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The quantum *N*-body problem

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This selective review is written as an introduction to the mathematical theory of the Schrödinger equation for N particles. Characteristic for these systems are the cluster properties of the potential in configuration space, which are expressed in a simple geometric language. The methods developed over the last 40 years to deal with this primary aspect are described by giving full proofs of a number of basic and by now classical results. The central theme is the interplay between the spectral theory of N-body Hamiltonians and the space–time and phase-space analysis of bound states and scattering states.
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I. INTRODUCTION

The quantum N-body problem has been posed since 1926 in a precise mathematical form: the Schrödinger equation for N particles interacting pairwise by two-body potentials which vanish at infinity. Together with the general principles of quantum mechanics this equation represents the simple, unifying basis for understanding all forms of nonrelativistic matter from the atomic point of view. Of course spin and statistics as well as the coupling to electromagnetic fields must be included to substantiate this claim, but these aspects will not be considered in our review.

The theories of atoms, molecules and solids evolving from this basis did not solve the N-body problem (for $N>2$) in any mathematical sense, but from the point of view of physics they achieved much more. Due to its classical flavor the Schrödinger equation lends itself beautifully to heuristic simplifications, thus leading to intermediate models describing particular situations. This process is of course necessary to reduce the quantitative complexity of the underlying ''exact'' theory to human (or machine) proportions, not only for doing computations, but also for understanding the results. Some of these model theories have also been studied from the mathematical point of view, but again this is not a topic of our review.

The mathematical theory of N-body quantum systems presented here is the result of a complementary effort, essentially over the last 40 years, to derive some basic dynamical properties of N-body systems directly from the Schrödinger equation and from general assumptions on the interactions. An overview is presented by the following condensed history:

1926 *Schrödinger:* The time-dependent Schrödinger equation for N-body systems.[84]

1932 *von Neumann:* Abstract Hilbert space and the mathematical foundations of quantum mechanics.[108]

1951 *Kato:* Self-adjointness and lower bound for a large class of N-body Schrödinger Hamiltonians including Coulomb systems.[63] These systems therefore fit into von Neumann's abstract framework with all its methods and results (dynamics described by a one-parameter unitary group, spectral theorem, etc.).

1959 *Hack:* Existence of scattering states for any prescribed asymptotic motion of independent, bound fragments in the case of short-range potentials (falling of faster than r^{-1}).[40] The conjecture stands that these scattering states together with the bound states span the entire Hilbert space (asymptotic completeness[60]).

1960 *Zhislin:* Determination of the essential spectrum of atomic Hamiltonians.[118] In the context of general N-body systems this result was rediscovered independently by Hunziker[47] and van Winter.[104] It forms the basis for all variational methods applied to the discrete spectrum. For example, the energy spectrum of atoms and positive ions below the first ionization threshold consists of infinitely many isolated eigenvalues of finite multiplicities.

1963 *Faddeev:* The first mathematical theory of three-body systems,[29] based on a system of coupled integral equations for the three-body Green's function (Faddeev equations), which becomes of Fredholm type after a number of iterations. This approach was later extended to arbitrary N by Yakubowsky[117] and Hepp,[43] but its power is limited by supplementary assumptions concerning the spectral properties of all subsystems of less than N particles.

1969 *Ruelle:* Ergodic space–time characterization of bound states versus continuum states,[82] simplified and generalized by Amrein and Georgescu[7] and by Enss.[26]

1970 *Efimov:* In contrast to the two-body case, three-body Hamiltonians with short-range potentials can have an infinite number of discrete eigenvalues (Efimov effect).[23,24] The first mathematical treatment is due to Yafaev.[113]

1971 *Lavine:* Asymptotic completeness of N-body systems with purely repulsive potentials.[68,69] The first time-dependent proof using a positive commutator argument (developed in general by Putnam[80] and Kato[64]).

1971 *Balslev, Combes:* Application of spectral deformation[4] to N-body Hamiltonians with dilation-analytic potentials.[10] This method reveals the general structure of the essential spectrum of H (thresholds, embedded eigenvalues, absence of singular continuous spectrum), and provides the basis for a theory of resonances.[96]

1972 *Iorio, O'Carroll:* Asymptotic completeness of N-body systems in the limit of weak potentials.[57] A simple perturbative approach using the Dyson expansion.

1973 *O'Connor:* Isotropic exponential bounds for N-body eigenfunctions in the discrete spectrum, with an exponent determined by the masses and the energy difference to the lowest threshold.[76] Later generalized in the dilation-analytic case to nonthreshold eigenvalues embedded in the continuous spectrum,[14] where absence of positive eigenvalues can be proved in a variety of cases (see e.g., Ref. 81, Vol. IV, Thm. XIII. 61).

1977 The advent of ''geometric'' (configuration space) methods of spectral analysis and scattering theory.[18,25,97,17,87] These methods combine the local analysis of a Schrödinger Hamiltonian (as a partial differential operator) with the global (operator) analysis in a very effective way, leading to essential simplifications and new results.

1978 *Deift et al.:* Anisotropic exponential bounds for N-body eigenfunctions in terms of the energy, all thresholds and the masses.[17] A concise form of this result is later given by Agmon[2] (Agmon distance).

1978 *Enss:* A short inspiring proof of asymptotic completeness for $N=2$, using only Ruelle's theorem and the propagation properties of free wave packets,[26] later extended to $N=3$.[27] This proof marks the turning point from geometric to phase-space analysis.

1981 *Mourre:* Mourre's inequality for $N=3$,[75] soon extended to general N by Perry, Sigal and Simon.[79] Mourre's inequality establishes the structure of the essential spectrum for very general interactions. It also exhibits the strict positivity of the virial in any sufficiently narrow energy shell in the continuous spectrum which is separated from thresholds and eigenvalues. The resulting propagation estimate (local decay) plays a key role in the proofs of asymptotic completeness.

1982 *Froese, Herbst:* Exponential bounds for eigenfunctions belonging to embedded, nonthreshold eigenvalues, and absence of positive eigenvalues,[31] supplemented by Perry.[78] The proofs are based on Mourre's inequality.

1987 *Sigal, Soffer:* The first general proof of asymptotic completeness for arbitrary N and short-range potentials.[91] The proof rests on the construction of a set of phase space observables $\phi(x,p,t)$ which have locally positive commutators with H and which control the asymptotic propagation into the possible scattering channels.

1990 *Graf:* A much simpler proof of the Sigal–Soffer theorem.[38] The improvement resultsfrom the construction of new propagation observables which are better tuned to the geometry of N-body configurations. A variant of this construction is introduced later in the proof given by Yafaev.[116]

1993 *Dereziński:* Proof of asymptotic completeness for long-range potentials (falling off faster than $r^{-\mu}$, $\mu=\sqrt{3}-1$).[19] This proof was prepared by preliminary results of Sigal and Soffer,[93,94] who give an independent proof for the Coulomb case $\mu=1$.[95]

This short history is necessarily incomplete, and so is our review. As a rule we only describe results which have been obtained for general N and for general classes of potentials. Not covered are, in particular, the Faddeev theory and its generalizations,[29,117,43] the many beautiful results for Coulomb systems including the stability of matter,[70,30] and N-body systems in external electric and magnetic fields, e.g., Refs. 44, 8, 120, 36, 37, 67, 1, and 101. On the other hand, we present some of the methods originating from N-body theory in abstract form since they have a wider range of applicability: e.g., spectral deformation, resonances, higher order Mourre theory.

II. BASIC DYNAMICS

In this section we discuss two fundamental properties of Schrödinger operators

$$H=p^2+V(x) \text{ on } \mathcal{H}=L^2(X), \tag{2.1}$$

where X is a Euclidean space, $x\in X$ and $p^2=-\Delta$. The first one is Kato's celebrated theorem which states that

$$H=H^*\geqslant E_0>-\infty$$

for a large class of potentials including N-body systems with Coulomb interactions.[63] This result may be regarded as the mathematical foundation of nonrelativistic quantum mechanics: it shows that the standard models of atoms and molecules fit into von Neumann's abstract Hilbert space theory of quantum systems. In particular, the Schrödinger equation

$$i\partial_t\psi=H\psi$$

generates a unitary group $U_t=e^{-iHt}:\psi_0\rightarrow\psi_t$ describing the time evolution of any initial state $\psi_0\in\mathcal{H}$ for all $t\in R$. Moreover, H has a spectral representation $H=\int\lambda d\,E_\lambda$ which in turn defines the energy distribution $d(\psi,E_\lambda\psi)$ for any state ψ (i.e., any $\psi\in\mathcal{H}$ with $\|\psi\|=1$) as a probability measure on the spectrum $\sigma(H)$ of H. The result that the energy H has a finite lower bound E_0 explains, e.g., the stability of atoms (even before invoking the Pauli principle). In fact, this lower bound is obtained in the stronger form

$$p^2\leqslant aH+b \tag{2.2}$$

for some constants a,b depending on V. This upper bound for the kinetic energy p^2 in terms of the conserved total energy plays a fundamental role. In *classical mechanics* (2.2) holds only if the function $V(x)$ is bounded from below. Then the inequalities

$$|x|\leqslant R, \quad (x,p)\leqslant E$$

define a finite volume in phase space. Since the canonical flow $(x_0,p_0)\to(x_t,p_t)$ generated by $H(x,p)$ is volume preserving (Liouville's theorem), it follows that almost all orbits $t\to(x_t,p_t)$ fall into two classes: either x_t remains bounded for all t, or x_t becomes unbounded in both time directions $t\to\pm\infty$ ("capture is a process of probability zero"). This theorem is due to Schwarzschild (see, e.g., Ref. 85). Its ***quantum analog***, given by Ruelle,[82] is the second fundamental result we wish to discuss. In the quantum case (2.2) implies that the set of states ψ satisfying the inequalities

$$(\psi,|x|\psi)\leqslant R, \quad (\psi,H\psi)\leqslant E$$

is compact in $\mathcal{H}$, and Liouville's theorem is replaced by the unitarity of the flow U_t in $\mathcal{H}$. As a result $\mathcal{H}$ splits into two U_t-invariant orthogonal subspaces

$$\mathcal{H}=\mathcal{H}_B\oplus\mathcal{H}_C\,.$$

Here $\mathcal{H}_B$ is the subspace of bound states, spanned by the eigenvectors of H. An orbit $t\to\psi_t$ in $\mathcal{H}_B$ is characterized by the condition that, for any $\varepsilon>0, x$ stays with probability $1-\varepsilon$ in some finite ball $|x|\leqslant R(\varepsilon)$ for all t. $\mathcal{H}_C=\mathcal{H}_B^{\perp}$ is the continuous spectral subspace of H. For an orbit $t\to\psi_t$ in $\mathcal{H}_C$ the probability to find x in any finite ball $|x|\leqslant R$ at time t vanishes in the time average over both time directions $-\infty<t\leqslant 0$ and $0\leqslant t<+\infty$. This general result sets the stage for the further analysis of N-body systems, where we will eventually arrive at much sharper statements concerning the localization of bound states and continuum states.

A. Self-adjointness

The construction of self-adjoint Hamiltonians of the type (2.1) is a well-developed art (see, e.g., Ref. 81, Vol. II). Here we only recall the original construction of Kato.[63]

Definition: A Kato potential on X is a real function $V\in L^2_{\mathrm{loc}}(X)$ *which, as a multiplication operator on* $L^2(X)$, *satisfies an estimate*

$$\|V\psi\|\leqslant\alpha\|p^2\psi\|+\beta(\alpha)\|\psi\| \tag{2.3}$$

for any $\alpha>0$ *and all* $\psi\in C_0^\infty(X)$.

Theorem 2.1:[63] *If V is a Kato potential on X, then* $H=p^2+V$ *is self-adjoint with domain* $D(H)=D(p^2)$ *and bounded from below. Moreover,* p^2 *is H-bounded with a bound*

$$\|p^2\psi\|\leqslant(1-\alpha)^{-1}(\|H\psi\|+\beta(\alpha)\|\psi\|)\,; \quad 0<\alpha<1. \tag{2.4}$$

Proof: V is a closed operator on its natural domain. Since $C_0^\infty(X)$ is a core of p^2, (2.3) extends to all $\psi\in D(p^2)$. Thus H is defined as a symmetric operator on $D(p^2)$, where

$$z-H=[1-V(z-p^2)^{-1}](z-p^2) \tag{2.5}$$

for Re(z)<0. From (2.3) we find $\|V(z-p^2)^{-1}\|\leqslant\alpha+\beta(\alpha)|\mathrm{Re}(z)|^{-1}<1$, if we choose $\alpha<1$ and $|\mathrm{Re}(z)|$ sufficiently large. Then (2.5) shows that $\mathrm{Ran}(z-H)=L^2(X)$ and that $z-H$ has a bounded inverse. Thus the resolvent set $\rho(H)$ of H contains a left half-plane, which proves the first part of the theorem. Equation (2.4) follows from (2.3). □

Here is a summary on Kato potentials:

Theorem 2.2: *(a) A real function* $V\in L^p(X)$ *is a Kato potential if* $p\geqslant 2$ and $2p>\dim(X)$. *(b) Let* $X=X_1\oplus X_2$ *be an orthogonal decomposition of X with adapted coordinates* $x=x_1+x_2$. *Sup-*

pose that V depends only on $x_1 : V(x) = V(x_1)$. *Then V is a Kato potential on X if and only if it is a Kato potential on* X_1. *(c) The Kato potentials on X form a real vector space.*

For a proof of (a) see Ref. 81, Vol. II, Thm.X.20. (b) and (c) are elementary.

Example: $V(x) = |x|^{-1}$ is a Kato potential on $X = R^3$ since it is the sum of an L^2-function [which is Kato by (a)] and a bounded function. Let $X = R^{3N}$ with coordinates $x_1, \ldots, x_n \in R^3$. By (b) the potentials $V_{ik} = |x_i - x_k|^{-1}$ $(i \neq k)$ are Kato potentials on X. By (c) this is also true for any real linear combination of the potentials V_{ik}. Therefore the total Coulomb potential of a system of N charged particles in R^3 is a Kato potential on R^{3N}. According to (b) this remains true if we fix the center-of-mass by restricting the configuration space R^{3N} to the subspace $\{x | \Sigma_{k=1}^{N} m_k x_k = 0\}$ where m_k is the mass of the particle k.

B. Bound states and continuum states

Lemma 2.3: Suppose that H is a self-adjoint operator on $L^2(X)$ *satisfying (2.2) for some constants a, b. Let* $f \in L^\infty(X)$ *with* $f(x) \to 0$ *as* $|x| \to \infty$. *Then the operator*

$$f(x)(z-H)^{-1} \text{ is compact} \tag{2.6}$$

for any z in the resolvent set $\rho(H)$. *We will refer to this by saying that H has the local compactness property.*

Proof: We use Cartesian coordinates $x = (x_1, \ldots, x_n)$ in X and the corresponding momentum operators $p = (p_1, \ldots, p_n)$, $p_k = -i \partial / \partial x_k$. Let $g \in L^\infty(X)$ with $g(x) \to 0$ as $|x| \to \infty$. Then the operator $f(x) g(p)$ is compact. This follows by observing that $f(x) g(p)$ is a norm limit of Hilbert–Schmidt operators $f_n(x) g_n(p)$, obtained by setting $f(x)$ and $g(x)$ equal to zero for $|x| > n$ and letting $n \to \infty$. [Notice that $f_n(x) g_n(p)$ is an integral operator with the square-integrable kernel $K(x,y) = f_n(x) \hat{g}_n(x-y)$, where $\hat{g}_n$ is the Fourier transform of g.] As a norm limit of compact operators $f(x) g(p)$ is compact. By (2.2) the operator $(1+p^2)(z-H)^{-1}$ is bounded. Therefore the product $f(x)(1+p^2)^{-1}(1+p^2)(z-H)^{-1}$ is compact. □

Self-adjointness and the local compactness property of H are the only ingredients of Ruelle's theorem:

Theorem 2.4:[82,7,26] *Suppose that* $H = H^*$ *on* $L^2(X)$ *has the local compactness property (2.6). Let* $\mathcal{H}_B$ *be the subspace spanned by all eigenvectors of H, and* $\mathcal{H}_C = \mathcal{H}_B^{\perp}$. *If* $\chi_R(x)$ *is the characteristic function of some ball* $|x| < R$, *then*

$$\varphi \in \mathcal{H}_B \Leftrightarrow \lim_{R \to \infty} \|(1-\chi_R) e^{-iHt} \varphi\| = 0 \quad \textit{uniformly in } 0 \leq t < \infty; \tag{2.7}$$

$$\psi \in \mathcal{H}_C \Leftrightarrow \lim_{t \to \infty} t^{-1} \int_0^t ds \, \|\chi_R e^{-iHs} \psi\|^2 = 0 \quad \textit{for any } R < \infty. \tag{2.8}$$

Replacing H by $-H$, we obtain the analogous theorem for negative times. We also note that two states φ and ψ with the space–time characteristic (2.7) and (2.8) are orthogonal:

$$(\phi, \psi) = 0. \tag{2.9}$$

In fact, (2.8) implies $\chi_R e^{-iHt} \psi \to 0$ for some sequence $t \to \infty$. Thus we can make

$$(\varphi, \psi) = (e^{-iHt} \varphi, \chi_R e^{-iHt} \psi) + ((1-\chi_R) e^{-iHt} \varphi, e^{-iHt} \psi)$$

arbitrary small by first choosing R and then t large enough.

Proof of Theorem 2.4: Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and suppose that zero is not an eigenvalue of H. By the mean ergodic theorem,

$$\lim_{t \to \infty} t^{-1} \int_0^t ds \, e^{-iHs} \psi = 0 \quad \forall \psi \in \mathcal{H}. \tag{2.10}$$

(This follows for $\psi = H\varphi$ by explicit integration, and these ψ are dense in $\mathcal{H}$ since zero is not an eigenvalue of H.) Now suppose that H has no eigenvalues. Then zero is not an eigenvalue of the operator $H\otimes 1 - 1\otimes H$ on $\mathcal{H}\otimes\mathcal{H}$ (a consequence of the spectral theorem), so that by (2.10)

$$0 = \lim_{t\to\infty} t^{-1}\int_0^t ds\,(\varphi\otimes\psi, e^{-iHs}\psi\otimes e^{iHs}\varphi)$$

$$= \lim_{t\to\infty} t^{-1}\int_0^t ds\,|(\varphi, e^{-iHs}\psi)|^2 \forall \varphi,\psi\in\mathcal{H}. \tag{2.11}$$

Now let $H = H^*$ be arbitrary and suppose that $K(i+H)^{-1}$ is compact for some bounded operator K. Then we claim that

$$\lim_{t\to\infty} t^{-1}\int_0^t ds\,\|K e^{-iHs}\psi\|^2 = 0 \tag{2.12}$$

for any vector ψ in the continuous spectral subspace $\mathcal{H}_C$ of H. Since it suffices to prove this for the dense set of vectors $\psi = (i+H)^{-1}\varphi, \varphi\in\mathcal{H}_C$, we may assume that K itself is compact. Then K is the norm limit of finite rank operators, which leaves us to prove (2.12) for operators K of rank one: $K e^{-iHs}\psi = (u, e^{-iHs}\psi)v$; $u,v\in\mathcal{H}$. Since $\psi\in\mathcal{H}_C$ we can choose $u\in\mathcal{H}_C$. Then (2.12) follows from (2.11) because H has no eigenvectors in $\mathcal{H}_C$. In the context of (2.4) this proves the direction $\Rightarrow$ of (2.8), since $\chi_R(i+H)^{-1}$ is compact. On the other hand the direction $\Rightarrow$ of (2.7) holds trivially for any eigenvector φ of H and thus for any $\varphi\in\mathcal{H}_B$. The opposite directions $\Leftarrow$ of (2.7) and (2.8) now follow from (2.9). □

III. *N*-BODY SYSTEMS

A system of N particles in R^3 with pair-interactions is described by the Hamiltonian

$$H = \sum_{k=1}^{N} \frac{p_k^2}{2m_k} + \sum_{i<k}^{1,\ldots,N} V_{ik}(x_i - x_k), \tag{3.1}$$

with $V_{ik}(x)\to 0$ as $|x|\to\infty$. From this standard case we extract the following basic notions:

A. Configuration space

The configuration space X of an N-body system is a Euclidean space with scalar product denoted by $x\cdot y$. In the case of (3.1), regarded in the center-of-mass (CM) frame:

$$X \equiv \left\{ x = (x_1,\ldots,x_N) \middle| x_k\in R^3; \sum m_k x_k = 0 \right\};$$

$$x\cdot y \equiv \sum m_k (x_k\cdot y_k)_{R^3}. \tag{3.2}$$

Here $\frac{1}{2}\dot{x}\cdot\dot{x} = \frac{1}{2}\dot{x}^2$ is the classical kinetic energy, and $p = \dot{x}$ is the momentum conjugate to x. In quantum mechanics,

$$H = \tfrac{1}{2}p^2 + V(x) \quad \text{on} \quad L^2(X), \tag{3.3}$$

where $p = -i\nabla$ and $p^2 = -\Delta$ have the usual form in Cartesian coordinates (not particle coordinates) of X.

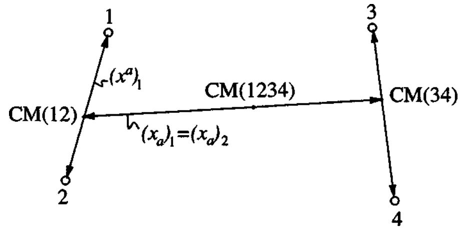

FIG. 1. The coordinates x_a and x^a.

1. Channels

In X there is a distinguished, finite lattice L of subspaces $a,b,\ldots$ (channels). L is closed under intersections and contains at least $a=\{0\}$ and $a=X$. In the case of (3.1) the channels correspond to all partitions of $(1,...,N)$ into clusters. For example, if $N=4$:

partition channel

$$(12)(34)\leftrightarrow a=\{x|x_1=x_2;x_3=x_4\}. \tag{3.4}$$

In general the partial ordering of L is defined by

$$a<b\leftrightarrow a\subset b; \quad a\neq b. \tag{3.5}$$

For each $a\in L$ there is an orthogonal decomposition:

$$X=a\oplus a^\perp : x=x_a+x^a . \tag{3.6}$$

This corresponds to the introduction of CM-coordinates. See Fig. 1 for the example (3.4).

The relation $p^2=(p_a)^2+(p^a)^2$ expresses the familiar decomposition of the kinetic energy into CM-parts and internal parts with respect to the clusters.

2. Intercluster distance

The basic feature of N-body systems is that they can split into widely separated, almost independent clusters. As a measure of the separation we might use the minimal distance $d_a(x)$ in R^3 of the clusters, e.g.,

$$d_a(x)=\min_{i\in(12);k\in(34)}|x_i-x_k| \tag{3.7}$$

in the example (3.4). However, we prefer to express the separation in terms of the geometry of X. Some reflection shows that $d_a(x)=0\Leftrightarrow x\in b, b\cap a<a$.

Figure 2 shows the unit sphere in X, intersected by two channels a,b with $b\cap a=c<a$. This leads to the definition of the *intercluster distance*

$$|x|_a\equiv\min_{b\cap a<a}|x^b| \quad \text{for any} \quad a>\{0\}. \tag{3.8}$$

In the example (3.4) one finds

$$|x|_a=\min_{i\in(12);k\in(34)}\left(\frac{m_im_k}{m_i+m_k}\right)^{1/2}|x_i-x_k|.$$

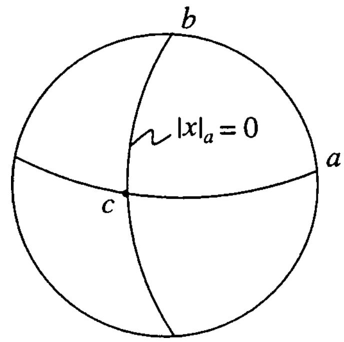

FIG. 2. Intercluster distance.

The set of all configurations $x \in a$ with $|x|_a > 0$ is given by

$$a^* = a \setminus \bigcup_{c < a} c \tag{3.9}$$

(empty for $a = \{0\}$), and these sets form a disjoint covering of $X \setminus \{0\}$. We note that $|x + sy|_a \to \infty$ as $s \to \infty$ for the translations

$$x \to x + sy; \quad s \in R, y \in a^*. \tag{3.10}$$

These translations separate the clusters in channel a without affecting their internal configuration x^a.

B. Hamiltonians

We assume that for each $a > \{0\}$ the potential $V(x)$ has the cluster property

$$\begin{gathered} V(x) = V^a(x^a) + I_a(x); \\ I_a(x) \leqslant f(|x|_a) \to 0 \quad \text{as} \quad |x|_a \to \infty. \end{gathered} \tag{3.11}$$

In particular $I_a = V$ for $a = X$. For $a = \{0\}$ we define $I_a = 0$. In the example (3.4),

$$V^a = V_{12} + V_{34}; \quad I_a = V_{13} + V_{14} + V_{23} + V_{24}.$$

Corresponding to $L^2(X) = L^2(a) \otimes L^2(a^\perp)$, we write

$$\begin{gathered} H = H_a + I_a; \\ H_a = \tfrac{1}{2}(p_a)^2 \otimes 1 + 1 \otimes H^a; \\ H^a = \tfrac{1}{2}(p^a)^2 + V^a(x^a) \quad \text{on} \quad L^2(a^\perp). \end{gathered} \tag{3.12}$$

Here H_a describes the dynamics of the system of noninteracting clusters, and H^a describes their (joint) internal dynamics.

1. Conditions on the potential

The rate at which $I_a(x)$ [and later also derivatives of $I_a(x)$] vanishes as $|x|_a \to \infty$ will be essential for many dynamical aspects. In addition to the cluster properties some global condition is required to make all the Hamiltonians (3.12) self-adjoint. For the purpose of this review we assume that V is a Kato potential. This property is automatically inherited by the potentials V^a. Let

$$T_s: \quad \psi(x) \to \psi(x - sy) \tag{3.13}$$

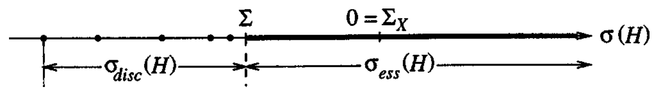

FIG. 3. Discrete and essential spectrum of *H*.

be the unitary translation operator corresponding to (3.10). By (3.11) the potential V^a is then determined by

$$V^a \psi = \lim_{s\to\infty} T_{-s} V T_s \psi \quad \forall \psi \in C_0^\infty(X). \tag{3.14}$$

Since p^2 is translation invariant it follows that $V^a(x^a)$ is a Kato potential on X and thus on $a^\perp$. Therefore all the Hamiltonians (3.12) are self-adjoint and possess the local compactness property. In the following we will not reiterate these basic assumptions on $V(x)$. All of the results we report have been established for substantially larger classes of potentials. For a particularly lucid discussion of this aspect we refer to Ref. 39.

