Barry Simon’s contributions to non-relativistic quantum mechanics: two-body and \(N\)-body Schrödinger operators and resonances

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Dedicated with respect and admiration to Barry Simon on the occasion of his 60th birthday.

1 Introduction

Non-relativistic quantum mechanics and Schrödinger operators occupy a central place in Barry Simon’s prodigious output. This article is a review of Simon’s work on two-body and \(N\)-body Schrödinger operators, and on resonances. A few early papers reviewed here do include results about the general theory of Schrödinger operators (that is, without any decay assumptions on the potential), but I have excluded some more recent papers on one dimensional Schrödinger operators that seemed more closely related to work on inverse problems and random potentials. Also notable among the excluded results are papers dealing with electric and magnetic fields, the semi-classical limit and Thomas-Fermi theory. These will be covered in other articles.

Imposing these severe restrictions on the subject matter still leaves a formidable collection of papers. I have grouped them into three sections: two-body and general Schrödinger operators ([4], [5], [13], [24], [35], [59], [70], [71], [80], [99], [103], [106], [114], [115], [135], [137], [179], [181], [218], [226], [227]), \(N\)-body Schrödinger operators ([9], [25], [43], [44], [45], [46], [51], [55], [83], [84], [85], [95], [96], [97], [119], [122], [124], [125], [131], [132], [133], [134], [160], [175], [199], [304]), and resonances ([19], [20], [105], [107], [121], [156], [276]). Here and throughout this article, references are to Simon’s publication list at \url{http://www.math.math.caltech.edu/people/biblio.html}
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and on page ?? of this volume. Note that upper case (resp. lower case) roman numerals that appear below refer to books (resp. review articles and conference proceedings.) The following graph displays the distribution of these papers among all of Simon’s research articles. (The horizontal axis is the publication date. The graph shows research articles only, not review papers or books.) As the graph shows, this review mainly considers topics that occupied Simon during the early and middle parts of his career.

I should emphasize that this article is about Barry Simon’s contributions, and not a review of the field. Barry Simon himself is a masterly reviewer, and in addition to his research articles, he has authored books as well as several book-length reviews, dealing with the topics discussed here. These books and reviews have been (and continue to be) profoundly influential in my own education, and in shaping the entire field.

I was fortunate to participate in the writing of [X], together with Cycon, Kirsch and, of course, Simon. This book started out as a week long lecture series by Simon, delivered at breathtaking pace in a small castle in Thurnau, Germany. It aims to survey the field of Schrödinger operators with an emphasis on results that were recent at the time of writing in the early 1980’s. Other reviews that are relevant to this article are 1982 Bulletin article \(\text{Schrodinger semigroups}\) [xxi] and the 2000 review \(\text{Schrödinger operators in the twentieth century}\) [xxxix]. For this article I have often had to compress the contents of entire long research papers into a sentence or two. So I am fortunate to be able to refer the reader to these articles for more information, in particular, to references to works by other authors. Each of Simon’s reviews contains a reference list of several hundred articles.

Finally, it is impossible to discuss Simon’s pedagogical work on Schrödinger operators without mentioning the series Reed and Simon ([II] [III], [V], [VII]) from which several generations of Mathematical Physicists have learned the
subject.

Almost all the papers under review here concern the theory of Schrödinger operators of the form

\[ H = -\Delta + V \]

acting in \( L^2(\mathbb{R}^n) \). In the context of non-relativistic quantum mechanics the most important questions about such an operator for a given potential \( V \) are

(i) self-adjointness: To begin with, the expression for \( H \) is only a formal sum. How can \( H \) be defined as a self-adjoint unbounded operator?

(ii) spectral theory: What is the nature of the spectrum and where is it located? What are the smoothness and decay properties of the eigenfunctions?

(iii) scattering theory: What is the long time behaviour of the Schrödinger time evolution \( e^{-itH} \)?

The definition of resonances requires some extra structure and is discussed below.

2 Two-body and general Schrödinger operators

This section deals with work on two-body potentials, that is, potentials \( V(x) \) that tend to zero in some sense as \( |x| \to \infty \), as well as some results (mostly about self-adjointness) that continue to hold under the addition of an \( L^\infty \) term to the potential. Note that two-body operators become one-body operators after the removal of the center of mass. This is briefly discussed in the \( N \)-body section below.

2.1 Quadratic forms, singular and positive potentials

(with P. Deift) *On the decoupling of the finite singularities from the question of asymptotic completeness in two body quantum systems*, J. Funct. Anal. 23 (1976), 218-238


In the early part of his career, Simon contributed much to the understanding of how to handle singularities of the potential in basic questions about Schrödinger operators. Singularities are important because the most important potentials in physics, like the Coulomb potentials $C|x|^{-1}$, are singular. Moreover, the kinetic energy (Laplacian) term in a Schrödinger operator dominates a potential as singular as $-\alpha |x|^{-2}$ for small enough $\alpha$ so one would like to be able to handle potentials up to this borderline. It is a fact of life, though, that for most properties there is no simple best possible class of potentials.

