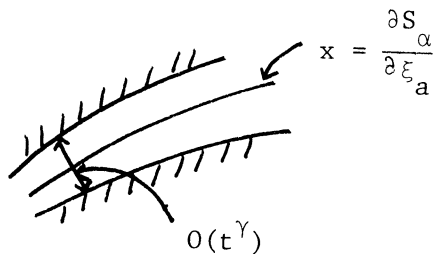
Note that in the one-body case Sigal [Sig] has shown that for

$$\| \, |x - \frac{\partial S}{\partial \xi}| \, \psi_t \| \leqslant const$$

for $\psi \in \mathrm{Ran} \ E_\Lambda(H) \cap D(|x|^2)$.

1. <u>Asymptotic Energy Distribution</u>. There is an obstruction in the long-range case for deriving asymptotic completeness from the asymptotic clustering at non-threshold energies. Namely, the energy for decomposed systems is not conserved anymore : $\psi \in E_\Lambda(H_a(0)) \not\Rightarrow U_a(t)\psi \in E_\Lambda(H_a(t))$. This makes controlling the diffusion at zero relative velocities non trivial. However, Sigal and Soffer [SigSof3] have shown that for $\mu > 1/2$ the cluster energy is conserved asymptotically in the sense that the limits

$$E^{\pm}_{a,\Omega} = \lim_{t \to \pm\infty} U^*_a(t) \ E_\Omega(H^a) \ P^{cont}_a \ U_a(t)$$

exist. Here P^{cont}_a is the projection onto the orthogonal complement of the span of all eigenfunctions of H^a. This provides a half-way through the obstacle. The remaining part requires the strong continuity of the asymptotic energy distribution :

$$E^{\pm}_{a,\Omega} \overset{s}{\to} 0 \quad \text{as} \quad |\Omega| \to 0$$

So for we have failed to prove this fact when Ω shrinks to a threshold of H^a. Actually, we conjecture that it might not be true, in general, for $N \geqslant 4$ due to the phase-space tunneling. The later refers to the phenomenon when the system in question oscillates between two open channels (i.e. different components of PS_E) one of which is a threshold channel (the relative velocity between two of the stable clusters is zero) :

zero relative vel.
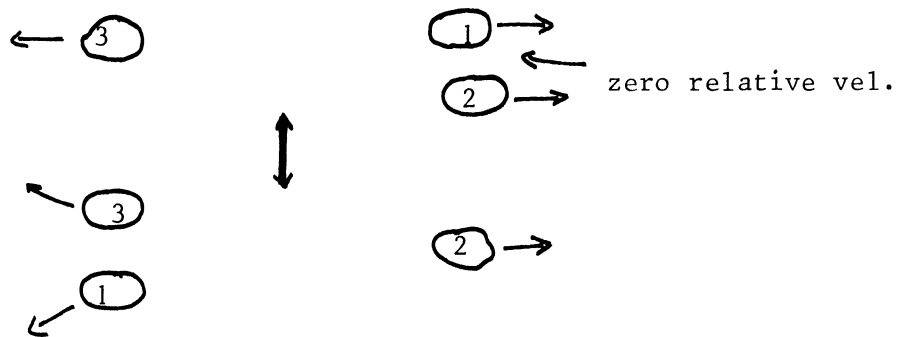
As a result the probability for the system to be outside of the propagation set vanishes too slowly to garantee the strong continuity of $E^{\pm}_{a,\Omega}$. Consequently, asymptotic completeness might fail for long-range systems.

Open problem. Determine whether the asymptotic energy distributions, $E^{\pm}_{a,\Omega}$, are continuous or not near the thresholds of H^a for Coulomb-type potentials ($\mu=1$) and for $N \geqslant 4$.

The domain of long-range scattering for $\mu < 1$ and $N \geqslant 4$ is almost unexplored. I wish good luck to young researchers.

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