2. Induction principle

As a result we have arrived at a simple mathematical definition of N-body systems involving only three ingredients:

$$\begin{aligned}&(1)\ \text{a configuration space } X,\\ &(2)\ \text{a lattice } L \text{ of channels } a\subset X,\\ &(3)\ \text{conditions on } I_a(x).\end{aligned} \tag{3.15}$$

In this sense each Hamiltonian H^a also describes an N-body system with reduced configuration space $a^\perp$, with channels $b\cap a^\perp$, $b \geqslant a$ and with corresponding intercluster potentials $I_b(x^a)$, which we call a *subsystem*. Any proposition P derived from (3.16) can therefore be established by induction on the lattice L. To begin with, P is verified in the trivial case $a=X{:}H^a=0$ on $L^2(\{0\})=C$. Then P is proved for $a=\{0\}{:}H^a=H$, under the induction hypothesis that P holds for any H^a with $a>\{0\}$. This *induction in subsystems* is in fact more convenient than an induction in the particle number N.

C. Discrete and essential spectrum

Here we prove that the spectrum $\sigma(H)$ is of the form in Fig. 3:

$$\Sigma = \min_{a>\{0\}} \Sigma_a ; \quad \Sigma_a = \min(\sigma(H^a)).$$

Σ is the lowest energy threshold for breaking the system into independent parts. Therefore $\sigma(H)$ contains the continuous part $[\Sigma,\infty)$. Less obvious is the fact that H has only *discrete spectrum* below Σ. By definition, the discrete spectrum $\sigma_{\text{disc}}(H)$ of a self-adjoint operator H is the set of all *isolated eigenvalues of finite multiplicity* (isolated from the rest of the spectrum). The *essential spectrum* of H is the complement

$$\sigma_{\text{ess}}(H) \equiv \sigma(H) \backslash \sigma_{\text{disc}}(H). \tag{3.16}$$

Theorem 3.1:[47,104,118]

$$\sigma_{\text{ess}}(H) = [\Sigma,\infty). \tag{3.17}$$

Proof: Step 1: $[\Sigma,\infty)\subset\sigma(H)$. By (3.12) $\sigma(H_a)=[\Sigma_a,\infty)$ for $a>\{0\}$, since the kinetic energy makes the spectrum continuous. To prove that $\sigma(H_a)\subset\sigma(H)$, let $\lambda\in\sigma(H_a)$. Then $\|(\lambda-H_a)\psi\|<\varepsilon$ for any $\varepsilon>0$ and some $\psi\in C_0^\infty(X)$, $\|\psi\|=1$. By (3.14)

$$HT_s\psi\to H_aT_s\psi \quad (s\to\infty)$$

in norm. Therefore $\|(\lambda-H)T_s\psi\|<\varepsilon$ for some s, which shows that $\lambda\in\sigma(H)$.

Step 2: $\sigma_{\text{ess}}(H)\subset[\Sigma,\infty)$. We introduce a *partition of unity on X*, i.e., a finite family $\{j_a\}$ of real C^∞-functions on X with the property

$$\sum_a j_a^2(x)\equiv 1. \tag{3.18}$$

Then H can be decomposed into pieces localized in the supports of j_a plus a localization error:

$$H=\sum_a j_aHj_a+\frac{1}{2}\sum_a [j_a,[j_a,H]]=\sum_a j_aHj_a-\frac{1}{2}\sum_a |\nabla j_a|^2. \tag{3.19}$$

In our case a labels all channels $a>\{0\}$. Then the sets

$$S_a=\{x\in X|\ |x|=1\ ;|x|_a>0\}$$

form an open covering of the unit sphere S of X. Therefore there exists a partition of unity $\{j_a\}$ on S with supp $(j_a)\subset S_a$. Since these supports are compact it follows that

$$|x|_a\geqslant\varepsilon>0 \quad \text{on supp}\,(j_a) \quad \forall a>\{0\}.$$

Next, the partition of unity $\{j_a\}$ is extended from S to the region $|x|>1$ by setting $j_a(x)=j_a(x|x|^{-1})$. In the region $|x|<1$ we choose an arbitrary smooth extension satisfying (3.19). The resulting partition on X has the properties

$$\begin{aligned} j_a(\lambda x)&=j_a(x) \quad \text{for } |x|\geqslant 1,\lambda\geqslant 1;\\ |x|_a&\geqslant\varepsilon|x| \quad \text{for } |x|\geqslant 1, x\in\text{supp}\,(j_a). \end{aligned} \tag{3.20}$$

Therefore the functions $|\nabla j_a(x)|^2$ and $j_aI_a(x)j_a$ vanish as $|x|\to\infty$: as operators they are compact relative to H. As a result

$$H=\sum_{a>\{0\}} j_aH_aj_a+K$$

with K compact relative to H. By a theorem of Weyl (Ref. 81, Vol. IV, Thm. XIII. 14)

$$\sigma_{\text{ess}}(H)=\sigma_{\text{ess}}\left(\sum_{a>\{0\}} j_aH_aj_a\right). \tag{3.21}$$

Since $H_a\geqslant\Sigma$ it follows with (3.19) that the operator appearing on the right is bounded below by Σ, and we conclude that $\sigma_{\text{ess}}(H)\subset[\Sigma,\infty)$. □

IV. DISCRETE SPECTRUM

A. Exponential bounds for eigenfunctions

We consider a discrete eigenvalue $E<\Sigma$ of H and a corresponding bound state wave function $\psi(x)$. In the two-body case (where $\Sigma=0$) $\psi(x)$ has a universal exponential bound

$$f(x)=|x_1-x_2|\sqrt{-2mE}$$

in the following sense: for any $\alpha<1$ there is a constant C_α such that

$$|\psi(x)|\leqslant C_\alpha e^{-\alpha f(x)}.$$

The reason why we cannot set $\alpha=1$ is exemplified by the polynomial factors in the hydrogen wave functions. In this section we construct the analogous exponential bound in the N-body case: a positive function $f(x)$, homogeneous of degree 1, determined implicitly by the energy E and by the thresholds

$$\Sigma_a=\min(\sigma(H^a));\quad a>\{0\}.$$

Although an analytic expression of $f(x)$ is not known, weaker bounds can be given explicitly. All these bounds are expressed by the Euclidean metric (3.2) which describes their dependence on the masses.

Theorem 4.1:[17] *Let $H\psi=E\psi, E<\Sigma$. If $f(x)$ is homogeneous of degree 1, and has the Lipschitz properties*

$$|f(x)-f(y)|\leqslant\lambda_a|x-y|;\quad \lambda_a\equiv\sqrt{2(\Sigma_a-E)} \tag{4.1}$$

for all $a\in L, a>\{0\}$, and all $x,y\in a$, then f is an exponential bound for ψ in the sense that

$$e^{\alpha f}\psi\in L^\infty(X)\quad for\ \ any\quad \alpha<1. \tag{4.2}$$

In particular, the pointwise supremum $\bar{f}$ of all these exponential bounds f is an exponential bound.

The bound $\bar{f}$ is determined by the energy E and the thresholds Σ_a. Weaker bounds obtained from Theorem 4.1 are also useful, especially the isotropic bound

$$f(x)=|x|\sqrt{2(\Sigma-E)} \tag{4.3}$$

due to O'Connor.[76] In general, the bound $\bar{f}$ will be highly anisotropic with range in

$$|x|\sqrt{2(\Sigma-E)}\leqslant\bar{f}(x)\leqslant|x|\sqrt{-2E}.$$

Some examples are found in Ref. 17, but a general explicit form of $\bar{f}$ is not known. Agmon[2] has expressed the bound $\bar{f}$ as a geodesic distance in terms of the following Riemannian metric on X. To any $x\in X$ there is associated a unique minimal channel $m(x)\in L$ containing x:

$$m(x)=\bigcap_{a\ni x} a. \tag{4.4}$$

Expressed in particle coordinates $(x_1,\ldots,x_N)$: two particles i,k belong to the same cluster of $m(x)$ exactly if $x_i=x_k$. We remark that $m(x)\leqslant m(y)$ for all y in some neighborhood of x. The *Agmon metric* on X is defined in terms of the Euclidean metric (3.2) by the line element

$$ds^2=2(\Sigma_{m(x)}-E)dx^2, \tag{4.5}$$

where, by the remark above, the coefficient function $(\Sigma_{m(x)}-E)$ is lower semi-continuous in x. A path $p\subset X$, given by a function $x(t)$ on $0\leqslant t\leqslant 1$, has the Agmon length

$$s(p)=\int_0^1 dt\,\lambda_{m(x(t))}|\dot{x}(t)|$$

with λ_a defined by (4.1). Since $\lambda(x(t))$ is semi-continuous in t this is well defined for square integrable $\dot{x}(t)$. The Agmon distance $d(x,y)$ between x and y is the infimum of $s(p)$, taken over all paths p joining x,y. We refer to Ref. 13 for a proof that this infimum is a minimum, and for a discussion of Agmon geodesics.

Theorem 4.2:[2] *The exponential bound $\overline{f}$ given in Theorem 4.1 is $\overline{f}(x)=d(0,x)\equiv\rho(x)$.*

Proof: Evidently $\rho(x)$ is homogeneous of degree 1. By the geodesic triangle inequality,

$$|\rho(x)-\rho(y)|\leqslant d(x,y)\leqslant\lambda_a|x-y|$$

for $x,y\in a$. This proves $\rho\leqslant\overline{f}$. To show the converse we choose a path p from 0 to x with $s(p)<\rho(x)+\varepsilon$. Approximating $\dot{x}(t)$ by a step function in L^2-sense, we see that p may be taken as a polygon of straight lines $p_1,\ldots,p_n$. For each p_k we define

$$a_k=\bigcap_{a\supset p_k} a\in L.$$

Then $\lambda_{m(x)}=\lambda_{a_k}$ for all $x\in p_k$, with the possible exception of a single point (a straight line $p\not\subset a$ can intersect a only in one point). Therefore $s(p_k)=\lambda_{a_k}|p_k|$, where $|p_k|$ is the Euclidean length of p_k. On the other hand, (4.1) implies $|\Delta\overline{f}|\leqslant\lambda_{a_k}|p_k|$ for the increment $\Delta\overline{f}_k$ of $\overline{f}$ along p_k. Therefore $\overline{f}(x)=\Sigma_k\Delta\overline{f}_k\leqslant\Sigma_k\lambda_{a_k}|p_k|=s(p)\leqslant\rho(x)+\varepsilon$. □

We now return to the derivation of Theorem 4.1. Instead of (4.2) we will only prove the L^2-bound:

$$e^{\alpha f}\psi\in L^2(X)\quad\text{for any}\quad\alpha<1. \tag{4.6}$$

Since f is uniformly Lipschitz, the L^∞-bound (4.2) then follows by a general argument given in Ref. 17. The basic tool for estimating exponential tails of eigenfunctions is simple:

Lemma 4.3: Suppose that $H\psi=E\psi$. Let $J,f\in C^2(X)$ be non-negative with bounded derivatives, and let $\operatorname{supp}(\nabla J)$ *be compact. If*

$$J(H-\tfrac{1}{2}|\nabla f|^2-E)J\geqslant\delta J^2 \tag{4.7}$$

for some $\delta>0$, then

$$\|e^fJ\psi\|\leqslant\delta^{-1}\|e^f[H,J]\psi\|. \tag{4.8}$$

The hypothesis allows $f(x)\to\infty$ as $x\to\infty$. The bound (4.8) is finite, since f is bounded on $\operatorname{supp}(\nabla J)$. Typically, J will be a smoothed characteristic function of a set $|x|>R$. Then (4.8) implies $\exp(f)\psi\in L^2(X)$.

Proof: Suppose first that f is bounded, and let

$$H_f\equiv e^fHe^{-f}=H-\frac{1}{2}|\nabla f|^2+\frac{i}{2}(\nabla f\cdot p+p\cdot\nabla f).$$

Then $(H_f-E)u=0$ for $u=e^f\psi$, so that (4.7) implies

$$\delta\|Ju\|^2\leqslant\operatorname{Re}(Ju,(H_f-E)Ju)\leqslant\|Ju\|\,\|[H_f,J]u\|,$$

which proves (4.8). If f is unbounded, we replace it by $f_\varepsilon=f(1+\varepsilon f)^{-1},g>0$. Since $|\nabla f_\varepsilon|\leqslant|\nabla f|$, (4.8) holds for f_ε uniformly in ε, and extends to f in the limit $\varepsilon\to0$. □

The next step is to prove a smooth version of Theorem 4.1:

Lemma 4.4: Theorem 4.1 holds if the Lipschitz condition (4.1) is replaced by the stronger differentiability condition

$$f\in C^2(X\backslash\{0\});\quad |\nabla f(x)|^2\leqslant 2(\Sigma_{m(x)}-E) \tag{4.9}$$

for all $x\in S=$ *unit sphere of* X.

Proof: Let $g=\alpha f, \alpha<1$. Then

$$|\nabla g|^2\leqslant 2(\Sigma_{m(x)}-E-\varepsilon) \tag{4.10}$$

for some $\varepsilon>0$ and all $x\in S$. Each $y\in S$ has a neighborhood $S_y\subset S$ given by

$$S_y\equiv\{x\in S|2|x|_{m(y)}>|y|_{m(y)};|\nabla g(x)|^2<|\nabla g(y)|^2+\varepsilon\}, \tag{4.11}$$

where we have used the definitions (3.8) and (4.4). As in the proof of Theorem 3.1, we pick a finite covering $\{S_y\}$ of S, and then construct a partition of unity $\{j_y\}$ on X with the properties

$$\mathrm{supp}\,(j_y)\subset S_y;\quad j_y(x)=j_y(x/|x|)\quad \text{for}\quad |x|>1.$$

From (3.20) we obtain

$$H-\frac{1}{2}|\nabla g|^2-E=\sum_y j_y\left(H-\frac{1}{2}|\nabla g|^2-E\right)j_y-\frac{1}{2}\sum_y |\nabla j_y|^2.$$

By construction, $|\nabla j_y(x)|\to 0$ and $I_{m(y)}j_y(x)\to 0$ as $x\to\infty$. Let J be a real, smooth, bounded function supported in $\{|x|>R\}$. Using (4.10), (4.11) and $H_a\geqslant\Sigma_a$ we find

$$J\left(H-\frac{1}{2}|\nabla g|^2-E\right)J\geqslant\left(\frac{\varepsilon}{2}-o(R)\right)J^2.$$

Taking R sufficiently large, we conclude from Lemma 4.3 that $e^g\psi\in L^2(X)$. □

The proof of Theorem 4.1 is by regularization: f can be approximated by a smooth exponential bound according to Lemma 4.4. Since this regularization is somewhat technical, we refer to Ref. 53.

B. The number of discrete eigenvalues

1. Infinite discrete spectrum

For $N=2$ the discrete spectrum of H is finite if the potential $V(x)$ has short range, whereas a long-range attractive potential will always produce an infinite number of bound states below the continuous spectrum. The border line between short- and long-range potentials is marked by the asymptotic behavior $V(x)\sim|x|^{-\mu}(|x|\to\infty)$ with $\mu=2$, since $|x|^{-2}$ scales with x like the Laplacian. (In scattering theory there is a different border line $\mu=1$.) For $N>2$ the question whether $\sigma_{\mathrm{disc}}(H)$ is finite or infinite cannot be answered solely in terms of the asymptotic fall-off of some intercluster potentials $I_a(x)$: the nature of the threshold Σ at the bottom of the continuous spectrum also plays a decisive role. We begin with some results for the case where Σ is a *two-cluster threshold*. This means that for the energy Σ and slightly above, the system can only desintegrate into two bound clusters C_1, C_2 (see Fig. 4).

This situation can be represented by a product wave function

$$\psi(x)=u(x_a)\phi(x^a);\quad H^a\phi=\Sigma\phi \tag{4.12}$$

with (u,p_a^2u) arbitrary small. The condition that Σ is a two-cluster threshold means that Σ is a *discrete* eigenvalue of H^a, so that ϕ has an exponential bound

$$|\phi(x^a)|\leqslant\mathrm{const}\exp(-\alpha|x^a|),\quad \alpha>0. \tag{4.13}$$

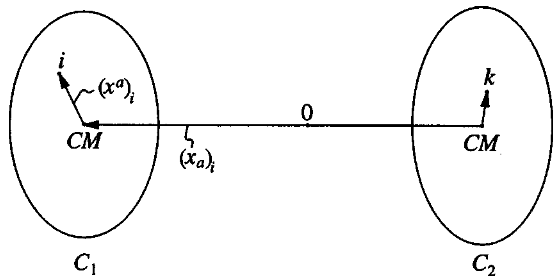

FIG. 4. Two bound clusters.

Using states ψ of the form (4.12) as trial states to make $(\psi,H\psi)<\Sigma$, it is a simple matter to show that $\sigma_{\rm disc}(H)$ is infinite if $I_a(x)$ has a long-range attractive part. For simplicity we write this out in the case of Coulomb potentials

$$I_a(x)=\sum_{i\in C_1;k\in C_2}\frac{e_ie_k}{|x_i-x_k|};\quad \sum_{i\in C_1;k\in C_2}e_ie_k<0,$$

assuming that the clusters have opposite total charges. Using the exponential bound (4.13) it follows that

$$|(\psi,(I_a(x)-I_a(x_a))\psi)|\leqslant \text{const}|x_a|^{-2},$$

and therefore

$$(\psi,(H-\Sigma)\psi)\leqslant\left(u,\left(\frac{1}{2}p_a^2-\frac{q}{|x_a|}+\text{const}|x_a|^{-2}\right)u\right);\quad q<0.$$

Now let $u\in C_0^\infty(R^3)$, $\|u\|=1$ and supp(u) in $1<|x_a|<2$. Then the orthonormal functions

$$u_n(x_a)=n^{-3/2}u(n^{-1}x_a),\quad n=1,2,4,8,\ldots,$$

have disjoint supports, so that the corresponding trial states ψ_n satisfy

$$(\psi_n,H\psi_m)=0\quad(n\neq m);\ \ (\psi_n,(H-\Sigma)\psi_n)\leqslant\frac{q}{n}+\text{const}\,n^{-2}<0,$$

if n is sufficiently large. Therefore, by the min–max principle, H possesses infinitely many (discrete) eigenvalues below Σ. The same proof applies to attractive pair potentials $\sim-|x_i-x_k|^{-\mu}$, $0<\mu<2$, and also if additional short-range potentials are present in $I_a(x)$. The result shows that neutral atoms and positive ions always have infinite discrete spectrum.[118] The accumulation of eigenvalues at Σ can be discussed by using trial wave functions ψ_{nlm} of the form (4.12) with hydrogenic eigenfunctions $u_{nlm}(x_a)$ corresponding to an energy $-n^{-2}$ in suitable units. Then it can be shown that

$$\|(H-E_n)\psi_{nlm}\|\leqslant\text{const}\,n^{-\alpha};\quad \alpha>3$$

for $E_n=\Sigma-n^{-2}$, if $l\leqslant n$ grows sufficiently fast with n ($l=n$ corresponding to a circular classical hydrogen orbit). This means that H has groups of eigenvalues close to E_n compared to the spacing $E_{n+1}-E_n$ as $n\to\infty$ (Rydberg states). By taking symmetries into account this result can be established for any multiplet system.[48]

2. Finite discrete spectrum

Here we show that $\sigma_{\rm disc}(H)$ is finite if the relevant intercluster potentials have short range and if Σ is a two-cluster threshold. A channel $a \in L$ is said to be a *two-cluster channel* if

$$b < a \Rightarrow b = \{0\}. \tag{4.14}$$

These channels correspond to the partitions of $(1,...,N)$ into two clusters. The set of two-cluster channels will be denoted by m. The lowest threshold Σ of H always coincides with Σ_a for some $a \in m$, since $\Sigma_a \leqslant \Sigma_b$ if $a < b$. Σ is called a two-cluster threshold if $\Sigma_a = \Sigma$ *only* for $a \in m$.

Theorem 4.5:[114,119,121,87] *Suppose that $\Sigma_a = \Sigma$ only if $a \in m$ and in that case*

$$I_a(x) \geqslant -c(1+|x|_a)^{-\mu}, \quad \mu > 2 \tag{4.15}$$

for large $|x|_a$. Then the discrete spectrum of H is finite.

Proof: We give an outline of the proof, deferring the details to the subsequent discussion. The starting point is the localization formula (3.20) for a specially adapted partition of unity $\{j_a\}$ on X. The first step is a purely geometric estimate of the localization error in the form

$$F \equiv \sum_a |\nabla j_a|^2 \leqslant \sum_a j_a F_a j_a \tag{4.16}$$

with multification operators $F_a = F_a(x)$, leading to $H \geqslant \Sigma_a j_a (H - F_a) j_a$. Each term in this sum is then further estimated from below by

$$j_a(H - F_a) j_a \geqslant j_a B_a j_a, \tag{4.17}$$

where B_a is self-adjoint with purely discrete and finite spectrum below Σ, i.e.,

$$B_a \geqslant C_a + \Sigma; \quad C_a \text{of finite rank.} \tag{4.18}$$

Therefore H has an estimate $H \geqslant C + \Sigma$ with $C = \Sigma_a j_a C_a j_a$ of finite rank. It follows from the min–max principle that the number of eigenvalues (including multiplicities) of H below Σ is bounded by the finite number of negative eigenvalues of C. □

We now describe the steps of the proof in detail. The geometry of two-cluster channels is very simple: for $a, b \in m$

$$a^* = a \setminus \bigcup_{b<a} b = a \setminus \{0\}; \quad a \cap b = \{0\} \quad \text{if } a \neq b.$$

It follows from (3.9) that, on the unit sphere $|x| = 1$, the channels $a \in m$ are *disjoint*, and that the intercluster distance $|x|_a$ is strictly positive for all $x \in a$. The partition of unity $\{j_a\}$ used in the proof of Theorem 3.1 can therefore be adapted to have the following properties:

(1) $j_{\{0\}}(x)$ is equal to one for $|x| \leqslant R - 1$ and vanishes for $|x| > R$, where R may be fixed arbitrary large.
(2) The functions j_a for $a \in m$ have disjoint supports.
(3) For $a > \{0\}$ the functions j_a are homogeneous of degree zero for $|x| > R$, and, on supp(j_a), $|x|_a > \lambda |x|$ for some $\lambda > 0$.

In particular we take R sufficiently large so that for all a with $\Sigma_a = \Sigma$

$$I_a(x) \geqslant -C|x|^{-\mu} \quad \text{on supp}(j_a). \tag{4.19}$$

Lemma 4.6: For any $\varepsilon > 0$ the estimate (4.16) holds with

$$F_a=(1+|x|)^{-2}\begin{cases}\varepsilon & if \quad a\in \boldsymbol{m},\\ c_\varepsilon & if \quad a\neq \boldsymbol{m}.\end{cases} \tag{4.20}$$

Proof: Since $F(x)$ is homogeneous of degree -2 for $|x|>R$ while $j_a(x)$ is homogeneous of degree zero, it suffices to prove that

$$F\leqslant \varepsilon \sum_{a\in m} j_a^2 + c_\varepsilon \sum_{a\neq m} j_a^2$$

for $|x|\leqslant R$ and any $\varepsilon>0$. Since the functions j_a with $a\in m$ have disjoint supports,

$$F=0 \quad \text{on the set} \quad \left\{x \,\middle|\, \sum_{a\in m} j_a^2(x)=1\right\}.$$

Therefore, by continuity,

$$F\leqslant \frac{\varepsilon}{1-\delta}\sum_{a\in m} j_a^2,$$

where $\delta=\delta(\varepsilon)\rightarrow 0$ as $\varepsilon\rightarrow 0$. On the complement of this set

$$\sum_{a\neq m} j_a^2 \geqslant \delta \Rightarrow F\leqslant F\frac{1}{\delta}\sum_{a\neq m} j_a^2.$$

□

To derive the estimates (4.17) and (4.18) we distinguish between different types of channels.

The channel $a=\{0\}$. Here we set $B_{\{0\}}=f(x)(H-c_\varepsilon)f(x)$, where $f\in C_0(X)$ is equal to one on supp$(j_{\{0\}})$. Let P be the projection onto the spectral subspace $H<c_\varepsilon$. Then $B_{\{0\}}\geqslant f(x)P(H-c_\varepsilon)Pf(x)$. By the local compactness property of H this lower bound is a compact operator with purely discrete spectrum below zero, of which only a finite part is below $\Sigma<0$.

The channels a with $\Sigma_a>\Sigma$. Here we set

$$B_a=H_a+\tilde{I}_a(x)-c_\varepsilon(1+|x|)^{-2};\quad \tilde{I}_a(x)=I_a(x)\chi_a(x),$$

where $\chi_a(x)$ is the characteristic function of supp(j_a). Since $\tilde{I}_a(x)$ vanishes as $|x|\rightarrow\infty$ we have $\sigma_{\text{ess}}(B_a)=\sigma_{\text{ess}}(H_a)=[\Sigma_a,\infty)$. Therefore, the spectrum of B_a below $\Sigma<\Sigma_a$ is discrete and finite.

The channels a with $\Sigma_a=\Sigma$. Here we choose $B_a=H_a-W_a(x)$, where $-W_a(x)$ is a lower bound of $I_a(x)-\varepsilon(1+|x|)^{-\mu}$, restricted to the support of j_a:

$$W_a(x)=\chi_a(x)[\text{const}(1+|x|)^{-\mu}+\varepsilon(1+|x|)^{-2}]. \tag{4.21}$$

By hypothesis Σ is the lowest, discrete eigenvalue of H^a. Let P^a be the corresponding eigenprojection and $Q^a=1-P^a$. On $L^2(X)=L^2(a)\otimes L^2(a^\perp)$ we define

$$P_a=1\otimes P^a;\quad Q_a=1\otimes Q^a.$$

Next we apply the Combes–Simon inequality: Let A be a self-adjoint operator and P an orthogonal projection which maps the domain of A into itself. Let $Q=1-P$ and $\delta>0$. Then

$$A\geqslant PAP+Q(A-\delta)Q-\delta^{-1}PAQAP, \tag{4.22}$$

which just another form of writing

$$0\leqslant(\delta^{-1}PA+1)\delta Q(\delta^{-1}AP+1).$$

Using (4.22) to estimate B_a from below we obtain

$$B_a \geqslant P_a(H_a - W_a - \delta^{-1} W_a Q_a W_a) P_a + Q_a(H_a - W_a - \delta) Q_a \tag{4.23}$$

since P_a commutes with H_a. Now we are left with proving that the two terms on the right of (4.23), viewed respectively as operators on Ran(P_a) and Ran(Q_a), have purely discrete, finite spectra below Σ. The same then follows by the min–max principle for the operator B_a on $\mathcal{H}$. The first term, as an operator on Ran(P_a), is bounded below by

$$\Sigma + (\tfrac{1}{2} - 4\varepsilon) p_a^2 - \text{const}(1 + |x_a|)^{-\mu} \tag{4.24}$$

for the following reasons:

$$H_a \geqslant \Sigma + \tfrac{1}{2} p_a^2 \quad \text{on} \quad \text{Ran}(P_a);$$

$$W_a(x) \leqslant W_a(x_a) \leqslant \text{const}(1 + |x_a|)^{-\mu} + \varepsilon(1 + |x_a|)^{-2};$$

$$\varepsilon(1 + |x_a|)^{-2} \leqslant \varepsilon |x_a|^{-2} \leqslant 4\varepsilon p_a^2;$$

$$W_a Q_a W_a \leqslant W_a^2 \leqslant \text{const}(1 + |x_a|)^{-4}.$$

Now we fix $\varepsilon < 1/8$. Then, apart from the constant Σ, (4.24) is a Schrödinger operator on $L^2(a)$ with a regular, spherically symmetric potential $V(|x|)$ vanishing faster than $|x|^{-2}$ at ∞. This operator has a discrete, finite spectrum below zero, and the same follows for the spectrum of (4.24) below Σ.