Simon’s thesis ([13] and the book [I]) is a systematic exploration of the Rollnik class of potentials. A potential $V$ defined on $\mathbb{R}^3$ is in the Rollnik class $R$ if the norm given by

$$
\|V\|_R^2 = \int_{\mathbb{R}^6} \frac{|V(x)||V(y)|}{|x-y|^2} d^3x d^3y
$$

is finite. Simon proposes the class $R$ as a replacement for $L^2(\mathbb{R}^3)$ in a collection of theorems about two-body Schrödinger operators. For example, considering the question of self-adjointness, the basic Kato-Rellich theorem allows $H = -\Delta + V$ to be defined as a self-adjoint operator sum on the usual domain $\mathcal{D}(\Delta)$ of the Laplacian provided $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. This definition allows singularities as bad as $|x|^{-3/2}$. To allow for potentials as singular as $|x|^{-2}$ (the physically relevant borderline), Simon proposes the condition $V \in R + L^\infty(\mathbb{R}^3)$. With this condition, $H$ can no longer be defined as an operator sum, but must be defined as the operator associated to the sum of quadratic forms, via the KLMN theorem. For these Hamiltonians defined as quadratic forms, Simon then considers bound state problems, existence and completeness of wave operators under an $L^1$ condition, and existence of eigenfunction expansions. The bound state results rely on the fact that for Rollnik potentials $|V|^{1/2}(-\Delta - E)^{-1}|V|^{1/2}$ is Hilbert-Schmidt. This allows Birman-Schwinger type arguments to bound the number of negative energy bound states and restrict the number and position of positive energy bound states.
states. In particular, for small enough Rollnik norm there are no positive energy bound states.

The question of the existence of positive energy bound states is a subtle one, since a tunneling argument predicts that they do not exist for a two-body potential. Yet, there is a well known example due to Wigner and von Neumann of a potential decreasing like $|x|^{-1}$ that does have a positive eigenvalue. Before his thesis, Simon already published a result on positive eigenvalues in [5], generalizing work of Kato and Odeh. In this paper he rules out eigenvalues in $[E_0, 1)$ for potentials $V \in L^2(S^2) + L^\infty(R^3)$ that are smooth near infinity and can be written as $V = V_1 + V_2$ where as $|x| \to \infty$, $|x|V_1(x) \to 0$, $V_2(x) \to 0$ and $\lim sup x \cdot \nabla V_2(x) = E_0 < \infty$. The proof treats the equation for an eigenfunction as an ODE in the radial variable for an $L^2(S^2)$ valued function, and proceeds via differential inequalities.

Simon returns to the question of self-adjointness in [24],[35], this time essential self-adjointness on $C^0_{\text{loc}}$ for Schrödinger operators in higher dimensions. The natural condition given by the Kato-Rellich theorem for dimension $n \geq 4$ is $V \in L^p(R^n) + L^\infty(R^n)$ for $p > n/2$ (but $p = n/2$ for $n \geq 5$ is also known). For positive potentials one expects to be able to handle more singular potentials. In [24] Simon proves essential self-adjointness on $C^0_{\text{loc}}$ for positive $V$ in $L^2(R^n) + L^\infty(R^n)$. Clearly, a local $L^2$ condition is required to define $H$ on $C^0_{\text{loc}}$. In this paper Simon conjectures that $V = V_+ - V_-$ with $V_+ \in L^2_{\text{loc}}$ and $V_-$ as above should suffice for essential self-adjointness on $C^0_{\text{loc}}$. This was proved by Kato, and again by Simon in [35]. A crucial ingredient in Kato’s proof is the distributional inequality $\Delta |u| \geq \text{Re}(\text{sgn} u \Delta u)$. (For complex $u$, $\text{sgn} u$ equals $\bar{u}/|u|$ at points where $u \neq 0$ and vanishes at points where $u$ does.) Simon explores the connection between this type of inequality and positivity preserving semigroups in [76] and [86]. The paper [35] also proves self-adjointness for positive potentials $V \in L^2(R^n\setminus 0)$ provided $V \geq C_n r^{-2}$ for an explicit constant $C_n$.