In discussing the second term of (4.23) we only use that W_a is compact relative to H_a on $L^2(X)$. Since Q_a commutes with H_a it follows that $Q_a W_a Q_a$ is compact relative to H_a on Ran(Q_a), where $\sigma_{\text{ess}}(H_a) = [\Sigma_1, \infty)$, $\Sigma_1 > \Sigma$. By Weyl's theorem $H_a - \delta - Q_a W_a Q_a$ has essential spectrum $[\Sigma_1 - \delta, \infty)$ on Ran(Q_a). Fixing now $\delta < \Sigma_1 - \Sigma$ it follows that the operator $Q_a(H_a - \delta - W_a)Q_a$ on Ran(Q_a) has a purely discrete, finite spectrum below Σ. This concludes the proof of Theorem 4.5.

Notes: Exponential bounds for eigenfunctions. For a review of other results, see Ref. 46.

Finite vs. infinite discrete spectrum. If Σ is not a two-body threshold in the sense of Theorem 4.5, then the discrete spectrum of H is still finite if none of the operators H^a with $\Sigma_a = \Sigma$ has a resonance at the bottom of its spectrum, i.e., a solution of $H^a \psi = \Sigma \psi$ which vanishes as $|x^a| \to \infty$ too slowly to be square integrable (see Refs. 110, 111, and 109, and references quoted therein). For bounds on the number of eigenvalues, see Refs. 115, 66, and 88. However, if the no-resonance condition stated above is violated, then shortrange forces can create infinite discrete spectrum. This was discovered for three-body systems by Efimov[23,24,5] and proven by Yafaev.[113,112]

Coulomb sytems. Atoms and stable ions provide examples where Σ is a two-cluster threshold. The proof of Theorem 4.5 can be extended to prove that negative ions have finite discrete spectrum.[114,87] It was shown by Ruskai[83] and Sigal[87] that a given nucleus can bind only a finite number of electrons. To find a sharp estimate for this number as a function of the nuclear charge is a challenging open problem (see Ref. 70 for some of the original papers and Ref. 90 for a review).

V. ESSENTIAL SPECTRUM I. SPECTRAL DEFORMATION

A. Spectral deformation

The nature of the essential spectrum of N-body Hamiltonians was first established by Balslev and Combes[10] for the special class of dilation-analytic potentials. We review this theory since it

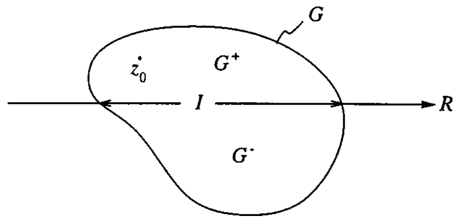

FIG. 5. The spectral condition.

also provides the framework for a description of resonances.[96] In abstract form, the idea is to test the spectral properties of a self-adjoint operator H on a Hilbert space $\mathcal{H}$ by analyzing the family of transformed Hamiltonians

$$H(\xi)=U(\xi)HU(\xi)^{-1}$$

for a suitably chosen one-parameter unitary group

$$U(\xi)=e^{-i\xi A};\quad A=A^*;\quad \xi\in R.$$

We use the notation

$$C^{\pm}=\{z|\pm\mathrm{Im}(z)>0\};\ \ R(z)=(z-H)^{-1};R(z,\xi)=(z-H(\xi))^{-1}.$$

The analysis rests on the following two conditions:

Analyticity condition: $H(\xi)$ extends from $\xi\in R$ to a family of operators defined on a complex strip $\Xi=\{\xi||\mathrm{Im}(\xi)|<\alpha\}$ such that the resolvent $R(z,\xi)$ exists for some $z=z_0\in C^+$ and is holomorphic in $\xi\in\Xi$.

Spectral condition: See Fig. 5.

For some $\xi_0\in\Xi$ there is an open, connected complex region $G\ni z_0$ with the properties

$$G\cap\sigma_{\mathrm{ess}}(H(\xi_0))=\emptyset,$$

$$G^{\pm}\equiv G\cap C^{\pm}\text{is connected,}\tag{5.1}$$

$$G^{\pm}\neq\emptyset.$$

Equation (5.1) is the condition of spectral deformation: if H has essential spectrum in $I=G\cap R$, then this spectrum is removed from G by passing from H to $H(\xi_0)$. Here we use the definition $\sigma_{\mathrm{ess}}(L)=\sigma(L)\setminus\sigma_{\mathrm{disc}}(L)$ of the essential spectrum for a general operator L on $\mathcal{H}$. The discrete spectrum $\sigma_{\mathrm{disc}}(L)$ is the set of all *isolated spectral points* $\lambda\in\sigma(L)$ for which the projection

$$P=(2\pi i)^{-1}\oint_{\Gamma}dz(z-L)^{-1}$$

has *finite rank*, where Γ is a loop in the resolvent set around λ which separates λ from the rest of $\sigma(L)$. Then λ is an eigenvalue of L and the resolvent $(z-L)^{-1}$ has a pole of (finite) order $n\geqslant 1$ at $z=\lambda$. λ is called a *semi-simple eigenvalue* if $n=1$: then (and only then) all vectors in Ran(P) are eigenvectors. Nevertheless we will call P the ''eigenprojection'' for the eigenvalue λ. We will show that the two conditions stated above have important consequences for the spectrum of H in $I=G\cap R$.

1. Preparation

The two relations

$$H(\xi+a)=U(a)H(\xi)U(a)^{-1}, \quad a\in R;$$

$$H(\xi)=H(\overline{\xi})^*$$

hold for $\xi\in \boldsymbol{R}$ and extend by analyticity to all $\xi\in\Xi$ via their resolvent equivalents. In particular the spectrum of $H(\xi)$ depends only on Im(ξ). We also see that the preference given above to C^+ is purely conventional, since $R(z,\xi)=R(\overline{z,\xi})^*$ is also holomorphic in $\xi\in\Xi$ for $z=\overline{z_0}$. Therefore we can also start from the equivalent *conjugate picture* in which z_0, ξ_0, G, $G^{\pm}$ are replaced by their complex conjugates. The unitary group $U(\xi)$ is extended to all $\xi\in C$ via the spectral representation

$$U(\xi)=e^{-i\xi A}=\int_R e^{-i\xi s}\,dF(s),$$

$F(s)$ being the spectral family of A. $U(\xi)$ is a closed operator with domain

$$\varphi\in U(\xi)\Leftrightarrow\int_R e^{2s\,\mathrm{Im}}(\xi)d\|F(s)\psi\|^2<\infty$$

and satisfies $U(\xi)^*=U(\overline{\xi})$. [We note that $U(\xi_0)$ and therefore A must be unbounded if there is to be any spectral deformation.]

The set $\mathcal{A}$ of *analytic vectors* ψ is defined by the condition that the measure $d\|F(s)\psi\|^2$ has *compact support*. For $\psi\in\mathcal{A}$ the function

$$\xi\rightarrow U(\xi)\psi\equiv\psi(\xi)\in\mathcal{H} \tag{5.2}$$

is entirely analytic. $\mathcal{A}$ is a core of $U(\xi)$ and invariant under $U(\xi)$. With this preparation the following facts are easily derived:

Lemma 5.1: (a) Let B be a bounded operator on $\mathcal{H}$ such that the function $\xi\in R\rightarrow U(\xi)BU(\xi)^{-1}$ has a bounded-holomorphic extension $B(\xi)$ on Ξ. Then

$$B(\xi)=U(\xi)BU(\xi)^{-1} \quad \text{on} \quad D(U(\xi)^{-1}). \tag{5.3}$$

(b) Let $\varepsilon>0$ and $\Xi_\varepsilon=\{\xi||\mathrm{Im}(\xi)|<\alpha-\varepsilon\}$. Then there exists a neighborhood Ω_ε of z_0 such that

$$R(z,\xi)=U(\xi)R(z)U(\xi)^{-1} \quad \text{on} \quad D(U(\xi)^{-1}) \tag{5.4}$$

for all $(z,\xi)\in\Omega_\varepsilon\times\Xi_\varepsilon$.

Theorem 5.2: *Suppose that the analyticity and spectral conditions stated earlier are satisfied, and let $\xi\in\Xi$ be such that*

$$G\cap\sigma_{\mathrm{ess}}(H(\xi))=\varnothing \tag{5.5}$$

(e.g, $\xi=\xi_0$). Then we have the following.

(a) For any φ, $\psi\in\mathcal{A}$ the holomorphic function $z\rightarrow(\varphi,R(z)\psi)$ on G^+ has a meromorphic extension to G given by

$$M(\varphi,\psi,z)=(\varphi(\overline{\xi}),R(z,\xi)\psi(\xi)) \tag{5.6}$$

and by the definition (5.2).

(b) The (discrete) spectrum of $H(\xi)$ in G is given by

$$\sigma_{\rm disc}(H(\xi))\cap G=\bigcup_{\varphi,\psi\in\mathcal{A}}\{\text{poles of } M(\varphi,\psi,\cdot)\},\tag{5.7}$$

which is independent of ξ *[as long as (5.5) holds].*

(c) $H(\xi)$ *has no spectrum in* G^+, *where*

$$R(z)=U(\xi)^{-1}R(z,\xi)U(\xi)\quad\text{on}\quad D(U(\xi)).\tag{5.8}$$

The same is true for G^- *if* $\sigma(H)$ *has a gap in* I.

(d) H *and* $H(\xi)$ *have the same eigenvalues in* I. *Any such eigenvalue is semi-simple for* H *and for* $H(\xi)$, *with corresponding eigenprojections* P *and* $P(\xi)$ *satisfying*

$$P=U(\xi)^{-1}P(\xi)U(\xi)\quad\text{on}\quad D(U(\xi));$$

$$\dim(P)=\dim(P(\xi))<\infty;\tag{5.9}$$

$$\mathrm{Ran}(P)\subset D(U(\xi)).$$

These relations also hold if ξ *is replaced by* $\overline{\xi}$, *so that* $\mathrm{Ran}(P)$ *is contained in*

$$D(U(\xi))\cap D(U(\overline{\xi})).\tag{5.10}$$

(e) Let $E(s)$ *be the spectral family of* H *and let* $\Delta\subset I$ *be an open interval whose endpoints are not eigenvalues of* H. *Then the spectral projection* E_Δ *of* H *corresponding to* Δ *is given by*

$$E_\Delta=\frac{i}{2\pi}\int_\Delta dx[U(\xi)^{-1}R(x,\xi)U(\xi)-U(\overline{\xi})^{-1}R(x,\overline{\xi})U(\overline{\xi})]\tag{5.11}$$

on the domain (5.10). Therefore $(\psi,E(s)\psi)$ *is real analytic in* $s\in\Delta$ *for any* ψ *in the domain (5.10). Since the eigenvalues of* H *in* I *form a discrete set it follows that* H *has no singular continuous spectrum in* I. *If* Δ *contains a single eigenvalue* λ *with eigenprojection* P, *then (5.11) holds for the reduced operators*

$$\overline{E}_\Delta=E_\Delta(1-P),$$

$$\overline{R}(x,\xi)=R(x,\xi)(1-P(\xi)),$$

so that $(\psi,\overline{E}(s)\psi)$ *is real analytic in* $s\in\Delta$ *for* ψ *in the domain (5.10).*

(f) If $\sigma(H)$ *has a gap in* I, *then the spectrum of* H *in* I *is purely discrete.*

Proof: (a) Since $\xi\in\Xi_\varepsilon$ for some $\varepsilon>0$, (5.6) holds for $z\in\Omega_\varepsilon$. $R(z)$ is holomorphic in $z\in G^+$, and $R(z,\xi)$ is meromorphic in $z\in G$: its poles are the eigenvalues of $H(\xi)$ in G.

(b) is a direct consequence of (a) since $\mathcal{A}$ is dense and invariant under $U(\xi)\forall\xi\in C$. Independence of ξ follows from the uniqueness of meromorphic continuations.

(c) follows from (b) since $M(\varphi,\psi,z)=(\varphi,R(z)\psi)$ for $z\in G^+$. This relation extends by analyticity to $z\in G^-$ if $\sigma(H)$ has a gap in I.

(d) Let $\lambda\in I$ be an eigenvalue of H. By the spectral theorem its eigenprojection P is given by $P=\lim_{\varepsilon\searrow 0}(-i\varepsilon)R(\lambda+i\varepsilon)$, so that by (5.8)

$$(\varphi,P\psi)=\mathrm{s}-\lim_{\varepsilon\searrow 0}(-i\varepsilon)(\varphi(\overline{\xi}),R(\lambda+i\varepsilon,\xi)\psi(\xi))\quad\forall\varphi,\psi\in\mathcal{A}.\tag{5.12}$$

Since this is nonzero for some φ, $\psi\in\mathcal{A}$, λ is a first order pole of $R(z,\xi)$, i.e., a semi-simple eigenvalue of $H(\xi)$. By (5.12) the corresponding eigenprojection $P(\xi)$ satisfies

$$(\varphi,P\psi)=(\varphi(\overline{\xi}),P(\xi)\psi)\quad\forall\varphi,\psi\in\mathcal{A},$$

which implies $P \supset U(\xi)P(\xi)U(\xi)^{-1}$ and therefore $\dim(P) = \dim P(\xi)$ which is finite by the definition of the essential spectrum. Moreover $D(U(\xi)) \cap \mathrm{Ran}(P)$ is dense in—and therefore equal to—$\mathrm{Ran}(P)$. The same analysis in the conjugate picture shows that (5.9) also holds for $\bar{\xi}$. Now let $\lambda \in I$ be an eigenvalue of $H(\xi)$, i.e., a pole of some order $n \geq 1$ of $R(z,\xi)$. Then

$$\lim_{\varepsilon \searrow 0} \varepsilon^n (\varphi, R(\lambda + i\varepsilon)\psi) = \lim_{\varepsilon \searrow 0} (\varphi(\bar{\xi}), R(\lambda + i\varepsilon, \xi)\psi(\xi)) \neq 0$$

for some $\varphi, \psi \in \mathcal{A}$. Since $\|R(\lambda + i\varepsilon)\| \leq \varepsilon^{-1}$, it follows that $n = 1$ and that λ is an eigenvalue of H.

(e) follows from the spectral formula

$$E_\Delta = \mathrm{s}-\lim_{\varepsilon \searrow 0} \frac{i}{2\pi} \int_\Delta dx [R(x + i\varepsilon) - R(x - i\varepsilon)].$$

After expressing $R(x + i\varepsilon)$ and $R(x - i\varepsilon)$ by (5.8) and its adjoint, ε can be set equal to zero.

(f) If $\sigma(H)$ has a gap in I, then (5.8) holds in $G^+ \cup G^-$ so that $E_\Delta = 0$ if Δ contains no eigenvalue of H. □

2. Resonances

According to Theorem 5.2 there are only two cases. Either $I \cap \sigma_{\mathrm{ess}}(H) = \emptyset$, then H and $H(\xi)$ have the same (discrete, real) spectrum in G. Or $I \subset \sigma_{\mathrm{ess}}(H)$, then the real (discrete) eigenvalues of $H(\xi)$ are the embedded eigenvalues of H in I, which have finite multiplicities. In addition $H(\xi)$ may have (discrete) complex eigenvalues in G^- which are also independent of ξ as long as $\sigma_{\mathrm{ess}}(H(\xi))$ stays away from G. They are commonly called *resonance eigenvalues* or simply *resonances of H* and actually occur in complex conjugate pairs together with the eigenvalues of $H(\bar{\xi})$ in $\overline{G^-}$. Alternatively, resonances are defined as the poles of the meromorphic continuations of the functions

$$z \to (\varphi, (z - H)^{-1}\psi); \quad \varphi, \psi \in \mathcal{A},$$

on $C^{\pm}$. This definition seems closer to the physicist's notion of a resonance, since poles of resolvent matrix elements near the real axis are expected to show up in the energy dependence of observable quantities like transition probabilities or scattering cross sections. However, it must be noted that these resonances are not uniquely defined by H since their construction involves the choice of a unitary group $U(\xi)$, or of a set $\mathcal{A}$ of analytic vectors. The physical interpretation of resonances is therefore a delicate matter.[98] A related and also commonly expected feature of resonances near the real axis is their association with long-living metastable states showing nearly exponential decay under the time evolution generated by H. This will be further discussed below.

B. Dilation-analytic *N*-body systems

In this section we apply the general theory to the case where

$$H = \tfrac{1}{2} p^2 + V(x)$$

is an N-body Schrödinger operator on $L^2(X)$, and $U(\xi)$ is the dilation group defined for $\xi \in R$ by

$$U(\xi): \psi(x) \to e^{\xi \dim(X)/2} \psi(e^\xi x). \tag{5.13}$$

This group has the generator

$$A = \tfrac{1}{2}(x \cdot p + p \cdot x) \tag{5.14}$$

and transforms H into

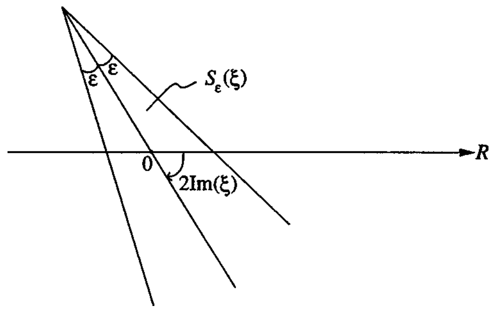

FIG. 6. The sector $S_\varepsilon(\xi)$.

$$H(\xi)=U(\xi)HU(\xi)^{-1}=e^{-2\xi}\tfrac{1}{2}p^2+V(e^{\xi}x). \tag{5.15}$$

$H(\xi)$ is extended from real ξ to the complex strip $\Xi=\{\xi||\mathrm{Im}(\xi)|<\alpha\}$ under the following two conditions:

(a) Dilation-analyticity. For any $\xi\in\Xi$, $V(e^{\xi}x)\equiv V(\xi,x)$ is defined as a function with values in $L^2_{\mathrm{loc}}(X)$. Moreover, the corresponding multiplication operator $V(\xi)$ is holomorphic in the sense that the function $\xi\to V(\xi)\psi\in L^2(X)$ is holomorphic in $\xi\in\Xi$ for any $\psi\in C_0^\infty(X)$ and satisfies an estimate

$$\|V(\xi)\psi\|\le\varepsilon\|\tfrac{1}{2}p^2\psi\|+\beta(\varepsilon)\,\|\psi\| \tag{5.16}$$

for any $\varepsilon>0$, uniformly in ξ.

(b) *N*-body structure. For any $a\in L$ there is a decomposition

$$V(\xi,x)=V^a(\xi,x^a)+I_a(\xi,x),$$

where $V^a(\xi,x)$ satisfies condition (a) as an operator on $L^2(a^\perp)$ and where

$$\lim_{|x|_a\to\infty} I_a(\xi,x)=0.$$

We will refer to these two conditions by saying that V is a ***dilation-analytic N-body potential***. An example is the Hamiltonian (3.1) with $V_{ik}(r)\sim 1/r\,(\alpha=\infty)$ or $V_{ik}(r)\sim(1/r)\,e^{-\mu r}$; $\mu>0(\alpha=\pi/2)$.

Here $\xi H(\xi)$ is defined for any $\xi\in\Xi$ on $C_0^\infty(X)$ by the explicit expression (5.15). This operator has a closure with domain $D(p^2)$ which we again denote by $H(\xi)$. The numerical range and the spectrum of $H(\xi)$ are contained in a complex sector $S_\varepsilon(\xi)$ of the form shown in Fig. 6 with ε arbitrary small. For $z\notin_\varepsilon(\xi)$ the resolvent $R(z,\xi)$ is bounded by

$$\|R(z,\xi)\|\le[\mathrm{dist}(z,S_\varepsilon(\xi))]^{-1} \tag{5.17}$$

and holomorphic in $\xi\in\Xi$ as long as $S_\varepsilon(\xi)$ does not cover z. For simplicity we restrict α to $\alpha<\pi/2$. Then the sectors $S_\varepsilon(\xi)$ do not sweep the entire complex plane for small ε and $|\mathrm{Im}\,(\xi)|<\alpha$. In particular, $R(z,\xi)$ is holomorphic in $\xi\in\Xi$ for z in some open set straddling the negative real axis.

For the application of Theorem 5.2 the main task is to determine the essential spectrum of $H(\xi)$ for $\mathrm{Im}\,(\xi)\ne0$. We define the set of thresholds of $H(\xi)$ as the set

$$\tau(H(\xi))=\bigcup_{a>\{0\}}\sigma_{\mathrm{disc}}(H^a(\xi)). \tag{5.18}$$

Theorem 5.3:[10] *Under the conditions (a) and (b) stated earlier,*

$$\sigma_{\text{ess}}(H(\xi)) = \bigcup_{a>\{0\}} \sigma(H_a(\xi)) = \tau(H(\xi)) + e^{-2\xi}R^+. \tag{5.19}$$

Proof: We fix $\xi \in \Xi$ and we shorten the notation by writing H, H^a for $H(\xi)$, $H^a(\xi)$, etc. The induction hypothesis is that for all $a>\{0\}$

$$\sigma_{\text{ess}}(H^a) = \tau(H^a) + e^{-2\xi}R^+; \quad \tau(H^a) = \bigcup_{b>a} \sigma(H^b_{\text{disc}}).$$

This is trivially satisfied for $a=X$. From

$$H_a = e^{-2\xi}\tfrac{1}{2}p_a^2 \otimes 1 + 1 \otimes H^a \quad \text{on } L^2(a) \otimes L^2(a^\perp)$$

it follows that

$$\sigma(H_a) = e^{-2\xi}R^+ + \sigma(H^a), \tag{5.20}$$

e.g., by reducing H_a to fibers of constant $p_a \in a$. Therefore,

$$\tilde{\sigma} \equiv \bigcup_{a>\{0\}} \sigma(H_a) = \bigcup_{a>\{0\}} (\sigma_{\text{disc}}(H^a) \cup \sigma_{\text{ess}}(H^a)) + e^{-2\xi}R^+ = \tau(H) + e^{-2\xi}R^+.$$

We note that the set $\tilde{\sigma}$ is a closed, countable union of parallel rays. Its complement is connected to the resolvent set of H: for $z \notin \tilde{\sigma}$ the ray $\{z - e^{-2\xi}R^+\}$ is in the complement of $\tilde{\sigma}$ and leaves the sector $\mathcal{S}_\varepsilon(\xi)$. It remains to prove that $\tilde{\sigma} = \sigma_{\text{ess}}(H)$. The inclusion $\tilde{\sigma} \subset \sigma_{\text{ess}}(H)$ follows exactly as in the case $\xi = 0$ (Theorem 3.1). To prove the opposite inclusion it suffices to show that

$$\partial\sigma_{\text{ess}}(H) \subset \tilde{\sigma}, \tag{5.21}$$

where $\partial\sigma_{\text{ess}}(H)$ denotes the boundary of $\sigma_{\text{ess}}(H)$. For suppose that $z \in \sigma_{\text{ess}}(H)$ but $z \notin \tilde{\sigma}$. Then the ray $\{z - e^{-2\xi}R^+\}$ must cross $\partial\sigma_{\text{ess}}(H)$ which contradicts (5.20). To prove (5.21) we refer to a generalization of Weyl's criterion,[55] valid for any closed operator H: if $\lambda \in \partial\sigma_{\text{ess}}(H)$, then there exists a sequence $\psi_n \in D(H)$ with $\|\psi_n\| = 1$ such that

$$\|(\lambda - H)\psi_n\| \to 0 \quad \text{and} \quad \psi_n \rightharpoonup 0 \quad (\text{weak convergence}). \tag{5.22}$$

This is exploited using the local compactness property of H (which holds since p^2 is H-bounded). Let χ_R be a smoothed characteristic function of the ball $\{|x|<R\}$. Since χ_R is H-compact it follows from (5.22) that $\|\chi_R\psi_n\| \to 0$ for any fixed R. By passing to a new sequence $\{\psi_n\}$ we can therefore replace the condition $\psi_n \rightharpoonup 0$ by the stronger form $\psi_n(x) = 0$ for $|x|<n$. Now let $J_a = j_a^2$ be the partition of unity used in the proof of Theorem 3.1. Since $[p^2, J_a]$ is H-compact it follows from (5.22) that $\|(\lambda - H)J_a\psi_n\| \to 0$. Moreover, $\|I_a J_a \psi_n\| \to 0 \ \forall a>\{0\}$ since $|x|_a \to \infty$ on supp $(J_a\psi_n)$. Therefore

$$\|(\lambda - H_a)J_a\psi_n\| \to 0 \quad \forall a>\{0\}. \tag{5.23}$$

On the other hand, $\|\Sigma_{a>\{0\}}J_a\psi_n\| \to 1$, which implies that $\|J_a\psi_n\| \geq \varepsilon > 0$ for some $a>\{0\}$ and for an infinite subsequence of $\{\psi_n\}$. Then it follows from (5.23) that $\lambda \in \sigma(H_a)$.

□

Hereafter we revert to the original notation which distinguishes between H and $H(\xi)$. The threshold set of H is defined by

$$\tau(H) = \bigcup_{a>\{0\}} \sigma_{\text{disc}}(H^a). \tag{5.24}$$

With $\Sigma(H)$ we denote the lowest threshold of H (formerly called Σ in Theorem 3.1).

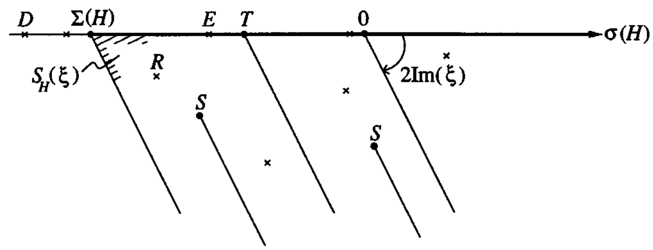

FIG. 7. The spectrum of $H(\xi)$.

Theorem 5.4:[10] *Suppose that V is a dilation-analytic N-body potential,* $\xi \in \Xi$ *and* $0 < |\mathrm{Im}(\xi)| < \pi/2$. *Let* $S_H(\xi)$ *be the complex sector*

$$S_H(\xi) = [\Sigma(H), \infty) + e^{-2\xi} \mathbf{R}^+.$$

Then

(a) $\sigma_{\mathrm{ess}}(H(\xi)) \subset S_H(\xi)$;
(b) $\sigma(H(\xi)) \setminus S_H(\xi) = \sigma_{\mathrm{disc}}(H)$;
(c) $\tau(H) = \tau(H(\xi)) \cap R$; *and*
(d) $\tau(H)$ *is closed and countable. The nonthreshold eigenvalues of H are the discrete real eigenvalues of* $H(\xi)$. *They have finite multiplicities and can accumulate only at thresholds of* H.

Proof: Proceeding by induction we assume that (a) and (b) hold for H^a if $a > \{0\}$. For $a = X$ this is trivial. (b) follows from (a) and Theorem 5.2. (a) Let $a > \{0\}$. By the induction hypothesis

$$\sigma(H^a(\xi)) \subset \sigma_{\mathrm{disc}}(H^a) \cup S_{H^a}(\xi) \subset S_H(\xi) .$$

Therefore, by (5.20), $\sigma(H_a(\xi)) \subset S_H(\xi)$ for all $a > \{0\}$ which proves (a). (c) Let $\lambda \in \tau(H(\xi)) \cap R$. Then λ is a discrete, real eigenvalue of $H^a(\xi)$ for some $a > \{0\}$ and therefore an eigenvalue of H^a by Theorem 5.2. This proves that $\tau(H) \supset \tau(H(\xi)) \cap R$. Now let $\lambda \in \tau(H)$. Then λ is an eigenvalue of H^a for some $a > \{0\}$. By the induction hypothesis $\tau(H^a) = \tau(H^a(\xi)) \cap R$. Therefore $\lambda \in \tau(H^a)$ implies $\lambda \in \tau(H(\xi)) \cap R$. If $\lambda \notin \tau(H^a)$, then λ is a real, discrete eigenvalue of $H^a(\xi)$ which also implies $\lambda \in \tau(H(\xi)) \cap R$. (d) $\tau(H)$ is countable by its definition. By (c) it is equal to $\sigma_{\mathrm{ess}}(H(\xi)) \cap R$ which is closed. The rest of (d) follows directly from (b) and from Theorem 5.2. □

1. Discussion

In the picture of $\sigma(H(\xi))$ (Fig. 7), drawn for $\mathrm{Im}(\xi) > 0$, we have indicated the points D = discrete eigenvalue of H; E = embedded non-threshold eigenvalue of H; T = thresholds of H, among them 0 and $\Sigma(H)$; R = discrete, complex eigenvalue of $H(\xi)$ (resonance); and S = complex threshold of $H(\xi)$.

The essential spectrum of $H(\xi)$ is a closed, countable union of parallel rays emerging from the thresholds of $H(\xi)$. The picture does not show possible accumulations of thresholds and eigenvalues and is therefore deceptively simple. Under a change of $\mathrm{Im}(\xi)$ the points R, S remain fixed as long as they are not touched by one of the rays forming the essential spectrum of $H(\xi)$. However, in the sectors swept by these rays the spectrum of $H(\sigma)$ may be altered completely. This indicates that the meromorphic extensions of $(\phi, (z-H)^{-1}\psi)$ across I live on a complicated Riemann surface with branch points T, S.

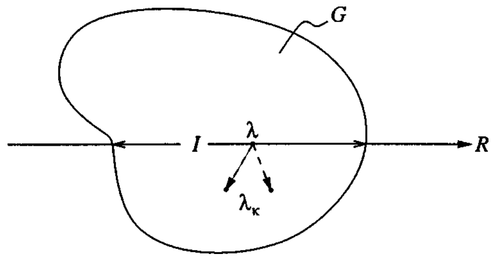

FIG. 8. Perturbation of a real eigenvalue of $H(\xi)$.

C. Resonances arising from bound states

Spectral deformation is particularly useful to study the perturbation of eigenvalues embedded in the continuous spectrum. Let $H_\kappa = H + \kappa V$ be a family of self-adjoint operators, defined for small $\kappa \in R$, and suppose that there exists a corresponding family

$$H_\kappa(\xi) = U(\xi) H_\kappa U(\xi)^{-1} = H(\xi) + \kappa V(\xi)$$

satisfying the analyticity and spectral conditions uniformly for small κ. Let $\lambda \in I \subset \sigma(H)$ be an embedded eigenvalue of H. After spectral deformation λ becomes a discrete, semi-simple eigenvalue of $H(\xi)$, whose perturbation by $\kappa V(\xi)$ may be studied by standard methods. We consider the simplest case where $V(\xi)$ is bounded relative to $H(\xi)$ so that analytic perturbation theory for semi-simple, discrete eigenvalues applies[65] (see Fig. 8).

For small κ the operator $H_\kappa(\xi)$ has a group of eigenvalues $\lambda_\kappa \notin G^+$ which converge to λ as $\kappa \to 0$. The λ_κ are the eigenvalues of a finite-rank operator $a(\kappa)$ acting on the unperturbed eigenspace Ran $P(\xi)$, where $P(\xi)$ is the eigenprojection of $H(\xi)$ corresponding to the eigenvalue λ. For small κ the operator $a(\kappa)$ has a convergent Rayleigh–Schrödinger expansion:[65]

$$\begin{gathered} a(\kappa) = a_0 + a_1\kappa + a_2\kappa^2 + \cdots; \\ a_0 = \lambda P(\xi); \\ a_1 = P(\xi)V(\xi)P(\xi); \\ a_2 = P(\xi)V(\xi)\overline{R}(\lambda,\xi)V(\xi)P(\xi). \end{gathered} \tag{5.25}$$

Here $\overline{R}(z,\xi)$ is the reduced resolvent

$$\overline{R}(z,\xi) = R(z,\xi)(1-P(\xi)), \quad R(z,\xi) = (z-H(\xi))^{-1}, \tag{5.26}$$

which is holomorphic in z near λ. The important point is that the description (5.25) of the perturbed eigenvalues can be reformulated entirely in terms of H and V without reference to spectral deformation. This is the essence of the following theorem due to Simon[96] for which we first state a more precise hypothesis.

1. Hypothesis

$H(\xi) = U(\xi) H U(\xi)^{-1}$ satisfies the analyticity and spectral conditions stated at the beginning of this section. V is symmetric and bounded relative to H, so that $B \equiv VR(z_0)$ is bounded. Moreover, it is assumed that the family of bounded operators $B(\xi) = U(\xi) B U(\xi)^{-1}$, $\xi \in R$, has a bounded-holomorphic extension to all $\xi \in \Xi$. Then $V(\xi)$ is defined by $V(\xi) = B(\xi)(z_0 - H(\xi))$, which is bounded relative to $H(\xi)$. We remark that by Lemma 5.1

$$B(\xi) = U(\xi) B U(\xi)^{-1} \text{ on } D(U(\xi)^{-1}).$$

Theorem 5.5:[96] *Under the previous hypothesis let* $\lambda \in I$ *be an eigenvalue of* H *with eigenprojection* P*. Then the corresponding perturbed eigenvalues* λ_κ *of* $H_\kappa(\xi)$ *are the eigenvalues of the finite rank operator*

$$b(\kappa)=U(\xi)^{-1}a(\kappa)U(\xi)|_{\mathrm{Ran}(P)},$$

which maps $\mathrm{Ran}(P)$ *into itself. The expansion of* $b(\kappa)$ *corresponding to (5.25) is*

$$\begin{gathered} b(\kappa)=b_0+b_1\kappa+b_2\kappa^2+\cdots; \\ b_0=\lambda P; \\ b_1=PVP; \\ b_2=\mathcal{P}\int (\lambda-s)^{-1}d(PV\bar{E}(s)VP)-i\pi\frac{d}{ds}(PV\bar{E}(s)VP)_{s=\lambda_0}. \end{gathered} \tag{5.27}$$

Here $\mathcal{P}$ *denotes the principal value, and* $\bar{E}(s)=E(s)(1-P)$ *is the reduced spectral family of* H*. (The negative imaginary term in* b_2 *is the precise form of the Fermi golden rule.)*

Proof: According to Theorem 5.2, $U(\xi)$ maps $\mathrm{Ran}(P)$ onto $\mathrm{Ran}(P(\xi))$ with the inverse $U(\xi)^{-1}$ restricted to $\mathrm{Ran}(P(\xi))$. Therefore $a(\kappa)$ and $b(\kappa)$ have the same eigenvalues. On $\mathrm{Ran}(P)$ we have

$$b_0=\lambda U(\xi)^{-1}P(\xi)U(\xi)=\lambda P;$$

$$\begin{aligned} b_1&=U(\xi)^{-1}P(\xi)B(\xi)(z_0-H(\xi))P(\xi)U(\xi) \\ &=PB(z_0-H)P=PVP. \end{aligned}$$

By the same argument we can express

$$\begin{aligned} b_2&=\lim_{\varepsilon\searrow 0}U(\xi)^{-1}P(\xi)V(\xi)\bar{R}(\lambda+i\varepsilon,\xi)V(\xi)P(\xi)U(\xi) \\ &=\lim_{\varepsilon\searrow 0}PV\bar{R}(\lambda+i\varepsilon)VP \end{aligned}$$

in terms of H and V. Using the spectral theorem this can be written as

$$b_2=\lim_{\varepsilon\searrow 0}\int (\lambda+i\varepsilon-s)^{-1}\,d(PV\bar{E}(s)VP).$$

According to Theorem 5.2 (e), the function $s\to PV\bar{E}(s)VP$ is real-analytic in some open interval $\Delta\ni\lambda$. Equation (5.27) thus follows from the identity

$$\lim_{\varepsilon\searrow 0}\int_\Delta ds\,(\lambda+i\varepsilon-s)^{-1}f(s)=-i\pi f(\lambda)+\mathcal{P}\int_\Delta ds\,(\lambda-s)^{-1}f(s),$$

valid for any integrable function f on Δ which is Hölder continuous at $s=\lambda$. □

2. Exponentially decaying metastable states

In the general framework of spectral deformation it is not clear how to associate long-living metastable states with resonance eigenvalues of H. However, for resonances arising from bound states, the unperturbed eigenvectors of H will turn into metastable states under the time evolution generated by H_κ. For simplicity we will treat the case where λ is a nondegenerate eigenvalue of H with normalized eigenvector ψ. Following Ref. 51 we will show that

$$(\psi, e^{-iH_\kappa t}\psi) = e^{-i\lambda_\kappa t} + O(\kappa^2) \tag{5.28}$$

uniformly in $0 \leq t < \infty$ as $\kappa \to 0$. In this sense ψ has exponential decay in time governed by the complex resonance eigenvalue λ_κ.

Theorem 5.6:[51] *Under the hypothesis of Theorem 5.5, suppose that λ is a simple eigenvalue of H with normalized eigenvector ψ. Let $g \in C_0^\infty(I)$ be a smoothed characteristic function with $g(x) \equiv 1$ on some open interval $\Delta \ni \lambda$ and such that λ is the only eigenvalue of H in* supp (g). *Then*

$$(\psi, e^{-iH_\kappa t} g(H_\kappa)\psi) = A(\kappa) e^{-i\lambda_\kappa t} + B(\kappa, t); \tag{5.29}$$

$$A(\kappa) = (\psi(\overline{\xi}), P_\kappa(\xi)\psi(\xi)) = 1 + O(\kappa^2); \tag{5.30}$$

$$|B(\kappa, t)| \leq \kappa^2 c_m (1+t)^{-m} \quad \forall m > 0 \tag{5.31}$$

as $\kappa \to 0$, uniformly in $0 \leq t < \infty$.

Proof of (5.28): Here we choose $0 \leq g \leq 1$. For $t = 0$ we obtain from (5.29)–(5.31)

$$(\psi, (1 - g(H_\kappa))\psi) = \|(1 - g(H_\kappa))^{1/2}\psi\|^2 = O(\kappa^2),$$

and therefore

$$(\psi, e^{-iH_\kappa t}(1 - g(H_\kappa))\psi) = O(\kappa^2)$$

uniformly in t. With this estimate (5.28) follows from (5.29) and (5.30). □

Proof of Theorem 5.6: Let $R_\kappa(z) = (z - H_\kappa)^{-1}$. By the spectral theorem

$$\begin{aligned} F(t) &\equiv (\psi, e^{-iH_\kappa t} g(H_\kappa)\psi) \\ &= \lim_{\varepsilon \searrow 0} \frac{1}{2\pi i} \int_R dx\, g(x) e^{-itx} (\psi, [R_\kappa(x - i\varepsilon) - R_\kappa(x + i\varepsilon)]\psi). \end{aligned} \tag{5.32}$$

Using (5.8) and its adjoint, $F(t)$ can be expressed in terms of $(z - H_\kappa(\xi))^{-1} = R_\kappa(z, \xi)$ as

$$\begin{aligned} F(t) &= f(t, \overline{\xi}) - f(t, \xi); \\ f(t, \xi) &= \frac{1}{2\pi i} \int_R dx\, g(x) e^{-itx} (\psi(\overline{\xi}), R_\kappa(x, \xi)\psi(\xi)). \end{aligned} \tag{5.33}$$

Here we have assumed that $\mathrm{Im}(\lambda_\kappa) < 0$. Otherwise the path of integration must be modified by a detour around λ_κ in C^+, which does not affect the estimates below. Now we split $R_\kappa(z, \xi)$ into singular and regular parts:

$$R_\kappa(z, \xi) = \frac{P_\kappa(\xi)}{z - \lambda_\kappa} + \overline{R}_\kappa(z, \xi). \tag{5.34}$$

By hypothesis we can pick a contour Γ enclosing supp(g) which separates λ from the rest of $\sigma(H(\xi))$. (See Fig. 9.) Then, for small κ, Γ also separates λ_κ from the rest of $\sigma(H_\kappa(\xi))$, so that $\overline{R}_\kappa(z, \xi)$ is holomorphic in z in the interior of Γ. Since $\|R_\kappa(z, \xi)\|$ is bounded by a constant for small κ and all $z \in \Gamma$ it follows from (5.34) by the maximum principle that

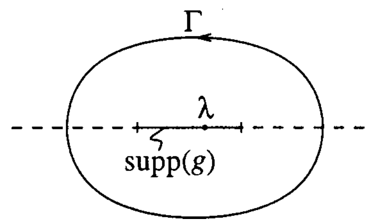

FIG. 9. Choice of the contour Γ.

$$\|\overline{R}_\kappa(z,\xi)\| \leq \text{const} \tag{5.35}$$

for small κ and all z in the interior of Γ.

Inserting (5.34) into (5.33) we obtain two contributions which are estimated separately.

3. Contribution of the regular part

Since $P_\kappa(\xi)\overline{R}_\kappa(z,\xi)=0$, the contribution of the regular part to $f(t,\xi)$ is given by

$$\frac{1}{2\pi i}\int_R dx\, g(x)e^{-itx}(u_\kappa(\overline{\xi}),\overline{R}_\kappa(x,\xi)u_\kappa(\xi));$$
$$u_\kappa(\xi)=(P_\kappa(\xi)-P(\xi))\psi(\xi)=O(\kappa). \tag{5.36}$$

By partial integration this integral is seen to have a bound of the form (5.31) for any $m>0$, since the x derivatives of $\overline{R}_\kappa(x,\xi)$ are powers of $\overline{R}_\kappa(x,\xi)$ and therefore bounded by (5.35).

4. Contribution of the singular part

The singular part of $R_\kappa(z,\xi)$ contributes to $F(t)$ the term

$$\overline{A(\kappa)}\frac{1}{2\pi i}\int_R dx\, g(x)e^{-itx}(x-\overline{\lambda_\kappa})^{-1}-A(\kappa)\frac{1}{2\pi i}\int_R dx\, g(x)e^{-itx}(x-\lambda_\kappa)^{-1}, \tag{5.37}$$

where $A(\kappa)$ is given by (5.30).

Since $g\equiv 1$ on some open interval $\Delta \ni \lambda$ we can deform the path of integration into C^- as shown in Fig. 10. From the second integral in (5.37) we then pick up the residue

$$A(\kappa)e^{-i\lambda_\kappa t}.$$

The remainder is given by (5.37) with both integrals now taken over the path γ where $g(x)=1$ for $\text{Im}(x)<0$. Using the identity

$$P(\xi)P_\kappa(\xi)P(\xi)=P(\xi)+(P_\kappa(\xi)-P(\xi))(P_\kappa(\xi)-1)(P_\kappa(\xi)-P(\xi))$$

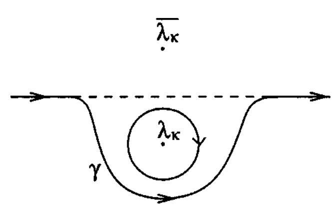

FIG. 10. Deforming the integration contour.

and the fact that $(\psi(\overline{\xi}),\psi(\xi))=(\psi,\psi)=1$, we see that $A(\kappa)=1+O(\kappa^2)$. The remainder can therefore be written in the form

$$-\frac{\mathrm{Im}(\lambda_\kappa)}{\pi}\int_\gamma dx\, g(x)e^{-itx}(x-\overline{\lambda_\kappa})^{-1}(x-\lambda_\kappa)^{-1}$$

$$+O(\kappa^2)\int_\gamma dx\, g(x)(e^{-itx}(x-\overline{\lambda_\kappa})^{-1}+e^{itx}(x-\lambda_\kappa)^{-1}).$$

Using that $\mathrm{Im}(\lambda_\kappa)=O(\kappa^2)$ and partial integration as before, we conclude that the remainder has a bound of the form (5.31) for any $m>0$. □

Notes: Spectral deformation is also discussed in Ref. 81, Vol. IV, and in Ref. 45. For a critical review of the corresponding notion of resonances see Ref. 98. As a tool to effect a spectral deformation the dilation group $x\rightarrow e^{\xi}x$ on R^n can be replaced by other flows or more general distortions.[99,86,15,49,34] In particular, the Balslev–Combes results hold under the weaker hypothesis that only the tails of the intercluster potentials $I_a(x)$ for large $|x|_a$ have some analyticity.[34] One of the few perturbative results for N-body systems is the Stark effect[44,51,89] which requires asymptotic rather than analytic perturbation theory.[50] Another example is the atom coupled to a quantized radiation field.[9] A time-dependent perturbation approach to the resonance problem was initiated by Soffer and Weinstein[102] (see also Ref. 73). Generally speaking, all results on the existence and interpretation of resonances so far rely on some sort of perturbation argument.

VI. ESSENTIAL SPECTRUM II. MOURRE'S INEQUALITY

The significance of Mourre's inequality[75,79] for the analysis of N-body systems can hardly be exaggerated. As a tool for exploring the nature of the essential spectrum of H it is both more general and more powerful than the (formally related) concept of dilation-analyticity. In addition, it provides a direct insight into the propagation properties of continuum states which form the basis for time-dependent scattering theory. As it appears later in Theorem 6.1, Mourre's inequality has no immediate heuristic appeal. However, the following considerations provide some preliminary understanding of its form. For trajectories $\psi_t=e^{-iHt}\psi$ in the continuous spectral subspace $\mathcal{H}_C$ we may expect that

$$\langle x^2\rangle_t=(\psi_t,x^2\psi_t)\approx\theta t^2\quad(t\rightarrow\infty) \tag{6.1}$$

for some constant $\theta\geqslant 0$. This constant should be equal to the second time derivative of $\langle x^2/2\rangle_t$ in the time mean, or for states ψ with sufficiently sharp energy distribution. Noting that

$$\frac{d^2}{dt^2}\left\langle\frac{x^2}{2}\right\rangle_t=\langle i[H,A]\rangle_t;$$

$$A=i\left[H,\frac{x^2}{2}\right]=\frac{1}{2}(p\cdot x+x\cdot p); \tag{6.2}$$

$$i[H,A]=p^2-(x\cdot\nabla V(x)), \tag{6.3}$$

we are led to a special case of Mourre's inequality: if E is not an eigenvalue of H, then

$$B_\Delta(H)\equiv E_\Delta(H)i[H,A]E_\Delta(H)\geqslant(\theta(E)-\varepsilon)E_\Delta(H) \tag{6.4}$$

for some $\theta(E)\geqslant 0$ and any $\varepsilon>0$, where E_Δ is the spectral projection of H for a sufficiently small open interval $\Delta\ni E$. The Mourre constant $\theta(E)$ is directly related to the effect of thresholds. A threshold of H is an eigenvalue λ^a of H^a for some $a > \{0\}$, corresponding to a stationary state $\psi^a \in L^2(a^\perp)$ of the subsystem H^a. In the energy range above λ^a, we expect the existence of scattering trajectories ψ_t with a behavior like

$$\psi_t \approx e^{-i(1/2\, p_a^2 + \lambda^a)t} \psi_a \otimes \psi^a \quad (t \to \infty), \tag{6.5}$$

where $\psi_a \in L^2(a)$ is arbitrary. For such trajectories, with energy distribution sufficiently localized near some energy $E > \lambda^a$, we will have

$$\langle x^2 \rangle_t \approx \langle x_a^2 \rangle_t \approx \langle p_a^2 \rangle t^2 \approx 2(E - \lambda^a) t^2 \quad (t \to \infty). \tag{6.6}$$

For fixed E all thresholds $\leqslant E$ might contribute scattering states with energies localized near E. For $E > \Sigma$, *the Mourre constant* $\theta(E)$ *is in fact twice the distance of* E *from the highest threshold* $\leqslant E$. Equation (6.4) also holds for $E < \Sigma$ if we define $\theta(E) = 0$. This is trivial if $E \notin \sigma(H)$. If E is an eigenvalue of H, then $\langle x^2 \rangle_t$ is constant for the corresponding bound states. In this case $E_\Delta(H)$ reduces to an eigenprojection for small Δ, and $B_\Delta(H) = 0$ follows from the *virial theorem:*

$$(\psi, i[H,A]\phi) = 0 \tag{6.7}$$

if ψ, ϕ are eigenvectors of H with the same eigenvalue E. Equation (6.7) is formally obvious for any $A = A^*$, since $(\psi, i[H,A]\phi) = iE[(\psi, A\phi) - (A\psi, \phi)] = 0$. All these are special cases of a more general Mourre inequality: *(6.4) holds for any real* E, *up to an error term which is a compact operator*. From this powerful inequality we will derive a number of basic results concerning the structure of the continuous spectrum of H:

(i) Eigenvalues away from thresholds have finite multiplicities and can accumulate only at thresholds, and only from below. Since thresholds are eigenvalues of subsystems, it follows that the set of thresholds is closed and countable.
(ii) Eigenfunctions for nonthreshold eigenvalues decay at least like $\exp(-|x|\sqrt{2(\lambda - E)})$, where λ is the lowest threshold $> E$.
(iii) H has no eigenvalues (and thus no thresholds) > 0.

Later we will exploit Mourre's inequality to analyze the large time behavior of continuum states, thereby confirming the heuristic arguments used in this introduction.

A. The virial theorem and Mourre's inequality

We define $i[H,A]$ by the explicit form (6.3) as a Schrödinger operator on $D(p^2)$, assuming that the *virial* $(x \cdot \nabla V(x))$ also satisfies the conditions imposed on the potential $V(x)$. Then the virial theorem (6.7) can be proven by using some regularization of A, e.g.,

$$A \to A_\varepsilon = \tfrac{1}{2}(p \cdot x e^{-\varepsilon x^2} + e^{-\varepsilon x^2} x \cdot p) \quad (\varepsilon > 0). \tag{6.8}$$

Here A_ε is bounded relative to p^2, and $i[H,A_\varepsilon]$ is defined by an expression similar to (6.3). The formal argument given for (6.7) is correct for A_ε, since $\psi, \phi \in D(A_\varepsilon)$. Thus $(\psi, i[H,A_\varepsilon]\phi) = 0$, and (6.7) follows in the limit $\varepsilon \to 0$.

Definition: A *threshold of* H is an eigenvalue of H^a for some $a > \{0\}$. $\tau(H)$ is the set of all thresholds of H. The *Mourre constant* $\theta(E)$ is defined for any real E by

$$\theta(E) = \begin{cases} 0 & \text{for } E < \Sigma; \\ \inf\limits_{\lambda \in \tau(H); \lambda \leqslant E} 2(E - \lambda) & \text{for } E \geqslant \Sigma. \end{cases} \tag{6.9}$$

Theorem 6.1:[75,79] *Suppose that the virial* $(x \cdot \nabla V(x))$ *satisfies the same condition as the potential* $V(x)$. *Let* $i[H,A]$ *be defined by (6.3), and let* $E_\Delta(H)$ *be the spectral projection of* H *for an interval* Δ. *Then we have the following.*

(*i*) *Given* $E \in R$ *and* $\varepsilon > 0$, *there exists an open interval* $\Delta \ni E$ *and a compact operator K such that*

$$B_\Delta(H) \equiv E_\Delta(H) i[H,A] E_\Delta(H) \geqslant (\theta(E) - \varepsilon) E_\Delta(H) + K. \tag{6.10}$$

(*ii*) *Nonthreshold eigenvalues of H have finite multiplicities and can accumulate only at thresholds. Therefore* $\tau(H)$ *is closed and countable.*

Notation: We will use the abbreviation "$\Delta \ni E$" to say that Δ is an open interval containing E and "$\Delta \to \{E\}$" for a sequence of such intervals with length $|\Delta| \to 0$.

Corollary: Equation (6.4) follows from (6.10) if E is not an eigenvalue of H.

Proof: Multiplying (6.10) from both sides by $E_\Delta(H)$ we see that K may be replaced by $E_\Delta K E_\Delta$. Then we let $\Delta \to \{E\}$ while keeping K fixed. Since E is not an eigenvalue of H, $E_\Delta(H) \xrightarrow{s} 0$ and therefore $\|K E_\Delta(H)\| \to 0$. □

Proof of Theorem 6.1:[32] We proceed by induction in subsystems, assuming that Theorem 6.1 holds for all H^a with $a > \{0\}$ in the following form: $\tau(H^a)$ consists of the eigenvalues of all H^b with $b > a$, $\theta^a(E)$ is defined with respect to $\tau(H^a)$, and (6.10) reads

$$B_\Delta(H^a) \geqslant (\theta^a(E) - \varepsilon) E_\Delta(H^a) + K \quad \text{on } L^2(a^\perp), \tag{6.11}$$

where $B_\Delta(H^a) = E_\Delta(H^a) i[H^a, A^a] E_\Delta(H^a)$; $i[H^a, A^a] = -\Delta^a - (x^a \cdot \nabla V^a(x^a))$. This induction hypothesis is trivially satisfied for $a = X$.