Singularities on a distinguished set also play a role in [59], where Simon and Faris examine the question of degeneracy of the ground state. A theorem of Faris insures the non-degeneracy of the ground state for $H = -\Delta + V$ defined via quadratic forms if $V = V_1 + V_2$ with $V_1 \geq 0$, $V_1 \in L^1_{\text{loc}}(R^n)$ and $V_2 \in L^\infty(R^n) + L^{n/2}(R^n)$ (here $n \geq 3$, there are similar conditions for $n = 1, 2$). On the other hand, Klauder noted that the singularity in $H = -d^2/dx^2 + x^2 + |x|^{-\alpha}$ for $\alpha \geq 1$ effectively decouples the positive and negative axis leading to a doubly degenerate ground state. (The phenomenon was analyzed by Simon in [41] in terms of form sums.) Looking to higher dimensions, Simon and Faris consider potentials in $L^1_{\text{loc}}(R^n\setminus K)$, where $K$ is a closed set of measure zero. They prove that if $R^n\setminus K$ is con-
nected, then $-\Delta + V$ has a non-degenerate ground state, even though $V$ can clearly be very singular on $K$. Two proofs are given: one using path integrals and one using differential operator methods. On the other hand if $\mathbb{R}^n \setminus K$ has more than one component, there exists $V \in L^1_{\text{loc}}(\mathbb{R}^n \setminus K)$ such that the ground state of $-\Delta + V$ is degenerate.

In [71] Deift and Simon also consider potentials $V$ that can be very singular on closed sets of measure zero, this time in the context of scattering theory. The main result asserts that if wave operators for $H_0 = -\Delta$ and $H = -\Delta + V$ are complete then so are the wave operators for $H_0$ and $H' = -\Delta + \chi V$, where $\chi$ is the characteristic function of the exterior of a ball. A mild regularity condition on the negative part of $V$ is required.

By the beginning of the 1980’s, in the book [X] and review article [xxi] Simon was advocating the class $K_\nu$ as a natural class of potentials for self-adjointness and other properties, based on his work with Aizenman in [135]. A potential on $\mathbb{R}^\nu$ for $\nu \geq 3$ is in this class if

$$\limsup_{\alpha \to 0} \sup_{|x-y| \leq \alpha} |x-y|^{2-\nu} |V(y)|dy = 0$$

(with similar definitions for $\nu = 1, 2$.) These potentials were previously studied by Kato and Schechter. They are not quite optimal for self-adjointness (clearly $\alpha |x|^{-p} \in K_\nu$ for $p < 2$ but not $p = 2$). However Aizenman and Simon show in [135] that they are very natural from the point of view of $L^p$ mapping properties for the Schrödinger semigroup $e^{-tH}$ and for Harnack inequalities. They prove, for example, that $V \in K_\nu$ is equivalent to

$$\lim_{E \to \infty} \|(-\Delta + E)^{-1}V\|_{\infty, \infty} = 0$$

Here $\| \cdot \|_{\infty, \infty}$ denotes the $L^\infty \to L^\infty$ operator norm.

2.2 Weak coupling and threshold behaviour

[227] (with G.M. Graf) Asymptotic series for the ground state energy of Schrödinger operators, J. Funct. Anal. 112 (1993), 442-446
The \( \lambda \) dependence of an eigenvalue of a Schrödinger operator \(-\Delta + \lambda V\) will can be understood using regular perturbation theory, as long as the eigenvalue stays isolated from the rest of the spectrum. However, as \( \lambda \) tends to zero, the eigenvalue will eventually be absorbed in the continuous spectrum, at the latest when \( \lambda \) becomes zero. Simon has written a number of papers about what happens near the point where the eigenvalue is absorbed.

The papers \([70]\) and \([80]\) deal with values of \( \lambda \) close to zero. They address the questions of whether there are eigenvalues for small but non-zero \( \lambda \), and, if so, how they behave as \( \lambda \) tends to zero. Simon’s paper \([70]\) begins with the observation that a negative square well potential in one or two dimensions, no matter how shallow, always has a bound state. In three or higher dimensions, shallow square well potentials have no eigenvalues. This observation is generalized as follows. In one dimension, if \( \int (1 + |x|^2)|V(x)|dx < \infty \) then \(-d^2/dx^2 + \lambda V\) has a bound state for all small positive \( \lambda \) if and only if \( \int V(x)dx < 0 \). A similar result holds in two dimensions. This paper also considers the analyticity of the lowest eigenvalue \( e(\lambda) \) at \( \lambda = 0 \) (true in one dimension and false in two) and the threshold behaviour. For example, in one dimension \( e(\lambda) \sim c\lambda^2 \) if \( \int Vdx < 0 \) and \( e(\lambda) \sim c\lambda^4 \) if \( \int Vdx = 0 \). In \([80]\) Blankenbecler, Goldberger and Simon revisit the one dimensional situation, but for longer range potentials for which \( \int (1 + |x|^2)|V(x)|dx = \infty \). Roughly speaking, this paper considers \( V(x) \sim -a|x|^{-\beta} \) for \( 1 < \beta < 3 \). New phenomena appearing include the existence of infinitely many bound states for small coupling (in the range \( 1 < \beta < 2 \)).