Lemma 6.2: Part (ii) of Theorem 6.1 follows from part (i).

Proof: By part (ii) of the induction hypothesis, $\tau(H)$ is closed and countable. Let $E_n \to E$ be an infinite sequence of eigenvalues of H with orthonormal eigenvectors ψ_n. From Theorem 2.1 we know that $E \geqslant \Sigma$, so that $\theta(E) = 0$ implies $E \in \tau(H)$. By (6.7) and (6.11),

$$0 \geqslant (\theta(E) - \varepsilon) + (\psi_n, K\psi_n)$$

for any $\varepsilon > 0$ and large n. Since $\psi_n \xrightarrow{w} 0$ we have $\|K\psi_n\| \to 0$ and therefore $\theta(E) = 0$, i.e., $E \in \tau(H)$. □

Lemma 6.3:

$$B_\Delta(H^a) \geqslant (\theta(E) - \varepsilon) E_\Delta(H^a) \tag{6.12}$$

for any $E \in R$, *any* $\varepsilon > 0$ *and some* $\Delta \ni E$.

Proof: If E is not an eigenvalue of H^a we have $B_\Delta(H^a) \geqslant (\theta^a(E) - \varepsilon) E_\Delta(H^a)$ by the induction hypothesis and by the Corollary to Theorem 6.1, and (6.12) follows since $\theta^a(E) \geqslant \theta(E)$. Now let E be an eigenvalue of H^a with eigenprojection P. Then we have to prove (6.12) with $\theta(E) = 0$. Since $\dim(P) = \infty$ is not excluded, we represent P as a strong limit of finite rank projections $P_n \leqslant P$. We abbreviate $B_\Delta(H^a) \equiv B_\Delta$ and $E_\Delta(H^a) \equiv E_\Delta$. By the virial theorem $P_n B_\Delta P = P_n P B_\Delta P = 0$, so that

$$B_\Delta = (1 - P_n) B_\Delta (1 - P_n) + P_n B_\Delta (1 - P) + (1 - P) B_\Delta P_n.$$

Using (6.11) in the form $B_\Delta \geqslant -\varepsilon + E_\Delta K E_\Delta$ to estimate the first term on the rhs, we obtain

$$B_\Delta \geqslant -\varepsilon - \|K(P - P_n)\| - \|K E_\Delta (1 - P)\| - 2\|P_n B_\Delta (1 - P)\|.$$

Since K and $P_n B_\Delta$ are compact, and since $E_\Delta(1 - P) \xrightarrow{s} 0$ as $\Delta \to \{E\}$, we can first fix n and then Δ to make the last three norms arbitrarily small, and multiplying the result from both sides with E_Δ proves (6.12). □

Lemma 6.4: Given a compact $I \subset R$ *and* $\varepsilon > 0$, *there exists* $\delta > 0$ *such that*

$$B_\Delta(H^a) \geqslant (\theta(E + \varepsilon) - 2\varepsilon) E_\Delta(H^a) \tag{6.13}$$

for any $E\in I$ *and any* $\Delta\ni E$ *of length* $|\Delta|<\delta$.

Proof: Suppose this is false. Then (6.13) is violated for some sequence $E_n\to E$ in I and corresponding $\Delta_n\ni E_n$ with $|\Delta_n|\to 0$. From (6.12) we obtain

$$B_\Delta(H^a)\geqslant\left(\theta(E)-\frac{\varepsilon}{2}\right)E_\Delta(H^a) \tag{6.14}$$

for some $\Delta\ni E$. Let n be so large that $|E_n-E|<\varepsilon/2$ and $\Delta_n\subset\Delta$. Since $\theta(E+x)\leqslant\theta(E)+x$ for any $x\geqslant 0$, we then have

$$\theta(E)\geqslant\theta(E_n+\varepsilon)-\varepsilon+E-E_n\geqslant\theta(E_n+\varepsilon)-3\frac{\varepsilon}{2}.$$

From this, $\Delta_n\subset\Delta$ and (6.14) we deduce that $B_{\Delta_n}(H^a)\geqslant(\theta(E_n+\varepsilon)-2\varepsilon)E_{\Delta_n}(H^a)$, which contradicts our assumption. □

Lemma 6.5:

$$B_\Delta(H_a)\geqslant(\theta(E+\varepsilon)-2\varepsilon)E_\Delta(H_a) \tag{6.15}$$

for any $E\in R$, *any* $\varepsilon>0$ *and some* $\Delta\ni E$.

Proof: We represent the functions $\psi(x)=\psi(x_a,x^a)$ by their partial Fourier transforms with respect to x_a, i.e., by functions $\psi_F(k)$ on a taking values in $L^2(a^\perp)$. In this representation:

$$(\psi,\phi)=\int_a dk(\psi_F(k),\phi_F(k))_{L^2(a^\perp)};$$

$$(H_a\psi)_F(k)=\left(\frac{k^2}{2}+H^a\right)\psi_F(k);$$

$$(E_\Delta(H_a)\psi)_F(k)=E_{\Delta-k^2/2}(H^a)\psi_F(k);$$

$$(i[H_a,A]\psi)_F(k)=(k^2+i[H^a,A^a])\psi_F(k).$$

For $\psi=E_\Delta(H_a)\psi$ we thus obtain

$$(\psi,B_\Delta(H_a)\psi)=\int_a dk(\psi_F(k),(k^2+B_{\Delta-k^2/2}(H^a))\psi_F(k))_{L^2(a^\perp)}.$$

Since H^a is bounded from below, the integrand has compact support: $\psi_F(k)=E_{\Delta-k^2/2}(H^a)\psi_F(k)=0$ for large k^2. By (6.13) it thus has a lower bound

$$\left(k^2+\theta\left(E-\frac{k^2}{2}+\varepsilon\right)-2\varepsilon\right)\|\psi_F(k)\|^2\geqslant(\theta(E+\varepsilon)-2\varepsilon)\|\psi_F(k)\|^2$$

which proves (6.15). □

Proof of (6.10): Let $f\in C_0^\infty(\Delta)$ be real with $f=1$ on some $\Delta_1\ni E$. Applying the localization formula (3.20) to the Schrödinger operator $i[H,A]$, we obtain in analogy to (3.21)

$$f(H)i[H,A]f(H)=\sum_a f(H)j_a i[H_a,A]j_a f(H)+\text{compact}.$$

We note that

$$L\equiv f(H)j_a-j_a f(H_a)\quad\text{is compact} \tag{6.16}$$

for any $f\in C_0^\infty(R)$. In fact, by the Helffer–Sjöstrand formula (9.1), it suffices to verify that

$$j_a(z-H)^{-1}-(z-H_a)^{-1}j_a=(z-H_a)^{-1}(\tfrac{1}{2}[j_a,p^2]+I_aj_a)(z-H)^{-1}$$

is compact. This follows from local compactness since both $\nabla j_a(x)$ and $I_a(x)j_a(x)$ vanish as $|x|\to\infty$. Using (6.16) and (6.15) we arrive at

$$f(H)i[H,A]f(H)\geqslant(\theta(E+\varepsilon)-2\varepsilon)f(H)^2+\text{compact}.$$

Multiplying both sides with $E_{\Delta_1}(H)$ we obtain

$$B_{\Delta_1}(H)\geqslant(\theta(E+\varepsilon)-2\varepsilon)E_{\Delta_1}(H)+\text{compact}.$$

This is equivalent to (6.10), since $\theta(E+\varepsilon)=\theta(E)+\varepsilon$ for small ε if $E\notin\tau(H)$. □

We now give a precise form of the estimate (6.1) which plays an important role in scattering theory. A finite, open interval Δ will be called a *Mourre interval* if

$$E_\Delta(H)i[H,A]E_\Delta(H)\geqslant\theta E_\Delta(H)\quad\text{for some}\quad\theta>0. \tag{6.17}$$

Let $\mathcal{H}_\Delta\equiv\text{Ran}(E_\Delta(H))$. Then (6.17) implies

$$\liminf_{t\to\infty}\left\langle\frac{x^2}{t^2}\right\rangle_t\geqslant\theta>0 \tag{6.18}$$

for all initial states ψ in the domain $\mathcal{H}_\Delta\cap D(|x|)$, which is invariant under e^{-iHt} and dense in $\mathcal{H}_\Delta$. By the virial theorem a Mourre interval Δ contains no eigenvalue of H so that $\mathcal{H}_\Delta\subset\mathcal{H}_C$. If E is not an eigenvalue nor a threshold of H, then E is contained in a Mourre interval by (6.4). Since the set of eigenvalues and thresholds is closed and countable, it follows that *the spectral subspaces* $\mathcal{H}_\Delta$ (Δ *a Mourre interval*) *span a dense linear set in* $\mathcal{H}_C$.

B. Exponential bounds for eigenfunctions and absence of positive eigenvalues

As a first application of Mourre's inequality we prove the following results of Froese, Herbst, and Perry:

Theorem 6.6:[31] *Under the hypothesis of Theorem 6.1, let* $H\psi=E\psi$ *and*

$$\alpha=\sup\{\beta\in R|e^{\beta r}\psi\in L^2(X)\},\quad(r=|x|).$$

Then $E+1/2\,\alpha^2$ *is either infinite or a threshold of* H.

Proof: The proof is indirect: we assume $0\leqslant\alpha<\infty$ and $E+1/2\,\alpha^2\notin\tau(H)$, which will lead to a contradiction. We construct a sequence of smooth, bounded functions $F_n(x)$ which approximate $F(x)=\alpha r$ from above in successively larger regions:

$$F_n(x)=\alpha_n r j(r)(1-j(\varepsilon_n r)). \tag{6.19}$$

Here $j(r)$ is a smoothed characteristic function of $\{r>1\}$, α_n is some sequence with $\alpha_n\searrow\alpha$, and $\varepsilon_n\searrow 0$ is chosen such that

$$\|e^{F_n}\psi\|\to\infty. \tag{6.20}$$

We define

$$\psi_n=e^{F_n}\psi\|e^{F_n}\psi\|^{-1};\quad\langle\cdots\rangle_n=(\psi_n,\ldots,\psi_n). \tag{6.21}$$

Lemma 6.7: (i) $\psi_n\overset{w}{\to}0$. *(ii)* $p^2\psi_n\overset{w}{\to}0$. *(iii)* $\|G(x)\psi_n\|\to 0$, *and* $\|G(x)(1+p^2)^{1/2}\psi_n\|\to 0$ *for any function* $G\in L^\infty(X)$ *which vanishes at* ∞.

Proof: (i) follows from (6.18); (iii) follows from (ii) and from the compactness property (2.6). To prove (ii) it remains to show that $\|p^2\psi_n\|$ is bounded. We set

$$H_n=e^{F_n}He^{-F_n}=H-\tfrac{1}{2}|\nabla F_n|^2+i\gamma_n; \tag{6.22}$$

$$\gamma_n=\tfrac{1}{2}(\nabla F_n\cdot p+p\cdot\nabla F_n). \tag{6.23}$$

Then $H_n\psi_n=E\psi_n$, and $E=\mathrm{Re}\langle H_n\rangle_n=\langle H\rangle_n-1/2\langle|\nabla F_n|^2\rangle_n$. Since $\nabla F_n(x)$ is uniformly bounded in (n,x), we obtain successive bounds for $\langle H\rangle_n$, $\langle p^2\rangle_n$, $\|\gamma_n\psi_n\|$, $\|H\psi_n\|$ and $\|p^2\psi_n\|$. □

Remark: In the following estimates we will need higher derivatives of $F_n(x)$. They are of the form

$$F_{n,k_1,\ldots,k_s}(x)=\alpha_n\left(\frac{\partial^s r}{\partial x_{k_1}\cdots\partial x_{k_s}}\right)j(r)(1-j(\varepsilon_n r)), \tag{6.24}$$

plus terms of fixed compact support [involving derivatives of $j(r)$], plus terms of order ε_n [involving derivatives of $j(\varepsilon_n r)$]. By Lemma 6.7 (iii), and since $\varepsilon_n\to 0$, these terms will give no contributions in the limit $n\to\infty$ to the expectation values $\langle\cdots\rangle_n$ estimated later. The same is true for the leading term (6.24) if $s>1$, since it is of order r^{1-s} as $r\to\infty$.

Lemma 6.8:

$$\lim_{n\to\infty}\|(H-\tfrac{1}{2}\alpha^2-E)\psi_n\|=0.$$

Proof:

$$\begin{aligned}0&=\langle(H_n^*-E)(H_n-E)\rangle_n\\&=\langle(H-\tfrac{1}{2}|\nabla F_n|^2-E)^2\rangle_n+\langle\gamma_n^2\rangle_n+\langle i[H-\tfrac{1}{2}|\nabla F_n|^2,\gamma_n]\rangle_n.\end{aligned} \tag{6.25}$$

We show that the third term vanishes as $n\to\infty$. By the remark above we need only consider $\langle i[V,\gamma_n]\rangle_n=-\langle\nabla V\cdot\nabla F_n\rangle_n$ since the other commutators involve higher derivatives of F_n. By (6.24),

$$\lim_{n\to\infty}\langle\nabla V\cdot\nabla F_n\rangle_n=\lim_{n\to\infty}\langle(x\cdot\nabla V)r^{-1}j(r)\rangle_n=0,$$

since $x\cdot\nabla V(x)$ is p^2-bounded and $r^{-1}j(r)\to 0$ as $r\to\infty$. Because the first two terms in (6.25) are positive, we now have $\lim_{n\to\infty}\|(H-1/2|\nabla F_n|^2-E)\psi_n\|=0$. Therefore it suffices to show that $\|(\alpha_n-|\nabla F_n|)\psi_n\|\to 0$. By Lemma 6.7, the contribution from any bounded region to this norm vanishes as $n\to\infty$, so we need only show that $\alpha_n I_n\to 0$ for $I_n=\|j(\varepsilon_n r)\psi_n\|$. This is trivial if $\alpha=0$. Otherwise, we split I_n into contributions from the regions $j(\varepsilon_n r)<\delta$ and $j(\varepsilon_n r)>\delta$, obtaining $I_n\leqslant\delta+\|e^{\alpha_n(1-\delta)r}\psi)\|\|e^{F_n}\psi\|^{-1}$. This bound becomes arbitrarily small by first fixing δ small and then n sufficiently large, since eventually $\alpha_n(1-\delta)<\alpha$. □

Lemma 6.9:

$$\lim_{n\to\infty}\inf\langle i[H,A]\rangle_n>0.$$

Proof: Let $B=i[H,A]$. Since $E+1/2\,\alpha^2\notin\tau(H)$, we have a Mourre inequality:

$$\langle E_\Delta(H)BE_\Delta(H)\rangle_n\geqslant\theta\langle E_\Delta(H)\rangle_n+\langle K\rangle_n \tag{6.26}$$

with $\theta>0$ and compact K, for some interval $\Delta=(E+\alpha^2/2-\varepsilon,E+\alpha^2/2+\varepsilon)$. By Lemma 6.7, $\langle K\rangle_n\to 0$ for $n\to\infty$. Setting $\overline{E}_\Delta=1-E_\Delta$ we also obtain

$$\|\overline{E}_\Delta\psi_n\|\leqslant\varepsilon^{-1}\|(H-\tfrac{1}{2}\alpha^2-E)\psi_n\|\to 0 \tag{6.27}$$

from Lemma 6.8. Now $\langle B\rangle_n\geqslant\langle E_\Delta BE_\Delta\rangle_n-\|\overline{E}_\Delta\psi_n\|(2\|BE_\Delta\|+\|B\overline{E}_\Delta\psi_n\|)$. By (6.27) the second term vanishes as $n\to\infty$, since $H\psi_n$ is bounded. Therefore

$$\liminf_{n\to\infty}\langle B\rangle_n\geqslant\liminf_{n\to\infty}\langle E_\Delta BE_\Delta\rangle_n\geqslant\liminf_{n\to\infty}\theta\langle E_\Delta\rangle_n\theta>0.$$

□

The next statement is in contradiction to Lemma 6.9 and thus completes the proof of Theorem 6.6:

Lemma 6.10:

$$\limsup_{n\to\infty}\langle i[H,A]\rangle_n\leqslant 0.$$

Proof: From the identity $0=2\,\mathrm{Im}(A\psi_n,(H_n-E)\psi_n)$ we obtain

$$\langle i[H,A]\rangle_n=\tfrac{1}{2}\langle i[|\nabla F_n|^2,A]\rangle_n-2\,\mathrm{Re}\langle\gamma_n A\rangle_n\,.$$

The only contribution involving only first order derivatives of F_n is

$$-\langle p_k(x_kF_{n,l}+F_{n,k}x_l)p_l\rangle_n\,.$$

By (6.24) this is equal to

$$-2\alpha_n\left\langle(p\cdot x)\frac{j(r)}{r}(x\cdot p)\right\rangle_n\leqslant 0,$$

modulo terms vanishing as $n\to\infty$. □

Theorem 6.11:[78] *Under the hypothesis of Theorem 6.1, eigenvalues can accumulate at thresholds only from below.*

Proof: Proceeding inductively, we assume that thresholds can accumulate at a given threshold E only from below: there is an interval $(E,\ldots,E+1/2\,\alpha^2]$ $(\alpha>0)$ containing no thresholds. Now suppose there is an infinite sequence of eigenvalues $E_n\searrow E$ in this interval, with corresponding orthonormal eigenfunctions $\phi_n\xrightarrow{w}0$. This leads to a contradiction. The proof is a straight copy of the proof of Theorem 6.6. The function $F(x)\equiv\alpha rj(r)$ corresponds to the functions $F_n(x)$ of (6.17) for $\alpha_n=\alpha$ and $\varepsilon_n=0$. By Theorem 6.6, $e^F\phi_n\in L^2(X)$. Therefore $\psi_n=e^F\phi_n\|e^F\phi_n\|^{-1}\xrightarrow{w}0$, and the rest of the proof (Lemmas 6.7–6.10) goes through with minimal changes: as an eigenvalue, E is replaced by E_n. □

Theorem 6.12:[31] *Under the hypothesis of Theorem 6.1, H has no eigenvalue $E>0$.*

Proof: Since thresholds arise from eigenvalues of subsystems, we can proceed by induction: assuming that H has no positive threshold, we prove that H has no positive eigenvalue. The proof is again indirect: we derive a contradiction from $H\psi=E\psi$; $E>0$. By Theorem 6.6, $e^{\alpha r}\psi\in L^2(X)$ for any $\alpha>0$. We first fix ρ such that

$$\int_{r<\rho}dx\,|\psi|^2\leqslant\int_{r>2\rho}dx\,|\psi|^2, \tag{6.28}$$

Then we choose a C^∞-function $F(r)\leqslant r$, with $F'(r)\geqslant 0$, and $F(r)=r$ for $r>\rho$, and we define $\psi_\alpha=e^{\alpha F}\psi\|e^{\alpha F}\psi\|^{-1}$; $\langle\ldots\rangle_\alpha=(\psi_\alpha,\ldots\psi_\alpha)$. By (6.28),

$$\int_{r<\rho} dx\,|\psi_\alpha|^2 \leqslant e^{-2\alpha\rho}. \tag{6.29}$$

Lemma 6.13: For some constant c_1 and all $\alpha>0$,

$$\langle H\rangle_\alpha \equiv (\psi_\alpha, H\psi_\alpha) \geqslant E + \frac{\alpha^2}{2} - c_1\alpha^2 e^{-2\alpha\rho}. \tag{6.30}$$

Proof: We define

$$H_\alpha = e^{\alpha F} H e^{-\alpha F} = H - \frac{\alpha^2}{2}|\nabla F|^2 + i\alpha\gamma;\ \gamma = \frac{1}{2}(\nabla F\cdot p + p\cdot\nabla F).$$

Then $H_\alpha\psi_\alpha = E\psi_\alpha$ and $\langle H\rangle_\alpha = E + (\alpha^2/2)\langle|\nabla F|^2\rangle_\alpha$. Since $|\nabla F|^2 = 1$ for $r>\rho$, we obtain from (6.29) $|\langle|\nabla F|^2\rangle_\alpha - 1| \leqslant c_1 e^{-2\alpha\rho}$. □

Lemma 6.14: For some constants c_2, c_3 and all $\alpha>0$,

$$\langle i[H,A]\rangle_\alpha = \langle p^2\rangle_\alpha - \langle x\cdot\nabla V(x)\rangle_\alpha \leqslant c_2\alpha^2 e^{-2\alpha\rho} + \alpha c_3. \tag{6.31}$$

Proof: From the identity $0 = 2\,\mathrm{Im}(A\psi_\alpha,(H_\alpha - E)\psi_\alpha)$ we obtain

$$\langle i[H,A]\rangle_\alpha = \frac{\alpha^2}{2}\langle i[|\nabla F|^2, A]\rangle_\alpha - 2\alpha\,\mathrm{Re}\langle\gamma A\rangle_\alpha.$$

Since $|\nabla F|^2 = 1$ for $r>\rho$, the first term is bounded by $c_2\alpha^2\exp(-2\alpha\rho)$. For the second term we compute

$$2\,\mathrm{Re}(\gamma A) = p_k(x_k F_{,l} + F_{,k}x_l)p_l - \frac{d}{2}F_{,ll} - \frac{1}{2}x_k F_{,llk},$$

where $d = \dim(X)$. The first term is positive since $F_{,l} = x_l r^{-1}F'(r)$, $F'(r)\geqslant 0$, and the remaining two terms are bounded. □

Completion of the proof of Theorem 6.12: Subtracting (6.30) from (6.31) we arrive at

$$\tfrac{1}{2}\langle p^2\rangle_\alpha - \langle V\rangle_\alpha - \langle x\cdot\nabla V(x)\rangle_\alpha \leqslant -E - \tfrac{1}{2}\alpha^2 + (c_1 + c_2)\alpha^2 e^{-2\alpha\rho} + \alpha c_3.$$

This is a contradiction: the left-hand side is bounded below, while the right-hand side goes to $-\infty$ for $\alpha\to\infty$. □

Notes: The use of the dilation generator A in Mourre's inequality is as arbitrary as the use of the dilation group to effect a spectral deformation. The following variant of Theorem 6.1 is due to Skibsted,[100] a simpler proof suggested by Graf is given in Ref. 39. The starting point is to replace the observable x^2 in (6.1) by a convex function $G(x)$ with the same growth:

$$c_1 x^2 \leqslant G(x) \leqslant c_2 x^2. \tag{6.32}$$

Then (6.2) and (6.3) take the form

$$\begin{aligned} A &= \frac{i}{2}[H,G] = \frac{1}{2}(p\cdot\nabla G + \nabla G\cdot p),\\ i[H,A] &= pG''p - \tfrac{1}{2}\Delta^2 G - \nabla G\cdot\nabla V(x), \end{aligned} \tag{6.33}$$

where (in Cartesian coordinates) $pG''p \equiv p_i G_{,ik} p_k \geqslant 0$ by the convexity of G. The proof of Theorem 6.1 in this case is based on a special construction of the function $G(x)$ due to Graf.[38] Up to a regularization $G(x)$ is given by

$$G(x) = \max_{a \in L} (x_a^2 + \varepsilon_a) \tag{6.34}$$

for a suitable choice of the parameters ε_a. This construction is similar to (and in fact the model of) a later construction by Yafaev[116] which we discuss more fully in Sec. VII. In particular the ε_a's can be adjusted so that only the tails of the intercluster potentials $I_a(x)$ enter into (6.33). As a result Theorem 6.1 holds in exactly the same form and with the same definition of $\theta(E)$ provided only that $\nabla I_a(x)$ exists for large $|x|_a$ with

$$|\nabla I_a(x)| = o(|x|_a^{-1}) \quad \text{as} \quad |x|_a \to \infty. \tag{6.35}$$

This generalization of Mourre's theorem avoids a global condition on $\nabla V(x)$, so that potentials with strong singularities (e.g., hard cores) can be allowed. And since $G(x)$ and x^2 have the same growth, most of the applications of Mourre's inequality hold under the weaker hypothesis (6.35).[39]

VII. SCATTERING THEORY

A. Scattering states

The existence and the asymptotic form of scattering orbits ψ_t for $t \to \infty$ depends crucially on the rate at which the intercluster potentials $I_a(x)$ vanish for large separation. We will state such fall-off conditions in the form

$$\partial_x^k I_a(x) = O(|x|_a^{-\mu - |k|}), \quad |x|_a \to \infty, \tag{7.1}$$

with k a multi-index. The required values of $\mu > 0$ and $|k|$ will be specified according to the context.

1. Short-range systems: $\mu > 1$

Here outgoing scattering states ψ are characterized by the asymptotic condition

$$\psi_t = e^{-iHt}\psi \underset{\|\|}{\rightarrow} \sum_{a \in L} e^{-iH_a t}\varphi_a \quad (t \to +\infty); \varphi_a \in \mathcal{H}_a \equiv L^2(a) \otimes \mathcal{H}_B(H^a), \tag{7.2}$$

where $\mathcal{H}_B(H^a)$ is the subspace of $L^2(a^\perp)$ spanned by the eigenvectors of H^a. Each term in the sum (7.2) represents a surface wave in X propagating freely along the channel $a \subset X$ or, viewed in R^3, a free motion of independent bound clusters. For convenience we have included the bound state channel $a = \{0\}$: if $\psi \in \mathcal{H}_B(H)$, then (7.2) holds trivially with $\varphi_{\{0\}} = \psi$, $\varphi_a = 0$ for $a > \{0\}$. The existence of a unique scattering state ψ for any given set $\{\varphi_a\}$ is one of the earliest results in N-body scattering theory:[40] if $I_a(x) = O(|x|_a^{-\mu})$, $\mu > 1$, then the wave operators

$$\Omega_a^+ = \text{s}-\lim_{t \to +\infty} e^{iHt} e^{-iH_a t} \tag{7.3}$$

exist on $\mathcal{H}_a$, so that (7.2) holds for

$$\psi = \sum_a \Omega_a^+ \varphi_a .$$

The wave operators are isometric from $\mathcal{H}_a$ to $\mathcal{H}$. Moreover, their ranges $\mathcal{H}_a^+ = \text{Ran}(\Omega_a^+)$ satisfy

$$\mathcal{H}_a^+ \perp \mathcal{H}_b^+ \quad (a \neq b),$$

expressing the fact that

$$\lim_{t\to+\infty}(e^{-iH_at}\varphi_a, e^{-iH_bt}\varphi_b)=0 \quad (a\neq b). \tag{7.4}$$

Therefore, the outgoing scattering states form a closed subspace

$$\mathcal{H}^+ = {\bigoplus_{a\in L}}' \mathcal{H}_a^+ \subset \mathcal{H}.$$

The proofs of (7.3) and (7.4) involve only the free center-of-mass motion of the clusters (see e.g., Ref. 81, Vol. III).