For short range potentials \( V \), if an eigenvalue \( e(\lambda) \) is absorbed in the continuous spectrum, that is, \( e(\lambda) \rightarrow 0 \), as \( \lambda \downarrow \lambda_0 \), what is the leading order of \( e(\lambda) \)? For example, is \( e(\lambda) \sim (\lambda - \lambda_0)^\alpha \)? This question is answered in detail in Klaus and Simon \([115]\). The answer is highly dimension dependent, with different results depending on whether the dimension is in \( \{1\}, \{2\}, \{3\}, \{4\}, \{5,7,9,\ldots\} \) or \( \{6,8,10,\ldots\} \).

In the early 1990’s, Simon again considered Schrödinger operators with weak coupling, that is, \(-\Delta + \lambda V\) for \( \lambda \) small. But now \( V \) is a potential that does not go to zero at infinity. Let \( e(\lambda) \) denote the infimum of the spectrum. Of course, in this setting \( e(\lambda) \) need not be an eigenvalue. In \([226]\) Gesztesy, Graf and Simon are address the question of when \( e(\lambda) < 0 \) (notice the strict inequality) for \( \lambda \neq 0 \). They prove for a large class of potentials that do not decrease at infinity that \(-c\lambda^2 \leq e(\lambda) \leq -d\lambda^2 \) for positive constants \( c \) and \( d \). In a follow up, Graf and Simon \([227]\) give a class of potentials, including some almost periodic potentials, for which \( e(\lambda) \) has a complete asymptotic series at \( \lambda = 0 \).
2.3 Some scattering results

[99] (with E.B. Davies) *Scattering theory for systems with different spatial asymptotics on the left and right*, Commun. Math. Phys. 63 (1978), 277-301


Here I will briefly describe some papers on scattering that have not been mentioned above, and are not discussed with $N$-body results below. In [99] Davies and Simon study scattering theory for systems with different spatial asymptotics on the left and the right. An example is a potential in one dimension that approaches different limiting values as $x \to \pm \infty$. A physically important example is a half-solid, that is, a potential in $\mathbb{R}^n$ that vanishes in a half space and is periodic in the other half space. This paper contains results about existence and completeness of scattering, where the comparison dynamics may be different on each side. In the case of a half solid, there is a proof of the decomposition of the absolutely continuous spectral subspace into scattering states and surface states.

Motivated by a result in classical mechanics, Radin and Simon in [103] show that there is a dense set of vectors such that $\|xe^{-itH}f\|$ is bounded by $C(1 + |t|)$ for $f$ in this set, provided $V$ is Laplacian bounded with bound less than one (in either the form or operator sense). Here $x$ is the vector valued position operator. This bound cannot be improved in general, since it describes ballistic motion, that is, the time behaviour for a freely moving particle. However, if $H$ has only point spectrum one might expect there to be no ballistic motion. This is proved by Simon in [218], where he shows that for such Hamiltonians $\lim_{t \to \infty} t^{-2}\|xe^{-itH}f\|^2 = 0$ for $f$ with compact support.

The paper [106] is a long exploration of the method introduced by Enss in two-body, and later in three-body, scattering. Enss’s method created a sensation when it appeared, since it was able to reproduce the strongest known results at the time in a transparent manner, with beautiful connections to classical mechanics. Simon extends the method to a large number of scattering systems, including pseudo-differential operators, Stark and Zeeman effects, optical and acoustical scattering, complex potentials, magnons and half solids (in some sense making obsolete the methods just introduced in [99]).
2.4 Multiple wells, continuum eigenfunctions and eigenvalue splittings


The paper [114] with Klaus was motivated in part by Sigal’s work on the Efimov effect. The Efimov effect is the phenomenon occurring for certain \(N\)-body Hamiltonians where short range (even compactly supported) pair potentials can produce infinitely many bound states. The main result in [114] concerns two compactly supported critical potentials \(V_1\) and \(V_2\). Here critical means that \(-\Delta + V \geq 0\) but \(-\Delta + \lambda V\) has a negative eigenvalue for any \(\lambda > 1\). In this situation Simon and Klaus prove that the potential \(W_r = V_1(x) + V_2(x - r)\), where \(r\) is large enough so that the supports are disjoint, produces a bound state with energy \(E(r) \sim |\beta r|^{-2}\). In three dimensions, \(\beta\) is a universal constant.

In [137] Simon shows that the spectrum of a fixed Schrödinger operator on a class of polynomially weighted spaces is independent of the weight. This holds for a large class of potentials \(V = V_+ + V_-\) with \(V_+ \geq 0\) and \(V_\mu \in K_\mu, V_- \in K_\nu\). A consequence of this theorem is the fact (first proved by Schrödinger) that if \(H\phi = E\phi\) has a polynomially bounded solution, then \(E\) is in the spectrum of \(H\).