Since the early days of scattering theory, when this formalism was developed (e.g., in Ref. 60) the main fundamental problem was to prove the conjecture of *asymptotic completeness, i.e., the conjecture that every state* $\psi\in\mathcal{H}$ *is an outgoing scattering state in the sense of* (7.2). This problem was first solved by Sigal and Soffer:[91]

Theorem 7.1:[91,38,116,103,52] *Under the hypothesis of Theorem 6.1 and if*

$$|I_a(x)| = O(|x|_a^{-\mu}), \quad \mu>1, \tag{7.5}$$

then $\mathcal{H}^+=\mathcal{H}$.

By time reversal the same result holds for the subspace $\mathcal{H}^-$ of incoming scattering states, defined by an asymptotic condition of the form (7.2) for $t\to-\infty$. This means that every orbit ψ_t of the system has an asymptotic form (7.2) in both time directions.

2. Long-range systems: $(\mu\leqslant 1)$

For μ not too small it is known[22,12] that the appropriate asymptotic condition generalizing (7.2) is

$$\psi_t = e^{-iHt}\psi \underset{\|\|}{\longrightarrow} \sum_a e^{-iH_at - i\alpha_{a,t}(p_a)}\varphi_a \quad (t\to t\infty) \tag{7.6}$$

with $\varphi_a\in\mathcal{H}_a$ as before. Compared to (7.2) only the free center-of-mass propagator of the fragments in channel a is modified from

$$e^{-(i/2)\,p_a^2 t} \quad \text{to} \quad e^{-(i/2)\,p_a^2 t - i\alpha_{a,t}(p_a)},$$

which still conserves the momentum p_a. Here $\alpha_t(p_a)$ is an adiabatic phase arising from the fact that classically the fragments are located at $x_a=p_at(1+O(t^{-\mu}))$ (as $t\to\infty$), so that

$$I_a(x) = I_a(p_at) + O(t^{-2\mu}), \tag{7.7}$$

provided that $\nabla I_a(x)=O(|x|_a^{-\mu-1})$ as $|x|_a\to\infty$. For $2\mu>1$ the error term in (7.7) decays integrably in time, while the leading term is of order $t^{-\mu}$ and therefore not integrable if $\mu\leqslant 1$. According to this classical picture the ansatz

$$\alpha_{a,t}(p_a) = \int^t ds\, I_a(p_a s)$$

should work for $\mu>\frac{1}{2}$. The reason why we have not fully defined $\alpha_{a,t}(p_a)$ is twofold. First, it is clear that the modified propagator is insensitive to a change of $\alpha_{a,t}(\cdot)$ on a null set of a. This allows us to restrict p_a to the set a^* (3.9), where $I_a(p_as)$ indeed decays like $s^{-\mu}$. Second, $\alpha_{a,t}(p_a)$ is arbitrary within gauge transformations of the kind

$$\alpha_{a,t}(p_a) \to \alpha_{a,t}(p_a) + f_t(p_a)$$

if $\lim_{t\to\infty} f_t(p_a) = f_\infty(p_a)$ exists, since in (7.6) the phase $f_\infty(p_a)$ can be absorbed in φ_a. This is why the integrable error in (7.7) has no effect and why (7.6) is equivalent to (7.2) if $\mu > 1$. A complete definition of $\alpha_{a,t}(p_a)$ modulo gauge transformations is therefore

$$\alpha_{a,t}(p_a) = \int_{R|p_a|_a^{-1}}^{t} ds\, I_a(p_a s) \quad (p_a \in a^*), \tag{7.8}$$

if, for $|x|_a > R$, $|I_a(x)| \leq \text{const}|x|_a^{-\mu}$. For $a = \{0\}$ we have $p_a = 0$ and we set $\alpha_{\{o\},t} = 0$. An important example is a system of charged particles (the Coulomb case). Then for $p_a \in a^*$

$$I_a(p_a t) = t^{-1} \sum_{\alpha<\beta} e_\alpha e_\beta \left| \frac{p_\alpha}{m_\alpha} - \frac{p_\beta}{m_\beta} \right|^{-1},$$

where the sum runs over all *pairs of clusters* in the channel a with (total) charges e_α, masses m_α and momenta $p_\alpha \in R^3$. A corresponding phase $\alpha_{a,t}(p_a)$ is obtained by changing the factor t^{-1} to $\log(t)$. [This phase differs from (7.8) by a gauge transformation.] The formulas (7.2)–(7.4) can now be transcribed to the long-range case simply by replacing

$$H_a \to H_a + \alpha_{a,t}(p_a). \tag{7.9}$$

The existence of Ω_a^+ is more difficult to prove than in the short-range case. In fact the first general proofs (without *ad hoc* assumptions on the fall-off of bound state wave functions) appeared as by-products of the proofs of asymptotic completeness.

Theorem 7.2:[19] *If (7.1) holds for* $|k| \leq 2$ *and some* $\mu > \sqrt{3} - 1$, *then* $\mathcal{H}^+ = \mathcal{H}$.

This is the result first obtained by Dereziński.[19] A proof for the Coulomb case $\mu = 1$ was also given by Sigal and Soffer.[95] The borderline $\mu = \sqrt{3} - 1$ was identified previously by Enss.[28] Other proofs are given in Refs. 122 and 52. In this review we give the proof of Theorem 7.1, followed by an outline of the strategy used in the long-range case. The common basis for both proofs are the propagation estimates and the asymptotic observables discussed in the next two sections, which are based in Ref. 52.

B. Propagation observables and propagation estimates

Mourre's inequality in the integrated form (6.18) only states that the expectation value $\langle x^2 \rangle_t = (\psi_t, x^2 \psi_t)$ diverges quadratically in t as $t \to \infty$ for any initial state $\psi \in \mathcal{H}_\Delta$, where Δ is any Mourre interval. To derive from this the detailed asymptotic form (7.2) or (7.6) of ψ_t, it is necessary to construct a set of phase-space propagation observables $\phi_t(x,p)$ which control the asymptotic propagation into all possible channels. The basic technique for deriving the corresponding propagation estimates requires that the Heisenberg derivative of ϕ_t is essentially positive, in the sense that

$$D_t \phi_t \equiv i[H, \phi_t] + \partial_t \phi_t = P_t + R_t,$$

where $P_t \geq 0$ and $\|R_t\| = O(t^{-\rho})$, $\rho > 1$. If ϕ_t is uniformly bounded in t, it then follows by integration that

$$\int_0^\infty dt \langle P_t \rangle_t \leq \text{const} \|\psi\|^2,$$

where $\langle P_t \rangle_t = (\psi_t, P_t \psi_t) \geq 0$. This is the type of propagation estimate which forms the basis of all proofs of asymptotic completeness.

1. The Graf–Yafaev construction

The following geometric construction in X was introduced by Graf,[38] then simplified in Ref. 19, and later modified by Yafaev.[116] Following Ref. 52 we use a time-dependent version of

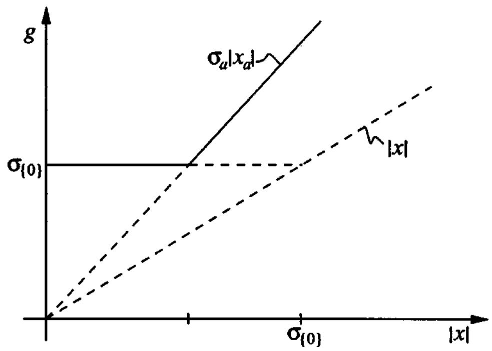

FIG. 11. A radial section of $g(x,\sigma)$.

Yafaev's construction, which results in a function $g_t(x)$; $x \in X$, $t>0$. The motivation for the construction will become evident when we introduce phase space observables built on $g_t(x)$. Let σ be a positive, decreasing function on L:

$$\sigma_{\{0\}}>\sigma_a>\sigma_b>\sigma_X=1$$

for $\{0\}<a<b<X$, to be adjusted in the course of the construction. We define

$$f_a(x)=\begin{cases}\sigma_{\{0\}} & (a=\{0\});\\ \sigma_a|x_a| & (a>\{0\}).\end{cases}$$

Then the prototype of the time-independent Graf–Yafaev function $g(x)$ is given by

$$g(x,\sigma)=\max_{a\in L} f_a(x). \tag{7.10}$$

A radial section of $g(x,\sigma)$ is shown in Fig. 11 for a direction $x\in a$.

Here $g(x,\sigma)$ is convex, constant on some compact set containing the ball $|x|<1$, and homogeneous of degree 1 in the complement of this set. We decompose $g(x,\sigma)$ into maximal pieces:

$$g(x,\sigma)=\sum_{a\in L} g_a(x,\sigma);\quad g_a(x,\sigma)=\begin{cases} f_a(x) & \text{if } f_a(x)=g(x,\sigma);\\ 0 & \text{otherwise.}\end{cases} \tag{7.11}$$

The piece $g_{\{0\}}(x,\sigma)$ has compact support on which it is constant. The pieces $g_a(x,\sigma)$ for $a>\{0\}$ are homogeneous of degree 1 on conical supports whose intersection with a sphere $|x|=R\geqslant\sigma_{\{0\}}$ is shown in Fig. 12. This figure corresponds to Fig. 2 and serves to explain the choice

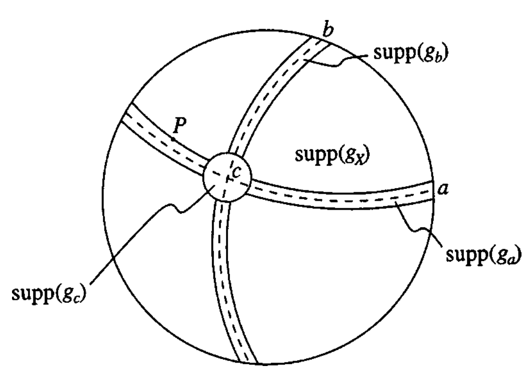

FIG. 12. The pieces of $g(x,\sigma)$.

of σ. Suppose first that $\sigma_a = \sigma_b = \sigma_c = 1$. Then Fig. 12 reduces to Fig. 2 since $\sigma_a |x_a| = |x|$ exactly if $x \in \mathbf{a}$, etc. We now increase σ_a, σ_b by arbitrary small amounts. Then the supports of g_a, g_b broaden into narrow belts shown in Fig. 12. Now we increase σ_c to $\sigma_c > \sigma_a$, σ_b, so that $\mathrm{supp}(g_c)$ grows to a disc covering the intersection of the two belts. This indicates the general construction scheme for the function σ on L which can be carried out analytically.[116,52,39] Figure 12, together with the definition (3.8) of the intercluster distance, suggests what can be achieved: There is a (largely arbitrary) choice of σ such that

$$|x|_a > \lambda |x| \quad \text{on} \quad \mathrm{supp}(g_a) \tag{7.12}$$

for some $\lambda > 0$. Moreover, since $g_a(x,\sigma)$ is, on its support, a function of x_a,

$$\nabla g(x,\sigma) \in \mathbf{a} \quad \text{on} \quad \mathrm{supp}(g_a) \tag{7.13}$$

except at boundary points, where $\nabla g(x,\sigma)$ is discontinuous. This discontinuity is removed by a regularization $g(x,\sigma) \to g(x)$ which preserves convexity:

$$g(x) = \int g(x,\mu) \prod_{a \in L} \delta(\mu_a - \sigma_a)\, d\mu_a,$$

where $0 < \delta \in C_0^\infty(\mathbf{R})$ is a regularization of the Dirac distribution with sufficiently narrow support. The same regularization is applied to $g_a(x,\sigma)$, so that

$$g(x) = \sum_{a \in L} g_a(x). \tag{7.14}$$

The effect of this regularization on Fig. 12 is that the boundaries are slightly smeared, but away from these strips the functional form of $g(x)$ remains the same. For further reference we list the relevant properties of g and g_a (Ref. 116, see also Ref. 52 or 39):

Lemma 7.3 (*Properties of g*):

(i) *g is smooth, convex, and homogeneous of degree 1 outside some ball:* $|x| > R_2$.

(ii) $g(x) = g(0)$ *inside some ball:* $|x| < R_1$.

(iii) *For any* $x \in \mathrm{supp}(\nabla g)$ *there exists* $a \in L$, $a > \{0\}$, *such that*

$$\nabla g(x) \in \mathbf{a} \quad \text{and} \quad |x|_a > \lambda |x|. \tag{7.15}$$

To explain (*iii*), consider the boundary point P shown in Fig. 12: There the intercluster distances with respect to $\mathbf{a}$ and X are both strictly positive, and after regularization we certainly have $\nabla g(P) \in X$. The functions g_a have corresponding properties *except* convexity:

Lemma 7.4 (Properties of g_a*):*

(*i*) g_a *is smooth, and homogeneous of degree 1 for* $|x| > R_2$.

(*ii*) $g_{\{0\}}$ *has compact support in* $|x| < R_2$. *For* $a > \{0\}$, g_a *is supported in* $|x| > R_1$, *and* $|x|_a > \lambda |x|$ *on* $\mathrm{supp}(g_a)$.

(*iii*) ∇g_a *is supported in* $|x| > R_1$. *For any* $x \in \mathrm{supp}(\nabla g_a)$ *there exists* $b \in L$, $b > \{0\}$ *such that*

$$\nabla g_a \in \mathbf{b} \quad \text{and} \quad |x|_b \geq \lambda |x|. \tag{7.16}$$

(*iv*) *For each* $a \in L$ *there exists a function* $\tilde{g}$ *sharing the properties of g given in Lemma 7.3 and such that the Hessians* g_a'' *and* $\tilde{g}''$ *satisfy*

$$\pm g_a'' \leq \tilde{g}''.$$

2. The basic propagation estimate

All our propagation observables are derived from

$$g_t(x) \equiv t^{\delta} g(t^{-\delta} x), \quad 0<\delta<1, \tag{7.17}$$

for $t>0$. By Lemma 7.3 g_t is smooth and convex in x,

$$g_t(x) = \begin{cases} t^{\delta} g(0) & (|x|<t^{\delta} R_1), \\ g(x) & (|x|>t^{\delta} R_2), \end{cases}$$

and, since g has bounded derivatives,

$$\partial_x^k g_t(x) = O(t^{\delta(1-|k|)}), \quad \partial_t^k g_t(x) = O(t^{\delta-k}), \tag{7.18}$$

as $t\to\infty$, uniformly in x. Now we compute

$$\gamma_t \equiv D_t g_t = \tfrac{1}{2}(\nabla g_t \cdot p + p\cdot \nabla g_t) + \partial_t g_t; D_t(\gamma_t - 2\partial_t g_t) = p g_t'' p - \tfrac{1}{4}\Delta^2 g_t - \nabla g_t \cdot \nabla V - \partial_t^2 g_t. \tag{7.19}$$

In the first term of (7.19) g_t'' denotes the Hessian of $g_t(x)$, i.e., $p g_t'' p \equiv p_k g_{t,kl} p_l$ (in Cartesian coordinates), which is positive due to the convexity of $g_t(x)$. The second and fourth terms are of orders $t^{-3\delta}$ and $t^{\delta-2}$, respectively, uniformly in x. The special geometric properties of $g_t(x)$ are essential to estimate the remaining term

$$i[\gamma_t, V] = \nabla g_t \cdot \nabla I_a. \tag{7.20}$$

Here ∇g_t is bounded and has support in $|x|>t^{\delta} R_1$. For any x in this support there exists $a\in L$ such that $\nabla g_t(x) \in a$ and $|x|_a > \lambda t^{\delta}$ for some $\lambda>0$. Decomposing $V(x) = V^a(x^a) + I_a(x)$ it follows that for t sufficiently large

$$\nabla g_t(x) \cdot \nabla V(x) = \nabla g_t \cdot \nabla I_a(x) \leqslant \text{const}\, t^{-\delta(\mu+1)}, \tag{7.21}$$

if (7.1) holds for $|k|=1$ (as we assumed in the long-range case). Then the constant in (7.21) is independent of x. As a result

$$D_t(\gamma_t - 2\partial_t g_t) = p g_t'' p + O(t^{-\rho}) \tag{7.22}$$

as $t\to\infty$, with $\rho = \min(3\delta, \delta(\mu+1), \delta-2)$. As long as $\mu>0, \delta$ can be chosen in $0<\delta<1$ such that $\rho>1$. In the short-range case the occurrence of ∇I_a can be avoided by treating the commutator $\gamma_t V - V\gamma_t$ directly as a form on $D(|p|)$ which (for the same geometric reason) is seen to be of order $t^{-\delta\mu}$ relative to the form p^2 if only $|I_a(x)| = O(|x|_a)^{-\mu}$. For $\mu>1$ and a proper choice of δ this leads again to (7.22) with $\rho = \min(3\delta, \delta\mu, \delta-2) > 1$.

Theorem 7.5: *Let c be a constant such that $H+c\geqslant 1$. If (7.22) holds in form sense on $D(|p|)$ with $\rho>1$, then*

$$\int_1^{\infty} dt\, \langle p g_t'' p\rangle_t \leqslant \text{const} \langle H+c\rangle_{\psi} \quad \forall \psi \in D(|p|). \tag{7.23}$$

Proof: Integrating (7.22) over $t_0 \leqslant t \leqslant t_1$ with t_0 sufficiently large we obtain

$$\int_{t_0}^{t_1} dt \langle p g_t'' p\rangle_t \leqslant \text{const} \langle H+c\rangle_{\psi}$$

uniformly in t_1. Since the integrand is $\geqslant 0$, the limit $t_1\to\infty$ exists. □

C. Asymptotic observables

Corresponding to (7.14) we decompose

$$g_t=\sum_a g_{a,t}; \quad g_{a,t}(x)=t^{\delta}g_a(t^{-\delta}x);$$
$$\gamma_t=\sum_a \gamma_{a,t}; \quad \gamma_{a,t}=D_t g_{a,t}. \tag{7.24}$$

We also introduce the Heisenberg observables

$$g(t)=e^{iHt}g_t e^{-iHt}; \quad \gamma(t)=e^{iHt}\gamma_t e^{-iHt}=\partial_t g(t), \tag{7.25}$$

and similarly for $g_a(t)$, $\gamma_a(t)$. The operator $\gamma(t)$ is defined on $D(|p|)$, both the operators $\gamma(t)$ and $g(t)$ are defined on the domain $D(|x|)\cap D(|p|)$, which is invariant under $\exp(-iHt)$.

Theorem 7.6: *Under the hypothesis of Theorem 7.5 the strong limits*

$$\gamma^{+}=\mathrm{s}-\lim_{t\to\infty}\gamma(t), \quad \gamma_a^{+}=\mathrm{s}-\lim_{t\to\infty}\gamma_a(t), \tag{7.26}$$

exist on $D(|p|)$ and have the following properties:

$$[\gamma^{+},H]=0, \tag{7.27}$$

$$\gamma^{+}=\mathrm{s}-\lim_{t\to\infty}\frac{1}{t}g(t)\geqslant 0 \tag{7.28}$$

on $D(|x|)\cap D(|p|)$, and similarly for γ_a^{+}. In particular,

$$\gamma_{\{0\}}^{+}=0; \quad i.e., \quad \gamma^{+}=\sum_{a>\{0\}}\gamma_a^{+}. \tag{7.29}$$

Moreover, γ^{+} and γ_a^{+} are independent of δ within the ranges allowed by the hypothesis of Theorem 7.5, since

$$\gamma^{+}=\mathrm{s}-\lim_{t\to\infty} e^{iHt}\frac{g(x)}{t}e^{-iHt} \quad \text{on} \quad D(|x|)\cap D(|p|), \tag{7.30}$$

where $g(x)$ is the unscaled Graf–Yafaev function (and similarly for γ_a^{+}).

Proof: (Step 1) *Existence of γ^{+}*. It suffices to prove strong convergence of γ_t on the range of $(H+c)^{-2}$. First we show that

$$\mathrm{s}-\lim_{t\to\infty} e^{iHt}\gamma_t e^{-iHt}(H+c)^{-2}=\mathrm{s}-\lim_{t\to\infty}(H+c)^{-1}e^{iHt}\gamma_t e^{-iHt}(H+c)^{-1} \tag{7.31}$$

if one of these limits exists. Since $\|\partial_t g_t\|=O(t^{\delta-1})$ we can replace γ_t by $\gamma_t-\partial_t g_t$. Then (7.31) follows since

$$i[H,\gamma_t-\partial_t g_t]=pg_t''p-\tfrac{1}{4}\Delta^2 g_t-i[\gamma_t,V], \tag{7.32}$$

so that by our previous estimates

$$\|[\gamma_t-\partial_t g_t,(H+c)^{-1}]\|\to 0.$$

To establish the second limit in (7.31) it suffices to prove convergence of

$$\varphi_t=(c+H)^{-1}e^{iHt}\tilde{\gamma}_t e^{-iHt}(c+H)^{-1}\psi$$

for all $\psi\in\mathcal{H}$, where we have set $\tilde{\gamma}_t\equiv\gamma_t-2\partial_t g_t$. Then

$$\partial_t\varphi_t=(H+c)^{-1}e^{iHt}(D_t\tilde{\gamma}_t)e^{-iHt}(H+c)^{-1}\psi, \tag{7.33}$$

and we show that this is norm-integrable. By (7.19) and by our previous estimates $D_t\tilde{\gamma}_t=pg_t''p$, modulo terms which give integrable contributions. Therefore it remains to prove that

$$u_t:=(H+c)^{-1}e^{iHt}pg_t''pe^{-iHt}(H+c)^{-1}\psi$$

is norm-integrable over some interval $t_0<t<\infty$. Factorizing the positive operator $pg_t''p$ into $pg_t''p=B_t^2;\ B_t=B_t^*$, we use the Schwarz inequality twice to estimate

$$\begin{aligned}\left\|\int_{t_1}^{t_2}dt\,u_t\right\|^2&=\sup_{\|v\|=1}\left|\int_{t_1}^{t_2}dt\,(v,u_t)\right|^2\\&\leqslant\sup_{\|v\|=1}\left(\int_{t_1}^{t_2}dt\,\|B_te^{-iHt}(H+c)^{-1}v\|\|B_te^{-iHt}(H+c)^{-1}\psi\|\right)^2\\&\leqslant\sup_{\|v\|=1}\int_{t_1}^{t_2}dt\,\|B_te^{-iHt}(H+c)^{-1}v\|^2\times\int_{t_1}^{t_2}dt\,\|B_te^{-iHt}(H+c)^{-1}\psi\|^2.\end{aligned} \tag{7.34}$$

By Theorem 7.5 the first factor is bounded uniformly in t_1, t_2, and the second factor vanishes as $t_{1,2}\rightarrow\infty$.

(Step 2) *Existence of* γ_a^+. This is proved in the same way with two notable differences. Instead of $i[\gamma_t,V]$ we encounter the commutator

$$i[\gamma_{a,t},V]=\nabla g_{a,t}\cdot\nabla V.$$

This commutator is estimated like $i[\gamma_t,V]$. Second, since g_a is not convex, $pg_{a,t}''p$ is not positive. Therefore we use Lemma 7.4 (*iv*) to split $pg_{a,t}''p$ into positive and negative parts:

$$pg_{a,t}''p=A_t^+-A_t^-\quad\text{with}\quad 0\leqslant A_t^\pm\leqslant p\tilde{g}_t''p.$$

Treating the contributions from $A_t^\pm$ separately, we then factorize $A_t^\pm=(B_t^\pm)^2$ and use the propagation estimate (7.23) for $\tilde{g}_t$.

(Step 3) *Properties of* γ^+, γ_a^+. Since γ^+ exists, it follows from (7.31) that

$$\gamma^+(H+c)^{-2}=(H+c)^{-1}\gamma^+(H+c)^{-1},$$

i.e., $[\gamma^+,H]=0$ (and similarly for γ_a^+). Using that $\gamma(t)=\partial_t g(t)$ we have on $D(|x|)\cap D(|p|)$:

$$\gamma^+=\mathrm{s}-\lim_{t\to\infty}\frac{1}{t}\int_1^t ds\,\partial_s g(s)=\mathrm{s}-\lim_{t\to\infty}\frac{1}{t}g(t)\geqslant 0$$

and similarly for γ_a^+. In particular, since $\|g_{\{0\}}(t)\|\leqslant\mathrm{const}\,t^\delta$,

$$\gamma_{\{0\}}^+=\mathrm{s}-\lim_{t\to\infty}\frac{1}{t}g_{\{0\}}(t)=0.$$

Equation (7.30) now follows from (7.28) and from the fact that $t^{-1}\|g_t-g\|\leqslant\mathrm{const}\,t^{\delta-1}$ since $g_t(x)=g(x)$ for $|x|\geqslant\mathrm{const}\,t^\delta$. □

Next we discuss the connection between γ^+ and Mourre's inequality.

Lemma 7.7: Let $\mathcal{H}_\Delta$ be the spectral subspace of H for a Mourre interval Δ (6.17). Then γ^+ reduces to a strictly positive operator $\mathcal{H}_\Delta \to \mathcal{H}_\Delta$. In particular, $\mathcal{H}_\Delta \subset \mathrm{Ran}(\gamma^+)$.

Proof: Since γ^+ is H-bounded and commutes with H it reduces to a bounded operator $\mathcal{H}_\Delta \to \mathcal{H}_\Delta$. Let $\psi \in \mathcal{H}_\Delta \cap D(|x|)$ and $\psi_t = e^{-iHt}\psi$. Then, by (7.27) and (6.18)

$$(\psi,(\gamma^+)^2\psi) = \lim_{t\to\infty} t^{-2}(\psi, g_t(x)^2\psi) \geqslant \lim_{t\to\infty}\inf t^{-2}(\psi_t, x^2\psi_t) \geqslant \theta > 0$$

since $g_t(x) \geqslant |x|$. □

D. The short-range case

Theorem 7.8: *If $I_a(x) = O(|x|_a^{-\mu}), \mu > 1$, then the Deift–Simon wave operators*

$$\omega_a^+ = \mathrm{s-}\lim_{t\to\infty} e^{iH_a t}\gamma_{a,t}e^{-iHt} \tag{7.35}$$

exist on $D(|p|)$ for δ satisfying $\min(\delta\mu, 3\delta, 2-\delta) > 1$.

The name *Deift–Simon wave operators* comes from Ref. 18 where limits of this general type were introduced in scattering theory.

Proof: The proof is almost the same as the proof of the existence of γ_a^+. The modifications are as follows. Instead of (7.31) we first show that

$$\mathrm{s-}\lim_{t\to\infty} e^{iH_a t}\gamma_{a,t}e^{-iHt}(H+c)^{-2} = \mathrm{s-}\lim_{t\to\infty}(H_a+c)^{-1}e^{iH_a t}\gamma_{a,t}e^{-iHt}(H+c)^{-1}$$

if one of these limits exists. This follows from

$$\begin{aligned}(\gamma_{a,t} - \partial_t g_{a,t})(H+c)^{-1} - (H_a+c)^{-1}(\gamma_{a,t} - \partial_t g_{a,t})\,(H_a+c)^{-1}\\ = ([H, \gamma_{a,t} - \partial_t g_{a,t}] - I_a(\gamma_{a,t} - \partial_t g_{a,t}))\,(H+c)^{-1}.\end{aligned} \tag{7.36}$$

The extra term involving I_a gives no contribution in the limit $t\to\infty$ since by Lemma 7.4 (ii) $|I_a(x)| \leqslant \mathrm{const}\, t^{-\delta\mu}$ on $\mathrm{supp}(g_{a,t})$. Therefore, it suffices to prove convergence of

$$\varphi_t = (H_a+c)^{-1}e^{iH_a t}\tilde{\gamma}_{a,t}e^{-iHt}(H+c)^{-1}\psi,$$

where $\tilde{\gamma}_{a,t} = \gamma_{a,t} - 2\partial_t g_{a,t}$. Instead of (7.33) we then obtain

$$\partial_t\varphi_t = (H_a+c)^{-1}e^{iH_a t}(D_t\tilde{\gamma}_{a,t} - iI_a\tilde{\gamma}_{a,t})e^{-iHt}(H+c)^{-1}\psi.$$

Here the term involving I_a gives an integrable contribution of order $t^{-\delta\mu}$. The rest of the proof goes through because the propagation estimate (7.23) also holds for the dynamics generated by H_a. □

Proof of Theorem 7.1: For $\psi \in \mathcal{H}_B$ the asymptotic condition (7.2) is trivially satisfied. Since the subspaces $\mathcal{H}_\Delta$ (Δ a Mourre interval) span $\mathcal{H}_C$ it suffices to show that every $\psi \in \mathcal{H}_\Delta$ is an outgoing scattering state. Then, by Lemma 7.7 and Theorem 7.6,

$$\psi = \sum_{a>\{0\}} \gamma_a^+\varphi \approx \sum_{a>\{0\}} e^{iHt}\gamma_{a,t}e^{-iHt}\varphi,$$

where the relation $\approx$ means that the difference of the two related expressions vanishes in norm as $t\to+\infty$. By Theorem 7.8

$$\psi_t = e^{-iHt}\psi \approx \sum_{a>\{0\}} e^{-iH_a t} e^{iH_a t} \gamma_{a,t} e^{-iHt}\varphi$$

$$\approx \sum_{a>\{0\}} e^{-iH_a t}\varphi_a; \quad \varphi_a = \omega_a^+ \varphi. \tag{7.37}$$

This last relation is called *asymptotic clustering:* the difference from (7.2) is that the φ_a need not be in $\mathcal{H}_a$. We now invoke the induction hypothesis that asymptotic completeness holds for all H^a with $a>\{0\}$, which is trivially satisfied for $a=X$. This is equivalent to saying that for any $\varphi_a \in \mathcal{H}$

$$e^{-iH_a t}\varphi_a \approx \sum_{b \geq a} e^{-iH_b t}\varphi_{ab}; \quad \varphi_{ab} \in L^2(b) \otimes \mathcal{H}_B(H^b).$$

Inserting this into (7.37) gives

$$\psi_t \approx \sum_b e^{-iH_b t} \sum_{a \leq b} \varphi_{ab},$$

which proves $\psi \in \mathcal{H}^+$. □

E. The long-range case

A strategy to deal with the long range case was developed in Refs. 93 and 94 and implemented in Refs. 19 and 95. Here we describe it in the form used in Ref. 52 to prove Theorem 7.2, and we refer to that proof for a central part which is too technical to be discussed in a short review. In the long-range case the occurrence of weakly time-dependent Hamiltonians, e.g., in (7.9) suggests an inductive scheme for Hamiltonians of the form

$$H_t = H + W_t(x) \quad \text{on} \quad L^2(X), \tag{7.38}$$

where H is the original N-body Hamiltonian and $W_t(x)$ is an external, time-dependent potential which, in the reduction process described below, will be generated by the long-range tails of the intercluster potentials $I_a(x)$. Therefore the conditions on $I_a(x)$ and $W_t(x)$ are linked in the following way:

$$|\partial_x^k I_a(x)| \leq \text{const}|x|_a^{-\mu-|k|} \quad (|x|_a \to \infty); \tag{7.39}$$

$$|\partial_{x,t}^k W_t(x)| \leq \text{const}(1+t+|x|)^{-\mu-|k|}. \tag{7.40}$$

In contrast to (7.39), the bounds (7.40) are global bounds holding for all $x \in X$ and all $t>0$, and $|k|$ also counts the derivatives with respect to t. The simple reduction $H \to H_a$ used in the short-range case (and inverted in the induction proof of Theorem 7.1) is now broken into several intermediate steps involving the following time evolutions (for the interval from zero to $t>0$) and their generators:

$$\begin{aligned} U_t &: H_t = H + W_t(x); \\ \tilde{U}_{a,t} &: \tilde{H}_{a,t} = H_a + W_{a,t}(x); \\ U_{a,t} &: H_{a,t} = H_a + W_{a,t}(p_a t + x^a); \\ U_{a,t}^\infty &: H_{a,t}^\infty = H_a + W_{a,t}(p_a t). \end{aligned} \tag{7.41}$$

Here $W_{a,t}(x)$ is defined by

$$W_{a,t}(x)=(I_a(x)+W_t(x))\chi_{a,t}(x), \tag{7.42}$$

where $\chi_{a,t}(x)$ is a smoothed characteristic function of the set

$$\{x||x|>(1+t)^{\delta}R_1;\quad |x|_a\geqslant|x|^{1-\varepsilon}\} \tag{7.43}$$

with $\varepsilon>0$ arbitrary small, and R_1 is the (arbitrary large) constant appearing in the Graf–Yafaev construction (Lemmas 7.3 and 7.4). In the region (7.43) the clusters are separated by a distance growing like $t^{\delta(1-\varepsilon)}$ so that $W_{a,t}(x)$ inherits the long-range part of $I_a(x)$ and is nonzero even if we start with $W_t(x)\equiv 0$: this is the reason for the generalized induction scheme. In the evolution $U_{a,t}$ the centers-of-mass of the clusters are positioned at $x_a=p_a t$, corresponding to the classical picture (7.7). The generating Hamiltonian $H_{a,t}$ commutes with p_a and can therefore be analyzed on fibers of constant $p_a=\xi\in a$, where it reduces to the operator

$$H_{a,t}(\xi)=H^a+\tfrac{1}{2}\xi_a^2+W_{a,t}(\xi t+x^a)\quad\text{on}\quad L^2(a^{\perp}). \tag{7.44}$$

Moreover, it suffices to perform this analysis for the fibers $\xi\in a^*$ (3.9) for which $|\xi t|_a\to\infty$ as $t\to\infty$. *Then the potential $W_{a,t}(\xi t+x^a)$ on $a^{\perp}$ essentially inherits the properties (7.40).* [The irrelevant difference is that the exponent $-(\mu+|k|)$ is changed by a factor $(1-\varepsilon)$ coming from (7.43).] This allows an inductive proof of the following theorem which reduces to Theorem 7.2 by setting $W_t(x)\equiv 0$ (after performing the induction).

Theorem 7.9: *If (7.39) and (7.40) hold for $0\leqslant|k|\leqslant 2$ and some $\mu>\sqrt{3}-1$, any $\psi\in\mathcal{H}$ is an outgoing scattering state in the sense that*

$$U_t\psi \underset{\|\ \|}{\rightarrow}\sum_a e^{-iH_a t-i\alpha_{a,t}(p_a)}\varphi_a\quad (t\to+\infty), \tag{7.45}$$

where $\varphi_a\in\mathcal{H}_a=L^2(a)\otimes\mathcal{H}_B(H^a)$ and

$$\alpha_{a,t}(p_a)=\int_{t_0(p_a)}^{t}ds\,(I_a(p_a s)+W_s(p_a s))\ (a>\{0\});\quad \alpha_{\{0\},t}=\int_0^t ds\,W_s(0). \tag{7.46}$$

In the remaining part of this section we describe the main steps of the proof following Ref. 52.

1. Construction of U_t

Since W_t is bounded the operators H_t are self-adjoint with constant domain $D(H)=D(p^2)$. Therefore, H_t generates a unitary propagator $U_t:\psi\to\psi_t$ for the interval $0,\ldots,t$ where $\langle p^2\rangle_t\leqslant\text{const}\langle H+c\rangle_0$. Since $D_t x=p$ it still follows that the domain $D(|x|)\cap D(p^2)$ is U_t-invariant. A useful concept is the asymptotic energy

$$H^+=\lim_{t\to\infty}U_t^{-1}H_tU_t=\lim_{t\to\infty}U_t^{-1}H\,U_t, \tag{7.47}$$

which exists since $\|\partial_t W_t\|=O(t^{-\mu-1})$ is integrable in t. H^+ is self-adjoint on $D(H)$ and has the same spectrum as H.

2. The basic propagation estimate

In (7.19) the operator γ_t remains unchanged but $i[\gamma_t,V]$ receives an additional term $\nabla g_t\cdot\nabla W_t\sim t^{-\delta(1+\mu)}$. Therefore the propagation estimate (7.23) still holds for δ in the range

$$\tfrac{1}{3}<\delta<1;\quad \delta(\mu+1)>1, \tag{7.48}$$

provided that (7.39) and (7.40) hold for some $\mu>0$ and $|k|\leqslant 1$. Under these conditions the existence of the asymptotic observable

$$\gamma^+ = \mathrm{s}-\lim_{t\to\infty} \gamma(t); \quad \gamma(t) = U_t^{-1}\gamma_t U_t$$

(and similarly for γ_a^+) follows as before. In the first step of that proof $(H+c)^{-2}$ is replaced by $(H^+ + c)^{-1}$, which then leads to

$$[\gamma^+, H^+] = [\gamma_a^+, H^+] = 0. \tag{7.49}$$

All the other properties of γ^+, γ_a^+ listed in Theorem 7.8 remain unchanged. In particular γ^+ and γ_a^+ are independent of the choice of the scaling parameter δ in the range (7.48).

3. Deift–Simon wave operators

This is the only place where the condition $\mu > 1$ was used in the short-range case. Following Ref. 20 we factorize

$$\omega_a^+ := \mathrm{s}-\lim_{t\to\infty} U_{a,t}^{-1}\gamma_{a,t}U_t = w_a^+ \tilde{\omega}_a^+;$$

$$w_a^+ = \mathrm{s}-\lim_{t\to\infty} U_{a,t}^{-1}\tilde{U}_{a,t}; \tag{7.50}$$

$$\tilde{\omega}_a^+ = \mathrm{s}-\lim_{t\to\infty} \tilde{U}_{a,t}^{-1}\gamma_{a,t}U_t.$$

The limit $\tilde{\omega}_a^+$ is established like ω_a^+ in the short-range case, but in place of the term $I_a(\gamma_{a,t} - \partial_t g_{a,t})$ in (7.36) we now obtain

$$(H_t - \tilde{H}_{a,t})(\gamma_{a,t} - \partial_t g_t) = (I_a + W_t)(1 - \chi_{a,t})(\gamma_{a,t} - \partial_t g_t).$$

This expression vanishes exactly for sufficiently large t, since then $\chi_{a,t} = 1$ on $\mathrm{supp}(g_{a,t})$. As a result, $\tilde{\omega}_a^+$ exists for δ in the range (7.48), provided that the limit w_a^+ exists for δ in the range

$$\tfrac{1}{3} < \delta < 1, \quad \delta(\mu+1) > \tfrac{3}{2}, \quad \delta(\mu+2) > 2, \tag{7.51}$$

and provided that (7.39) and (7.40) hold for some $\mu > \frac{1}{2}$ and $|k| \leqslant 2$. The proof[20,52] uses the identity

$$\partial_t U_{a,t}^{-1}\tilde{U}_{a,t}\psi = -iU_{a,t}^{-1}[W_{a,t}(x) - W_{a,t}(p_a t + x^a)]\tilde{U}_{a,t}\psi,$$

where the middle factor can be expressed as

$$[\cdots] = \int_0^1 ds\, \nabla_a W_{a,t}(sx_a + (1-s)p_a t + x^a)\cdot(x_a - p_a t) + \frac{it}{2}\int_0^1 ds\, \Delta_a W_{a,t}(sx_a + (1-s)p_a t + x^a).$$

This formula comes from evaluating the operator identity

$$f(x) - f(pt) = \int_0^t ds \frac{d}{ds} f(pt + s(x - pt)),$$

which is linear in f and holds for $f = \exp(ik\cdot x)$ by the Campbell–Hausdorff formula. The result is as follows.

Theorem 7.10: *For any $a > \{0\}$ the Deift–Simon wave operator*

$$\omega_a^+ = \mathrm{s}-\lim_{t\to\infty} U_{a,t}^{-1}\gamma_{a,t}U_t \tag{7.52}$$

exists on $D(|p|)$ *for* δ *in the range (7.51), provided that (7.39) and (7.40) hold for some* $\mu>\frac{1}{2}$ *and* $|k|\leqslant 2$. *Asymptotic clustering follows as in the short-range case: For* $\psi\in \mathrm{Ran}(\gamma^+)$

$$U_t\psi \underset{\|\,\|}{\rightarrow} \sum_{a>\{0\}} U_{a,t}\varphi_a\,;\varphi_a=\omega_a^+\psi \quad (t\rightarrow +\infty). \tag{7.53}$$

We now come to the induction proof of Theorem 7.9. The induction hypothesis is that asymptotic completeness in the sense given by Theorem 7.9 holds for the time evolution $U_{a,t}(\xi)$ generated by the Hamiltonian (7.44) for any $\xi\in a^*$. After integrating over the fibers ξ this amounts to the hypothesis that for any $a>\{0\}$ and any $\varphi_a\in\mathcal{H}$

$$U_{a,t}\varphi_a \underset{\|\,\|}{\rightarrow} \sum_{b\geqslant a} e^{-iH_bt-i\alpha_{b,t}(p_b)}\varphi_{ab}, \quad \varphi_{ab}\in\mathcal{H}_b,$$

as $t\rightarrow+\infty$. Inserting this into (7.53) it follows that any $\psi\in \mathrm{Ran}(\gamma^+)$ is an outgoing scattering state. However, with all this preparation we have only cleared the path to the hard core of the long-range problem: *to prove that (7.45) also holds if* $\gamma^+\psi=0$.

Theorem 7.11: *Let* $\gamma^+\psi=0$ *and suppose that (7.39) and (7.40) hold for some* $\mu>\sqrt{3}-1$ *and* $|k|\leqslant 1$. *Then for* $t\rightarrow+\infty$

$$U_t\psi \underset{\|\,\|}{\rightarrow} e^{-iHt-i\int_0^t ds W_s(0)}\varphi; \quad \varphi\in\mathcal{H}_B(H). \tag{7.54}$$

For a proof we refer to Ref. 52 or to the original proof in Ref. 19 (see also Ref. 20, where the same problem is dealt with in a different form). Basically the problem arises since strict energy conservation is lost for the dynamics generated by H_t: thresholds and embedded eigenvalues of H cannot be avoided by restricting the analysis to suitable energy shells Δ as in the short-range case. Essentially, a state ψ with $\gamma^+\psi=0$ propagates under U_t in a region $|x|\leqslant \mathrm{const}\, t^\delta$ with $0<\delta<1$, and (7.54) shows that this is only possible if ψ is a bound state of H. The still rather involved estimates which are used to establish this fact also allow us to prove the existence of the long-range wave operators in full generality:

Theorem 7.12:[19,122,52] *Suppose that (7.39) and (7.40) hold for some* $\mu>\sqrt{3}-1$ *and* $|k|\leqslant 2$. *Then the wave operators*

$$\Omega_a^+ = \mathrm{s}-\lim_{t\rightarrow\infty} U_t^{-1}U_{a,t}^{\infty}$$

exist on $\mathcal{H}_a$ *for all* $a\in L$ *and have mutually orthogonal ranges.*

Notes: For a comprehensive treatment of scattering theory of classical and quantum N-particle systems, see Ref. 21, where many additional references can be found. N-body scattering theory for potentials with strong (repulsive) singularities is treated in Refs. 56, 11, and 39.

Presently a considerable effort is under way to develop an extension of microlocal analysis covering N-body scattering theory,[71,72,41,105–107] which in particular leads to a better understanding of the singularities of the N-body scattering matrix.

VIII. HIGHER ORDER MOURRE THEORY

The results of this section follow from Mourre's inequality under the additional assumption that the multiple commutators

$$ad_A^{(k)}(H), \quad k=1,\ldots,n, \tag{8.1}$$

are H-bounded for some number $n>1$ depending on the context. The analysis will be quite general, i.e., not restricted to N-body Hamiltonians. However, we will be somewhat cavalier in handling commutators between unbounded operators like (8.1). For a rigorous treatment of this point we refer to Ref. 62 and especially to Ref. 6.

The results on *resolvent smoothness* state that for certain operators $B\in L(\mathcal{H})$ and for the resolvent $R(z)=(z-H)^{-1}$ the holomorphic functions

$$z\to F(z)=B^*R(z)B\in L(\mathcal{H}) \quad \text{on} \quad C^{\pm}=\{z|\pm \mathrm{Im}(z)>0\} \tag{8.2}$$

are bounded and have boundary values

$$F(x\pm i0)=\lim_{\varepsilon\searrow 0}F(x\pm i\varepsilon)\in L(\mathcal{H})$$

in norm sense for x in any Mourre interval Δ (6.17) with a certain degree of smoothness in x. Boundary values of this type are relevant for many dynamical aspects involving the continuous spectrum of H, e.g., for the perturbation of embedded eigenvalues (Fermi golden rule) and for the transition to time-independent scattering theory (which is not yet fully developed for N-body systems). The notion of *local decay* is related to resolvent smoothness in the following way. If $I\subset R$ is compact and covered by (finitely many) Mourre intervals, then it follows from resolvent smoothness that

$$\|B\,E_I(H)R(z)E_I(H)\,B^*\|\leq \mathrm{const} \tag{8.3}$$

uniformly in $z\in C^{\pm}$. Therefore, the operator $B\,E_I(H)$ is H-smooth, which is equivalent to

$$\int_{-\infty}^{+\infty}dt\,\|B\,e^{-iHt}\psi\|^2\leq \mathrm{const}\|\psi\|^2 \tag{8.4}$$

for all $\psi=E_I(H)\psi$ (see Ref. 81, Vol. IV, Theorem XIII.25 and Corollary). Equation (8.4) is generally referred to as *local decay* since it was first derived for Schrödinger Hamiltonians with $B=(1+x^2)^{-\alpha}$, $\alpha>\frac{1}{2}$.[75,79] This result requires (8.1) only for $n=2$ and will be discussed first. For any self-adjoint operator A we use the notation

$$\langle A\rangle\equiv(1+A^2)^{1/2}. \tag{8.5}$$

Theorem 8.1:[75,79] *Suppose that $ad_A^{(k)}(H)$ is H-bounded for $k=1,2$. Let $I\subset R$ be a compact interval covered by Mourre intervals, and*

$$I^{\pm}=\{z\in C^{\pm}|\mathrm{Re}\,(z)\in I\}.$$

Then for any $\alpha>\frac{1}{2}$ the function

$$F(z)=\langle A\rangle^{-\alpha}R(z)\langle A\rangle^{-\alpha}\in L(\mathcal{H}) \tag{8.6}$$

on $I^{\pm}$ has the properties

$$\|F(z)\|\leq \mathrm{const}; \tag{8.7}$$

$$\|F(z)-F(z')\|\leq \mathrm{const}|z-z'|^{\beta},\beta=\frac{2\alpha-1}{2\alpha+1}. \tag{8.8}$$

In particular the boundary values $F(x\pm i0)$ exist in norm sense for $x\in I$ and have bounds corresponding to (8.7) and (8.8). Moreover, (8.7) implies the local decay estimate

$$\int_{-\infty}^{+\infty} dt\, \|\langle A\rangle^{-\alpha} e^{-iHt}\psi\|^2 \leq \text{const}\|\psi\|^2 \tag{8.9}$$

for $\alpha > \frac{1}{2}$ and all $\psi = E_I(H)\psi$.

Corollary 8.2: Let $f \in C_0^\infty(R)$ be such that supp(f) *is covered by Mourre intervals. Then for any $\alpha > \frac{1}{2}$ the function*

$$F(z) = \langle A\rangle^{-\alpha} f(H) R(z) f(H) \langle A\rangle^{-\alpha},$$

now defined for all $z \in C^\pm$, also satisfies the estimates (8.7) and (8.8), with corresponding properties of the boundary values $F(x \pm i0)$ on R.

Proof: It suffices to consider α in $\frac{1}{2} < \alpha \leq 1$. Let I be a compact interval containing supp (f) in its interior, but still covered by Mourre intervals. For $\text{Re}(z) \notin I$ the bounds are trivial. For $\text{Re}(z) \in I$ they follow by factorizing

$$F(z) = \langle A\rangle^{-\alpha} f(H) \langle A\rangle^{\alpha} \langle A\rangle^{-\alpha} R(z) \langle A\rangle^{-\alpha} \langle A\rangle^{\alpha} f(H) \langle A\rangle^{-\alpha},$$

since

$$\langle A\rangle^{-\alpha} f(H) \langle A\rangle^{\alpha} \in L(\mathcal{H}) \tag{8.10}$$

for $0 \leq \alpha \leq 1$. It suffices to check this for $\alpha = 1$; the general case then follows by complex interpolation (Ref. 81, Vol. II, Appendix to IX. 4). For $\alpha = 1$ one can use, e.g., the Helffer–Sjöstrand formula (9.1) for $f(H)$ and the fact that $[H,A]$ is H-bounded. □

Corollary 8.3: Let H be a Schrödinger operator on $\mathcal{H} = L^2(X)$ and A be the dilation generator. Then $\langle A\rangle^{-\alpha}$ can be replaced by $\langle x\rangle^{-\alpha}$ in Theorem 8.1

Proof: Again it suffices to take α in $1/2 < \alpha \leq 1$. Let $g \in C_0^\infty(R)$, $g = 1$ on I and supp(g) still be covered by Mourre intervals. By factorizing $\langle x\rangle^{-\alpha} g(H) = \langle x\rangle^{-\alpha} g(H) \langle A\rangle^{\alpha} \cdot \langle A\rangle^{-\alpha}$ and assuming that

$$\langle A\rangle^{\alpha} g(H) \langle x\rangle^{-\alpha} \in L(\mathcal{H}), \tag{8.11}$$

it follows that the function $F(z) = \langle x\rangle^{-\alpha} g(H) R(z) g(H)\ \langle x\rangle^{-\alpha}$ satisfies (8.7) and (8.8). For $\text{Re}(z) \in I$ the factors $g(H)$ can be removed. To prove (8.11) it again suffices to take $\alpha = 1$. □

To prepare the proof of Theorem 8.1 we estimate the resolvent

$$R_s(z) = (z - H_s)^{-1}; \quad H_s = H - isB; \quad B = i[H,A]. \tag{8.12}$$

This part uses only the Mourre inequality and the condition that B is bounded relative to H.

Lemma 8.4: Let I be a compact subset of a Mourre interval Δ. If B is H-bounded, there exist constants $s_0, c_1 > 0$ such that

$$\|R_s(z)\| \leq c_1 s^{-1} \tag{8.13}$$

for $0 < s \leq s_0$, uniformly in $z \in I^+$.

Proof: Let $E_\Delta = E_\Delta(H)$ and $\overline{E}_\Delta = 1 - E_\Delta$. For $\text{Im}(z) \geq 0$ the Mourre inequality implies

$$\text{Im}(E_\Delta(z - H_s)E_\Delta) \geq s\theta E_\Delta.$$

Therefore,

$$\begin{aligned}\|E_\Delta(z - H_s)u\| &\geq \|E_\Delta(z - H_s)E_\Delta u\| - s\|E_\Delta B \overline{E}_\Delta u\| \\ &\geq s\theta\|E_\Delta u\| - sM_1\|E_\Delta u\|\end{aligned}$$

since $E_\Delta B$ is bounded. If $\mathrm{Re}(z)\in I$, then $\|(z-H)\bar{E}_\Delta u\|\geq \varepsilon\|\bar{E}_\Delta u\|$ for some $\varepsilon>0$. Setting $\varepsilon=\sqrt{s}$ with s sufficiently small we find

$$\begin{aligned}\|\bar{E}_\Delta(z-H_s)u\| &= \|(z-H)\bar{E}_\Delta(1+isR(z)B)u\|\\ &\geq s^{1/2}\|\bar{E}_\Delta(1+isR(z)B)u\|\\ &\geq s^{1/2}\|\bar{E}_\Delta u\|-s^{3/2}M_2\|u\|\end{aligned}$$

since $\bar{E}_\Delta R(z)H$ and therefore $\bar{E}_\Delta R(z)B$ is bounded uniformly in $z\in I^+$. Combining the two estimates we arrive at

$$\begin{aligned}\|E_\Delta(z-H_s)u\|+\|\bar{E}_\Delta(z-H_s)u\| &\geq (s\theta-s^{3/2}M_2)\|E_\Delta u\|+(s^{1/2}-sM_1-s^{3/2}M_2)\|\bar{E}_\Delta u\|\\ &\geq sM(\|E_\Delta u\|+\|\bar{E}_\Delta u\|)\end{aligned}$$

for some $M>0$. This implies

$$\|(z-H_s)u\|\geq sc_1\|u\| \quad \text{for some} \quad c_1>0$$

and (8.13) follows since $z\in\rho(H_s)$ for s sufficiently small. □

Lemma 8.5: In the situation of Lemma 8.4, $\|R_s(z)u\|^2$ and $\|R_s^*(z)u\|^2$ are bounded by

$$c_2(s^{-1}|\mathrm{Im}\,(u,R_s(z)u)|+\|u\|^2) \tag{8.14}$$

for all $u\in\mathcal{H}$ and $0<s\leq s_0$, uniformly in $z\in I^+$.