In [179] and [181] Kirsch and Simon consider the question of estimating the splitting between two eigenvalues of a Schrödinger operator. The paper [179] treats the one-dimensional case, where eigenvalues are simple. For \(V \in C_0^\infty\) supported in \([a, b]\) a bound of the form \(E_n - E_{n-1} \geq \pi^2 \exp(-\lambda(b-a))\) is obtained, where \(\lambda = \sup_{E \in (E_{n-1}, E_n), x \in (a,b)} \sqrt{|E - V(x)|}\). In higher dimensions, since eigenvalues other than the ground state can be degenerate, it only will be possible to estimate \(E_1 - E_0\) in general. The paper [181] gives variational lower bounds on this number that follow from realizing a Schrödinger operator as a Dirichlet form. These bounds lead to a quadratic lower bound \(\mathcal{E}_0(k) - \mathcal{E}_0(0) \geq Ck^2\) for the lowest band function \(\mathcal{E}_0(k)\) for a periodic Schrödinger operator.
3 \textbf{\textit{N}}-body Schrödinger operators

A Schrödinger operator describing \( N \) particles with masses \( m_i \) moving in \( \mathbb{R}^n \) and interacting via pair potentials \( V_{ij} \) has the form

\[
\hat{H} = -\sum_{i=1}^{N} \frac{1}{2m_i} \Delta_i + \sum_{1 \leq i < j \leq N} V_{ij}(x_i - x_j).
\]

This operator, acting in \( L^2(\mathbb{R}^{nN}) \), has purely absolutely continuous spectrum arising from the uniform motion of the centre of mass. To define the \( N \)-body operator \( H \), we must remove the centre of mass. I will give a brief description of this, as well as some of the terminology used below.

To remove the centre of mass (according to the Sigal-Sigalov prescription), consider the inner product on \( \mathbb{R}^{nN} \) defined by the masses via the formula

\[
\langle (x_1, \ldots, x_N), (y_1, \ldots, y_N) \rangle = \sum_{i=1}^{N} m_i \langle x_i, y_i \rangle,
\]

where the bracket on the right side denotes the usual inner product on \( \mathbb{R}^n \). Decompose \( \mathbb{R}^{nN} \) into an orthogonal direct sum \( X \oplus Y \), where

\[
Y = \{(x, \ldots, x) : x \in \mathbb{R}^n \}
\]

is the diagonal subspace and

\[
X = Y^\perp = \{(x_1, \ldots, x_N) : \sum_i = 1^N m_i x_i = 0 \}.
\]

The subspace \( Y \) can be thought of as co-ordinates for the displacement of the centre of mass, while the subspace \( X \) contains internal co-ordinates. From the direct sum decomposition, we obtain \( L^2(\mathbb{R}^{nN}) = L^2(X) \otimes L^2(Y) \). The first (kinetic energy) term in \( \hat{H} \), being \(-1/2\) times the Laplace operator for this metric defined by this inner product, can be written \(-\Delta_X \otimes I - I \otimes \Delta_Y\), where \( \Delta_X \) and \( \Delta_Y \) are the Laplace operators for the respective subspaces. Since the potential is constant along the diagonal, it can be written \( V \otimes I \), where \( V \) is given by the formula above, but thought of as the restriction of the original potential to \( X \). Thus

\[
\tilde{H} = H \oplus I + I \oplus (-\frac{1}{2} \Delta_Y).
\]

This defines the \( N \)-body Hamiltonian \( H = -\frac{1}{2} \Delta_X + V \) acting in \( L^2(X) \).

For any partition \( C = \{c_1, \ldots, c_k\} \) of \( \{1, \ldots, N\} \) into disjoint subsets, or clusters, there is an associated cluster Hamiltonian \( H(C) \) obtained from \( H \)
by dropping potentials $V_{i,j}$ when $i$ and $j$ lie in different subsets. Thus $H(C)$ is the Hamiltonian describing the particles within each cluster interacting, but clusters moving independently of the others.

There is an associated direct sum decomposition of $X$ into $X_{c_1} \oplus \cdots \oplus X_{c_k} \oplus Y_C$ giving rise to the tensor product decomposition $L^2(X) = L^2(X_{c_1}) \otimes \cdots \otimes L^2(X_{c_k}) \otimes L^2(Y_C)$. The subspaces $X_{c_i}$ contain the internal co-ordinates for the cluster $c_i$ while $Y_C$ contains co-ordinates for relative motion of the clusters. The cluster Hamiltonian has the associated decomposition

$$H(C) = h_{c_1} \otimes \cdots \otimes I \otimes I + \cdots$$
$$\cdots + I \otimes \cdots \otimes h_{c_k} \otimes I + I \otimes \cdots \otimes (-\frac{1}{2} \Delta_{Y_C}),$$

where $h_{c_k}$ is the $N_k$-body Hamiltonian for the particles in the cluster $c_k$. Here $N_k$ is the number of particles in the cluster $c_k$. This decomposition therefore sets the stage for an inductive treatment of $N$-body Hamiltonians.