Proof: Since $(z-H_s)-(z-H_s^*)=2i(\mathrm{Im}\,(z)+sB)$ for $\mathrm{Im}\,(z)>0$ we obtain the two estimates

$$\frac{1}{2is}(R_s^*-R_s)\geq R_s^*BR_s; \quad \frac{1}{2is}(R_s^*-R_s)\geq R_sBR_s^*. \tag{8.15}$$

In the first case $R_s^*BR_s$ is bounded from below as follows:

$$\begin{aligned}(u,R_s^*BR_su) &= (R_su,E_\Delta BE_\Delta R_su)+(R_su,E_\Delta B\bar{E}_\Delta R_su)+(\bar{E}_\Delta R_su,BR_su)\\ &\geq \theta\|E_\Delta R_su\|^2-M\|u\|(\|R_su\|+\|u\|).\end{aligned} \tag{8.16}$$

The first term comes from the Mourre estimate. In the remainder we have used that

$$\bar{E}_\Delta R_s=\bar{E}_\Delta R-is\bar{E}_\Delta RBR_s$$

is bounded for small s uniformly in $z\in I^+$. This follows from (8.13) and from the fact that $\bar{E}_\Delta RB$ is bounded. From (8.16) and (8.15) we obtain

$$\theta\|E_\Delta R_su\|^2\leq \mathrm{const}\,(s^{-1}|\mathrm{Im}\,(u,R_su)|+\|u\|\,\|R_su\|+\|u\|^2),$$

which implies

$$\|E_\Delta R_su\|^2\leq \mathrm{const}\,(s^{-1}|\mathrm{Im}\,(u,R_su)|+\|u\|^2). \tag{8.17}$$

The bound (8.14) for $\|R_su\|^2$ now follows since $\bar{E}_\Delta R_s$ is bounded for small s uniformly in $z\in I^+$. The bound (8.14) for $\|R_s^*u\|^2$ follows from the second inequality (8.15). □

Proof of Theorem 8.1:[79] We consider the case $z\in I^+$. By a covering argument we can assume that I is contained in a single Mourre interval Δ. We define the operators

$$\begin{aligned}\rho_s(A) &= \langle A\rangle^{-\alpha}\langle sA\rangle^{\alpha-1},\\ F_s(z) &= \rho_s(A)R_s(z)\rho_s(A),\end{aligned} \tag{8.18}$$

for $0<s\leq s_0$; $z\in I^+$. For $F_s(z)$ we will derive the differential inequality

$$\left\|\frac{d}{ds}F_s(z)\right\|\leq \text{const}\,(1+s^{\alpha-1})(s^{-1/2}\|F_s(z)\|^{1/2}+1). \tag{8.19}$$

This inequality gives the bound

$$\|F_s(z)\|\leq \text{const}, \tag{8.20}$$

since the function $s^{\alpha-3/2}$ is integrable at $s=0$ for $\alpha>\frac{1}{2}$. Substituting (8.20) back into (8.19) we obtain

$$\|F(z)-F_s(z)\|\leq \text{const}\, s^{\alpha-1/2}. \tag{8.21}$$

The bounds (8.20) and (8.21) prove (8.7). The differential inequality (8.19) is based on the following estimates. First,

$$\left\|\frac{d\rho_s}{ds}\right\|\leq \text{const}\, s^{\alpha-1}. \tag{8.22}$$

Second, by Lemma 8.5, both $\|\rho_s R_s(z)\|$ and $\|R_s(z)\rho_s\|$ have bounds of the form

$$\text{const}\,(s^{-1/2}\|F_s(z)\|^{1/2}+1). \tag{8.23}$$

Equation (8.19) is now obtained from

$$\frac{d}{ds}F_s(z)=\frac{d\rho_s}{ds}R_s\rho_s+\rho_s R_s\frac{d\rho_s}{ds}+\rho_s[A,R_s]\rho_s \quad -is\rho_s R_s[B,A]R_s\rho_s\,. \tag{8.24}$$

We note that in the last term (and only there) the double commutator $[[H,A],A]$ appears. It follows from (8.22) and (8.23) that all terms in (8.24) have bounds of the form (8.19). In particular, the term involving $[A,R_s]$ is estimated using

$$\|A\rho_s\|=\|\rho_s A\|\leq\|\langle A\rangle^{1-\alpha}\langle sA\rangle^{\alpha-1}\|\leq \text{const}\, s^{\alpha-1}.$$

This concludes the proof of (8.7). By the resolvent identity and (8.23),

$$\begin{aligned}\|F_s(z)-F_s(z')\|&\leq \text{const}\,|z-z'|\,\|\rho_s R_s(z)\|\,\|R_s(z')\rho_s\|\\ &\leq \text{const}\, s^{-1}|z-z'|\,.\end{aligned} \tag{8.25}$$

Combining this with (8.21) we find

$$\begin{aligned}\|F(z)-F(z')\|&\leq\|F(z)-F_s(z)\|+\|F_s(z)-F_s(z')\|+\|F_s(z')-F(z')\|\\ &\leq \text{const}\,(s^{\alpha-1/2}+|z-z'|s^{-1}).\end{aligned}$$

Equation (8.8) now follows by setting $s=|z-z'|^n, \quad n=(\alpha+\frac{1}{2})^{-1}$. □

We conclude this section with some results concerning the stability of the preceding estimates under small perturbations

$$H\to H_\kappa=H+\kappa V, \quad \kappa\in R,$$

where V is any symmetric operator such that the commutators

$$ad_A^{(k)}(V), \quad k=0,...,2, \tag{8.26}$$

are H-bounded. Here H_κ is self-adjoint for small κ and $R_\kappa(z)$ denotes the resolvent of H_κ. We begin with the stability of the Mourre estimate (6.17).

Lemma 8.6: Let Δ be a Mourre interval for H and Δ' a closed subinterval of Δ. Then there exist constants $\theta'>0$ and $c>0$ such that

$$E_{\Delta'}(H_\kappa)i[H_\kappa,A]E_{\Delta'}(H_\kappa)\geqslant\theta' E_{\Delta'}(H_\kappa) \tag{8.27}$$

for all κ with $|\kappa|<c$.

Proof: Let $f\in C_0^\infty(\Delta)$ with $f=1$ on Δ'. Equation (6.17) implies that $f(H)i[H,A]f(H)\geqslant\theta f^2(H)$. By the Helffer–Sjöstrand formula

$$f(H_\kappa)-f(H)=\kappa\int d\tilde{f}(z)R(z)VR_\kappa(z),$$

where the integral represents a bounded operator $\mathcal{H}\to D(H)$; $D(H)$ equipped with the H-norm. Therefore, and since $[V,A]$ is H-bounded,

$$f(H_\kappa)i[H_\kappa,A]f(H_\kappa)\geqslant\theta f^2(H_\kappa)-\text{const}\,\kappa$$

for small κ. Multiplying this from both sides with $E_{\Delta'}(H)$ yields (8.27) with $\theta'=\theta-\text{const}\,\kappa>0$ for small κ. □

Using this result it is straightforward to extend the estimates leading to Theorem 8.1 from H to H_κ for small κ, with constants independent of κ. We will refer to some of these estimates in the proof of the following stability result:

Theorem 8.7: *In the situation of Theorem 8.1 let $H_\kappa=H+\kappa V$, where V is symmetric and has H-bounded commutators*

$$ad_A^{(k)}(V); \quad k=0,...,2.$$

Let I be a compact interval covered by (finitely many) Mourre intervals. Then for $\alpha>\frac{1}{2}$ the function

$$(\kappa,z)\to F_\kappa(z)=\langle A\rangle^{-\alpha}R_\kappa(z)\langle A\rangle^{-\alpha}\in L(\mathcal{H}),$$

defined for small κ and $z\in I^\pm$, has the properties

$$\|F_\kappa(z)\|\leqslant\text{const}, \tag{8.28}$$

$$\|F_{\kappa'}(z')-F_\kappa(z)\|\leqslant\text{const}(|\kappa-\kappa'|+|z-z'|)^\beta, \quad \beta=\frac{2\alpha-1}{2\alpha+1}. \tag{8.29}$$

In particular the boundary values $F_\kappa(x\pm i0)$ for $x\in I$ exist and are Hölder continuous in (κ,x).

Proof: Again we may assume that I is contained in a Mourre interval Δ. We consider the case I^+ and prove Hölder continuity in κ, which is the new element not present in (8.8). Beginning with (8.12) we replace H by H_κ, defining

$$H_{\kappa s}=H_\kappa-isB_\kappa, \quad B_\kappa=i[H_\kappa,A], \quad R_{\kappa s}(z)=(z-H_{\kappa s})^{-1},$$

and noting that for small κ, s the operators $H_{\kappa s}$ are all uniformly bounded relative to each other. As a result the function

$$F_{\kappa s}(z)=\rho_s(A)R_{\kappa s}(z)\rho_s(A),$$

defined for small κ, small $s>0$ and $z\in I^+$, satisfies the estimates (8.20) and (8.21) uniformly in κ. To prove Hölder continuity of $F_{\kappa s}$ in κ we use the identity

$$R_{\kappa' s}-R_{\kappa s}=R_{\kappa s}(H_{\kappa s}-H_{\kappa' s})R_{\kappa' s},$$

$$H_{\kappa s}-H_{\kappa' s}=(\kappa-\kappa')(V+s[V,A])=(\kappa-\kappa')W_s,$$

where the operator W_s is bounded relative to H and therefore to $H_{\kappa s}$ uniformly for small κ, s. Therefore,

$$\|F_{\kappa s}(z)-F_{\kappa' s}(z)\|\leqslant \mathrm{const}|\kappa-\kappa'|\,\|\rho_s R_{\kappa s}\|\,\|W_s R_{\kappa' s}\rho_s\|$$
$$\leqslant \mathrm{const}|\kappa-\kappa'|s^{-1}$$

by the bounds (8.23) and (8.20) for $R_{\kappa s}$ and $F_{\kappa s}$. This corresponds to the estimate (8.25) used to prove Hölder continuity in z, so that Hölder continuity in κ of $F_\kappa(z)$ follows in the same way.□

A. The Fermi golden rule (FGR) and instability of embedded eigenvalues

In the framework of spectral deformation we have found the following instability criterion for an embedded eigenvalue λ of H with eigenprojection P under small perturbations $H\rightarrow H_\kappa=H+\kappa V$:

1. FGR criterion

Let $\bar{P}=1-P$ and $\bar{R}(z)=\bar{P}R(z)\bar{P}$. Then

$$\Gamma=-\operatorname{Im}(PV\bar{R}(\lambda+i0)VP) \tag{8.30}$$

exists, which implies $\Gamma=\Gamma^*\geqslant 0$. If $\Gamma>0$, then there exists an open interval $\Delta\ni\lambda$, such that the spectrum of H_κ in Δ is absolutely continuous for small $\kappa\neq 0$.

This criterion makes no reference to spectral deformation, and can in fact be established on the basis of Mourre's inequality.[3] The situation considered is the following: H and A are self-adjoint operators such that $[H,A]$ is H-bounded. $\Delta\subset R$ is an open interval for which there is a Mourre inequality

$$E_\Delta(H)i[H,A]E_\Delta(H)\geqslant\theta E_\Delta(H)+K,\quad \theta>0, \tag{8.31}$$

and K is a compact operator. $\lambda\in\Delta$ is an eigenvalue of H with eigenprojection P. It follows from (8.31) that $\dim(P)<\infty$ and that λ is the only eigenvalue of H in Δ if we choose $\Delta\ni\lambda$ sufficiently small. The result of this section is the following.

Theorem 8.8:[3] *In the situation described above the FGR criterion holds if the commutators*

$$ad_A^{(k)}(H)\quad\text{and}\quad ad_A^{(k)}(V)\quad\text{for}\quad k=0,1,2 \tag{8.32}$$

are H-bounded, and if

$$\operatorname{Ran}P\subset D(A^2). \tag{8.33}$$

Remark: This result applies to N-body Hamiltonians H, where A is the dilation generator and λ is any nonthreshold eigenvalue of H. Equation (8.33) then follows from the Froese–Herbst exponential bound (Theorem 6.6).

For the proof of Theorem 8.8 we work with the fixed reduction of $\mathcal{H}$ given by

$$1=P+\bar{P}:\mathcal{H}=M\oplus\bar{M}, \tag{8.34}$$

and we define reduced operators $\bar{M}\rightarrow\bar{M}$:

$$\overline{H}_\kappa=\overline{P}H_\kappa\overline{P},\quad \overline{R}_\kappa(z)=\overline{P}(z-\overline{H}_\kappa)^{-1}\overline{P},$$
$$\overline{V}=\overline{P}V\overline{P},\quad \overline{A}=\overline{P}A\overline{P}. \tag{8.35}$$

The first step is to establish the corresponding Mourre estimate on $\overline{M}$:

Lemma 8.9: There exists an open interval $\Delta\ni\lambda$ *and constants* $\theta>0$, $c>0$ *such that for* $|\kappa|<c$

$$E_\Delta(\overline{H}_\kappa)i[\overline{H}_\kappa,\overline{A}]E_\Delta(\overline{H}_\kappa)\geq\theta E_\Delta(\overline{H}_\kappa). \tag{8.36}$$

In particular, $\overline{H}_\kappa$ *has no eigenvalues in* Δ.

Proof: Multiplying (8.31) from both sides with $E_\Delta(\overline{H})$ and using the fact that $E_\Delta(\overline{H})\overset{s}{\rightarrow}0$ for $\Delta\rightarrow\{\lambda\}$ we see that (8.36) holds for $\kappa=0$. Next we note that the commutators

$$[\overline{H},\overline{A}]=\overline{P}[H,A]\overline{P},$$
$$[\overline{V},\overline{A}]=\overline{P}[V,A]\overline{P}-\overline{P}(VPA-APV)\overline{P}$$

are bounded relative to $\overline{H}$. Therefore (8.36) is a consequence of Lemma 8.6. □

Lemma 8.10: Suppose that for some fixed κ *in* $0<|\kappa|<c$, H_κ *has an eigenvalue* $\mu\in\Delta$ *with eigenvector* ψ. *Then*

$$\mathrm{Im}(\psi,PV\overline{R}_\kappa(\lambda+i0)VP\psi)=0. \tag{8.37}$$

Proof: In the reduction (8.34) the equation $H_\kappa\psi=\mu\psi$ is equivalent to two equations on M and $\overline{M}$:

$$PH_\kappa P\psi+PH_\kappa\overline{P}\psi=\mu P\psi;\quad \overline{P}H_\kappa P\psi+\overline{P}H_\kappa\overline{P}\psi=\mu\overline{P}\psi. \tag{8.38}$$

Since $\overline{P}H_\kappa P\psi=\kappa\overline{P}VP\psi$ the second equation can be written as

$$\overline{R}_\kappa(\mu+i\varepsilon)\kappa\overline{P}VP\psi=\overline{P}\psi-i\varepsilon\overline{R}_\kappa(\mu+i\varepsilon)\overline{P}\psi$$

for $\varepsilon>0$. The last term vanishes as $\varepsilon\rightarrow0$ since, by Lemma 8.9, μ is not an eigenvalue of $\overline{H}_\kappa$. Therefore

$$\overline{P}\psi=\kappa\overline{R}_\kappa(\mu+i0)\overline{P}VP\psi.$$

Inserting this expression for $\overline{P}\psi$ into the first equation (8.38) and taking the scalar product with ψ we find

$$(\lambda-\mu)(\psi,P\psi)+\kappa(\psi,PVP\psi)+\kappa^2(\psi,PV\overline{R}_\kappa(\mu+i0)VP\psi)=0.$$

Equation (8.37) follows by taking the imaginary part. □

Lemma 8.11: There exists an open interval $\Delta\ni\lambda$ *and a constant* $c>0$ *such that for* $|\kappa|<c$ *the boundary values*

$$F_\kappa(x)=PV\overline{R}_\kappa(x+i0)VP \tag{8.39}$$

exist for all $x\in\Delta$ *and satisfy*

$$\|F_\kappa(x)-F_{\kappa'}(x')\|\leq\mathrm{const}(|\kappa-\kappa'|+|x-x'|)^{1/3}. \tag{8.40}$$

Proof: For $\mathrm{Im}(z)>0$ we factorize

$$F_\kappa(z)=(PV\bar{P}\langle\bar{A}\rangle)(\langle\bar{A}\rangle^{-1}\bar{R}_\kappa(z)\langle\bar{A}\rangle^{-1})(\langle\bar{A}\rangle\bar{P}VP). \tag{8.41}$$

Here the first and last factors are bounded since $A\bar{P}VP\in L(\mathcal{H})$. To see this we expand

$$A\bar{P}VP=AVP-APVP^{(*)}$$

where the superscript $(*)$ indicates that the operator is bounded. Also

$$AVP=VAP+[A,V]P^{(*)},$$

and since V is H-bounded it suffices to note that

$$HAP=\lambda AP^{(*)}+[H,A]P^{(*)}.$$

Lemma 8.11 now follows from Theorem 8.7, applied to the middle factor in (8.41). The hypothesis of that theorem requires that the first and second commutators of $\bar{A}$ with $\bar{H}$ and $\bar{V}$ are bounded relative to $\bar{H}$. As an example we treat the double commutator $[[\bar{V},\bar{A}],\bar{A}]$. After dropping the outermost factors $\bar{P}$ this commutator takes the form

$$[[V,A],A]+2APVA+2AVPA-2APVPA-APAV-VAPA+VPAPA-VPA^2-A^2PV$$
$$+APAPV.$$

By hypothesis $[[V,A],A]$ is H-bounded. All other terms except those containing A^2 are easily bounded as in the first part of the proof. For the A^2-terms we need the hypothesis $\mathrm{Ran}(P)\subset D(A^2)$. □

Proof of Theorem 8.8: By Lemma 8.11 the limit (8.30) exists. Suppose that $\Gamma>0$. Then, in the notation (8.39),

$$-\mathrm{Im}(F_0(\lambda+i0))>0,$$

and therefore by (8.40)

$$-\mathrm{Im}(F_\kappa(\mu+i0))>0$$

for small κ and all μ in some open interval $\Delta\ni\lambda$. This is in contradiction to (8.37), so for small κ the operators H_κ have no eigenvalues in Δ. □

B. Escape velocity and resolvent smoothness

According to Theorem 2.4 the orbits ψ_t in the continuous spectral subspace $\mathcal{H}_C$ of H are escaping from finite regions in X in the mean ergodic sense (2.8). In this section we discuss sharp quantitative escape estimates of the form

$$\int_{|x|<vt}|\psi_t(x)|^2\le\mathrm{const}(1+|t|)^{-2m}, \tag{8.42}$$

valid for a dense set of initial states ψ in any spectral subspace $\mathcal{H}.$, Δ a Mourre interval (6.17). This estimate says that the orbit ψ_t escape at least with velocity v. In fact (8.42) holds for any $v<\sqrt{\theta}$ where θ is the Mourre constant (8.42) for the interval Δ. In this sense $\sqrt{\theta}$ is the ***minimal escape velocity*** for the orbits in $\mathcal{H}$. Minimal velocity estimates were first derived by Sigal and Soffer[92] also for certain time-dependent Hamiltonians. The first step towards (8.42) is an analogous result for the observable A instead of $|x|$, which we state in abstract form:

Theorem 8.12:[54] *For a pair H,A of self-adjoint operators on $\mathcal{H}$ suppose that*

$$ad_A^{(k)}(H) \text{ is } H-\text{bounded for } k=0,\ldots,n\geqslant 2, \tag{8.43}$$

and let $\chi^{\pm}$ *be the characteristic function of* $R^{\pm}$. *Then*

$$\|\chi^{-}(A-a-\vartheta t)e^{-iHt}g(H)\chi^{+}(A-a)\|\leqslant \text{const}\, t^{-m}(t>0) \tag{8.44}$$

for any $g\in C_0^{\infty}(\Delta)$, *any* ϑ *in* $0<\vartheta<\theta$ *and any* $m<n-1$, *uniformly in* $a\in R$.

Remarks: To explain the significance of (8.44) we note that the vectors of the form

$$\psi=g(H)\chi^{+}(A-a)\varphi, \quad \varphi\in\mathcal{H}, \tag{8.45}$$

form a dense set in $\mathcal{H}_{\Delta}$ since $g\in C_0^{\infty}(\Delta)$ and $a\in R$ are arbitrary. Equation (8.44) expresses the fact that for any initial state ψ of this form ψ_t is in the spectral subspace $A\geqslant a+\vartheta t$ of A, upt oa remainder of order t^{-m} in norm. This is the analog of (8.42) for the observable A in place of $|x|$.

Theorem 8.12 can also be used to derive some useful, although not optimal, results for resolvent smoothness. Setting $a=-\vartheta t/2$ and using that

$$\langle A\rangle^{-\alpha}=\langle A\rangle^{-\alpha}\chi^{\pm}(A\pm\vartheta t/2)+O(t^{-\alpha})$$

we conclude from (8.44) that

$$\|\langle A\rangle^{-\alpha}e^{-iHt}g(H)\langle A\rangle^{-\alpha}\|\leqslant \text{const}(1+|t|)^{-\min(\alpha,m)}. \tag{8.46}$$

For α, $m>1$ (i.e., $n>2$), this bound is integrable over $-\infty<t<+\infty$ and thus leads (via Fourier transform) to the resolvent estimate

$$\sup_{z\notin R}\|\langle A\rangle^{-\alpha}(z-H)^{-1}g(H)\langle A\rangle^{-\alpha}\|<\infty. \tag{8.47}$$

It also follows that the operator function $F(z)=\langle A\rangle^{-\alpha}(z-H)^{-1}\langle A\rangle^{-\alpha}$ has continuous boundary values $F(x\pm i0)$ in norm sense for $x\in\Delta$. With Theorem 8.1 we have already obtained this result under the weaker hypothesis $\alpha>\frac{1}{2}$ and $n=2$. On the other hand, Theorem 8.12 immediately gives similar bounds for the derivatives (powers) of $(z-H)^{-1}$: If $(\alpha,m)>1+p$, then

$$\sup_{z\notin R}\left\|\langle A\rangle^{-\alpha}\left(\frac{d}{dz}\right)^{p}(z-H)^{-1}g(H)\langle A\rangle^{-\alpha}\right\|<\infty \tag{8.48}$$

with corresponding smoothness in x of the boundary values $F(x\pm i0)$ in Δ. Resolvent smoothness estimates of this form have been derived in Ref. 62 under weaker conditions on α,m by time-independent methods as in the proof of Theorem 8.1. All these techniques and results will be useful in many respects, e.g., for the transition to time-independent scattering theory and the discussion of scattering amplitudes. Finally we return to the Schrödinger case $H=\frac{1}{2}p^2+V(x)$ where the relation

$$A=D_t(\tfrac{1}{2}x^2)$$

can be used to transform the spectral shift formula (8.44) with respect to A into a spectral shift with respect to x^2:

Theorem 8.13:[54] *If* H,A *given above satisfy the conditions of Theorem 8.12, then*

$$\|\chi^{-}(\tfrac{1}{2}x^2-at-\tfrac{1}{2}\vartheta t^2)e^{-iHt}g(H)\chi^{+}(A-a)\|\leqslant \text{const}\, t^{-m} \quad (t>0) \tag{8.49}$$

for any $g\in C_0^{\infty}(\Delta)$, $0<\vartheta<\theta$, $m<n-1$ *and* $a\in R$.

For the dense set of initial states (8.45) this implies the escape estimate (8.1). For the proofs of Theorems 8.12 and 8.13 we refer to Ref. 54. The methods used in these proofs also allow us to treat time-dependent Hamiltonians.[92]

Notes: Resolvent bounds and resolvent smoothness. Among the papers in this field which are not reviewed here we mention Refs. 62, 35, 58, 61, and 74. A basis for treating these and related problems in a generalized form of Mourre's theory is provided by Ref. 6.

Resonances in Mourre theory. Beyond the instability criterion for embedded eigenvalues given in Theorem 8.8 it is also possible to give a perturbative notion of resonances and corresponding exponential decay estimates in this case.[77,102]

Escape velocity and resolvent smoothness. Other results similar to Theorems 8.12 and 8.13, generally referred to as *minimal velocity estimates*, are due to Refs. 33 and 100 (see also Ref. 21).

IX. THE HELFFER–SJÖSTRAND FORMULA

A convenient operator calculus for functions $f(A)$ of self-adjoint operators A can be based on a formula of Helffer and Sjöstrand:[42,16]

$$f(A)=-\frac{1}{2\pi}\int_{R^2}(z-A)^{-1}\partial_{\bar{z}}\tilde{f}(z)\,dx\,dy, \tag{9.1}$$

where $z=x+iy$ and $\partial_{\bar{z}}=\partial_x+i\partial_y$. Here f is some given complex function on $\boldsymbol{R}$, and $\tilde{f}$ is a largely arbitrary extension of f to the complex plane, which must be *almost analytic* in the sense that it satisfies the Cauchy–Riemann equations *on the real axis:*

$$\partial_{\bar{z}}\tilde{f}(z)=0 \quad \text{for} \quad z\in R. \tag{9.2}$$

We abbreviate (9.1) by writing

$$f(A)=\int d\tilde{f}(z)(z-A)^{-1}; \quad d\tilde{f}(z)\equiv-\frac{1}{2\pi}\partial_{\bar{z}}\tilde{f}(z)dx\,dy. \tag{9.3}$$

For example, if $f\in C_0^2(\boldsymbol{R})$, we can construct the almost analytic extension

$$\tilde{f}(z)=(f(x)+iyf'(x))\chi(z) \tag{9.4}$$

in $C_0^1(C)$ by taking $\chi\in C_0^\infty(C)$ with $\chi=1$ on some complex neighborhood of supp(f). Then $\partial_{\bar{z}}\tilde{f}$ has compact support and vanishes on the real axis, so that $|\partial_{\bar{z}}\tilde{f}(z)|\leq\text{const}|y|$. On the other hand, $\|(z-A)^{-1}\|\leq|y|^{-1}$. Therefore, the integral (9.3) converges absolutely in norm sense, and (9.1) follows by verifying that

$$f_\varepsilon(t)\equiv\int_{|y|>\varepsilon}d\tilde{f}(z)(z-t)^{-1}$$

converges pointwise to $f(t)$ for $t\in\boldsymbol{R}$ as $\varepsilon\searrow0$. Often it is useful to replace (9.4) by the extended version

$$\tilde{f}(z)\equiv\chi(z)\sum_{k=0}^{n}f^{(k)}(x)\frac{(iy)^k}{k!}, \tag{9.5}$$

with χ as before and n arbitrary large. Then $|\partial_{\bar{z}}\tilde{f}(z)|\leq\text{const}|y|^n$ so that the integral $\int|\text{Im}(z)|^{-n}\partial_{\bar{z}}\tilde{f}(z)$ converges absolutely. As an application, suppose that A_1 and A_2 are self-adjoint and that K is compact relative to A_1 or A_2. Taking (9.5) with $n\geq2$ we find that the integral

$$\int d\tilde{f}(z)(z-A_1)^{-1}K(z-A_2)^{-1}$$

is a compact operator since it is the norm limit of compact operators. This argument was used in the proof of (6.16). Of course that particular case can be treated without using (9.1). The reason why we advertise the Helffer–Sjöstrand formula is that it also serves as the basis for a general method of commutator expansions and commutator estimates,[59,52] which is used extensively in the omitted proofs in Secs. VI and VIII.

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