3.1 The Pointwise bounds series


This series of papers considers the question of exponential decay of eigenfunctions. Let $\Psi(x)$ be an eigenfunction of an $N$-body Hamiltonian with eigenvalue $E < \Sigma = \inf \sigma_{\text{ess}}(H)$. One way of measuring the decay of $\Psi(x)$ is by a so-called $L^2$ bound, that is, a statement like $e^{a|x|} \Psi(x) \in L^2$ indicating that in some average sense, $\Psi(x)$ decays faster than $e^{-a|x|}$. A stronger statement is a pointwise bound of the form

$$|\Psi(x)| \leq C_a e^{-a|x|}.$$
which is required to hold for every $x$. This kind of bound (and the corresponding lower bound) is the subject of these papers.

In [43], the first paper of this series, Simon proves that such a pointwise estimate holds for all $a < \sqrt{\Sigma - E}$. In addition, Hölder continuity of $\Psi$ and $\nabla \Psi$ is proved. Prior to this paper, O’Connor had proved $L^2$ bounds by showing that $\Psi$ has an $L^2$ analytic continuation to a tube around $\mathbb{R}^{3N-3}$ and applying a Payley-Wiener argument. Simon shows that this continuation can be made in $L^1$, which leads to the desired bound.

The papers [46] and [51] are actually not about $N$-body Hamiltonians, but consider potentials $V(x)$ that grow at infinity. In this case, one expects faster than exponential decay, and this is what Simon proves.

The exponential bounds described so far are isotropic, that is, they depend only on $|x|$ and not on the direction of $x$. However, the behaviour of an $N$-body potential at infinity depends very much on the direction. Therefore, it is not unreasonable to expect that in the upper bound, $e^{-a|x|}$ could be replaced by $e^{-f(x)}$ where $f$ is homogeneous of degree one. Such non-isotropic bounds are the subject of the milestone paper [95] with Deift, Hunziker and Vock. In this paper, the Combes-Thomas technique is used to prove non-isotropic bounds $|\Psi(x)| \leq Ce^{-f(x)}$ for homogeneous functions $f$ whose gradient satisfies an inequality involving the spectrum of cluster Hamiltonians, that is, Hamiltonians defined by keeping only potentials that do not go to zero in a certain direction. Between this paper and the next in the series, the optimal $f$ satisfying the gradient inequality was found by Agmon, and is now known as the Agmon metric.

The next paper [133] with Carmona, is another landmark paper. In this paper, probabilistic methods are used to prove that the Agmon metric provides an exponential lower bound for the ground state $\Psi$. Combining this with the upper bound, we have

$$c_\epsilon e^{(1-\epsilon)f(x)} \leq \Psi(x) \leq C_\epsilon e^{(1+\epsilon)f(x)}.$$  

This bound shows that, in some sense, the Agmon metric captures exactly the behaviour of the ground state. Actually, the paper [133] considers not only $N$-body Hamiltonians, but also potentials that grow at infinity. For these potentials there is also a corresponding Agmon metric and upper bound, and Carmona and Simon provide the corresponding optimal lower bound for the ground state.

In final paper [134] of this series, Lieb and Simon go beyond upper and lower bounds above, to compute the first term in an asymptotic expansion. They consider the ground state $\Psi$ in a region of configuration space where
the particles form two widely separated clusters. They are able to prove asymptotics of the form

$$\Psi(\zeta_1, \zeta_2, R) = c\psi_1(\zeta_1)\psi_2(\zeta_2)e^{-kR}R^{-1}(1 + O(e^{-\gamma R}))$$

where $\zeta_1$ and $\zeta_2$, the internal co-ordinates for the two clusters, stay bounded while the intercluster distance $R$ tends to infinity. Here $\psi_1$ and $\psi_2$ are the ground states of the corresponding cluster Hamiltonians.

### 3.2 Geometric Methods


Geometric methods for $N$-body Hamiltonians aim to exploit the special form of an $N$-body potential near infinity in configuration space by using partitions of unity. In regions of configuration space where two particles are widely separated so that the corresponding potential is small, we should be able to ignore that potential. Such localizations are now pervasive in the subject, so it is interesting to sense the excitement they caused in the late 1970’s. This is from the introduction to Simon’s paper [84]:

“... there is some point in seeing the sweep of results presented here obtained by geometric methods without the pernicious influence of resolvent equations. Not that these equations do not have their usefulness but it seems to me that they have overly dominated our thinking. I will regard this paper as a success if it helps strike a balance in the reader’s mind; even better, I would hope to convey the excitement of the geometric ideas.”

The first paper [83] in this series, Deift and Simon take the first steps in a geometric time-dependent proof of asymptotic completeness for multiparticle systems. They consider wave operators for a three body system of the form

$$W_\alpha^\pm = s - \lim_{t \to \pm \infty} e^{itH_\alpha}J_\alpha e^{-itH}P_{ac}.$$
Here $H_\alpha$ is a cluster Hamiltonian obtained by dropping two of the three potentials in the original $H$, and $J_\alpha$ is a cutoff function that localizes to the region where the dropped potentials are small. For example, if the remaining potential in $H_\alpha$ is $V_{1,2}$, then $J_\alpha$ would localize to the region where $|x_1 - x_2|$ is small, but $|x_1 - x_3|$ and $|x_2 - x_3|$ are large. Deift and Simon prove that if asymptotic completeness holds, then these wave operators exist. They also show that if the wave operators exist, and scattering is complete for two body subsystems, then asymptotic completeness holds.

In the paper [84], Simon uses geometric methods to provide simple proofs of a number of basic results about $N$-body Schrödinger operators. The first of these is the HVZ theorem, first proved separately by Hunziker, Van Winter and Zhislin. Let $\Sigma$ denote the bottom of the essential spectrum of $H$

$$\Sigma = \inf \sigma_{\text{ess}}(H)$$

and denote by $\Sigma_2$ the infimum over the spectra of the cluster Hamiltonians $H(C)$ as $C$ ranges over all 2 cluster partitions.

$$\Sigma_2 = \inf_{C: \#(C)=2} \inf \sigma_{\text{ess}}(H(C)).$$

The quantity $\Sigma_2$ is the smallest energy the system of particles can have if we divide them into two groups and move the groups far apart. The HVZ theorem asserts that

$$\Sigma = \Sigma_2.$$

The second result is a theorem first proved by Combes. It concerns the situation where it always requires energy to break a two cluster partition into three groups. In other words, $\Sigma_2 < \Sigma_3$, where if

$$\Sigma_3 = \inf_{C: \#(C)=3} \inf \sigma_{\text{ess}}(H(C)).$$

Given the HVZ theorem, we see that scattering is possible in the energy range $[\Sigma, \Sigma_3]$. Combes’ theorem asserts that scattering is complete in this energy range. The final part of this paper deals with the question of when there are finitely many and when there are infinitely many bound states.

When proving Combes’ scattering result Simon required the interparticle potentials $V_{ij}(x)$ to decay like $|x|^{-n-\epsilon}$. In [85] Simon improves this to $|x|^{-1-\epsilon}$ in the case of central potentials, that is, potentials that only depend on $|x|$.

The papers [124] and [125] address the problem of estimating the total scattering cross section. Actually, most of this paper is not about $N$-body scattering, but the geometric time dependent approach makes it possible
to consider the \( N \) body problem too, and there is a result about the cross section for a two cluster channel in this paper. The total cross section in the two body case is defined as follows. Fix an incident direction \( \hat{e} \) and suppose that \( g(x) \) is a function of \( x \cdot \hat{e} \), that is, \( g(x) = G(x \cdot \hat{e}) \). Define \( \tilde{g}(k) \) to be the Fourier transform of \( G \). Then \( \sigma_{\text{tot}}(k) \) is defined via

\[
\|(S - 1)g\|^2 = \int \sigma_{\text{tot}}(k)|\tilde{g}(k)|^2 dk.
\]

Here \( S \) denotes the scattering operator. Since \( g \) is not square integrable, the left hand side must be defined as a limit \( \lim_{R \to \infty} \|(S - 1)gh_R\|^2 \) for a sequence of cutoff functions \( h_R \). The paper contains both upper and lower bounds on \( \sigma_{\text{tot}} \). In particular, the leading behaviour of the cross section for large coupling constant is obtained.

The recent preprint [304] with Yoram Last is proof that the geometric method has not run out of steam. This paper presents a unified framework for identifying the essential spectrum of a broad class of operators that includes the HVZ theorem as a special case. This method is able to handle potentials that do not have a limit at infinity. The proof is based on localization formulae. But in contrast to the earlier work, the support of the cutoff function is on balls of a fixed size, and only single commutators are used.

### 3.3 Absence of singular continuous spectrum


Perry, Sigal and Simon’s paper [132] was a landmark in the history of the subject. It contained the first proof, for general \( N \)-body systems, of the absence of singular continuous spectrum and the fact that eigenvalues can accumulate only at thresholds. The immediate antecedent of this work was a paper of Mourre who considered abstract positive commutator estimates, now known as Mourre estimates, of the form

\[
E_{\Delta}i[H, A]E_{\Delta} \geq \alpha E_{\Delta}^2 + K
\]

where \( E_{\Delta} \) is the spectral projection of \( H \) for the interval \( \Delta \), \( A \) is a self-adjoint operator which in applications to \( N \) body systems is the generator of dilations, and \( K \) is compact. Mourre showed how this sort of estimate could lead to the desired spectral information for \( H \) in the interval \( \Delta \). The
hypotheses in Mourre’s work allowed him to apply his theorem to 2 and 3 body systems. Perry, Sigal and Simon’s major technical achievement was the proof of the Mourre estimate for $N$-body systems for a large class of potentials.

### 3.4 Coulomb Systems


The most important multiparticle Hamiltonians from the physical point of view are Coulomb systems describing the interaction of $N$ electrons with $k$ nuclei via Coulomb potentials. A common approximation is to consider the limit of infinite nuclear mass. In this case the nuclei are static, fixed at positions $R_1, \ldots, R_k$. The corresponding Hamiltonian is

$$H = -\sum_{i=1}^{N} \Delta_i - \sum_{i=1}^{N} \sum_{j=1}^{k} z_j |x_i - R_j|^{-1} + \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1}$$

The $z_j$ are positive numbers giving the charges of the nuclei. In the case of static nuclei, no removal of the centre of mass is needed and $H$ acts in $L^2(\mathbb{R}^{3N})$. However, to take account of the effect of spin, we must let $H$ act in $L^2_0(\mathbb{R}^{3N}; \mathbb{C}^{2N})$. A function in this space can be thought of as $\Psi(x_1, \sigma_1; \ldots; x_N, \sigma_N)$ with $x_i \in \mathbb{R}^3$ and $\sigma_i \in \{1/2, -1/2\}$ with the requirement that $\Psi$ is antisymmetric under exchanges of $x_i, \sigma_i$ and $x_j, \sigma_j$.

The Hartree-Fock approximation to the ground state energy is obtained by minimizing $(\Psi, H\Psi)$ over a restricted set of $\Psi$ given by Slater determinants

$$\Psi(x_1, \sigma_1, \ldots, x_N, \sigma_N) = (N!)^{-1/2} \det(u_i(x_j, \sigma_j))$$

where $u_i(x, \sigma)$ for $i = 1, \ldots, N$ is an orthonormal set of trial functions. The Euler-Lagrange equations for this minimization problem are called the
Hartree-Fock equations. They are a complicated set of non-linear equations, and it is not clear that they have a solution.

In the paper [55] (and the announcement [45]), Lieb and Simon give a positive solution to this fundamental problem. Their proof is variational, that is, they prove the existence of a minimizer of the energy functional, rather than directly proving the existence of a solution to the Hartree Fock equations. In addition, they obtain properties of the minimizers, $u_i$, such as exponential decay. The proof is related to another approximation, the Thomas-Fermi approximation, which however is not covered in this review.

Lieb and Simon in [97] study the true ground state energy of $H$ as a function of the centres $R_i$. They consider first the case when there are two nuclei and one electron. In this case they prove that the ground state energy is an increasing function of $|R_1 - R_2|$. Secondly, they consider the case of one electron and $k$ nuclei whose positions are scaled to $\lambda R_1, \ldots, \lambda R_k$. In this case the ground state energy is non-decreasing as $\lambda$ increases. The proof uses correlation inequalities.

The paper [119] with M. Hoffmann-Ostenhof and T. Hoffmann-Ostenhof is an early work about nodal properties of eigenfunctions. The result is that near a zero of an eigenfunction the eigenfunction takes on both signs. Two proofs are sketched. Actually, the Coulomb nature of the potentials is not important in the proof.

In [160] M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof and Simon consider $H(A) = -\Delta_1 - \Delta_2 - |x_1|^{-1} - |x_2|^{-1} + A|x_1 - x_2|^{-1}$ at the critical value of the coupling constant $A$ where the ground state is absorbed in the continuum. They show that at the critical value the bound state persists.

The final paper in this group [199] (with an announcement in [175]) joint with Lieb, Sigal and Thirring concerns the maximum number $N(Z)$ of electrons that an atomic Hamiltonian with charge $Z$ can bind. This number is defined as follows. Consider the Hamiltonian $H$ above with $N$ electrons, one nucleus, that is, $k = 1$ and charge $z_1 = Z$. Call this Hamiltonian $H(N, Z)$. Let $E(N, Z)$ be the ground state energy, that is, the infimum of $\langle \Psi, H(N, Z) \Psi \rangle$ taken over antisymmetric $\Psi$. The Ruskai-Sigal theorem states that there is an $N$ such that $E(N + 1, Z) = E(N, Z)$. The smallest such $N$ for a fixed $Z$ is $N(Z)$. Sigal had showed that $\limsup N(Z)/Z \leq 2$ and Lieb had improved this to $N(Z) < 2Z + 1$. This paper contains a proof of the fact that

$$N(Z)/Z \to 1$$

as $Z \to \infty$. The proof begins by proving a classical analog of this theorem. This is then used in a proof modeled on Sigal’s.
3.5 Dilation Analyticity


These papers develop ideas introduced by Balslev, Combes and Thomas for studying the spectrum of $N$-body Hamiltonians and the decay of eigenfunctions. In [25] the original dilation analyticity argument of Balslev and Combes on the absence of singular continuous spectrum is extended to a wider class of potentials using quadratic form techniques. Paper [44] proves the absence of positive eigenvalues for a class of $N$-body Hamiltonians with dilation analytic potentials. In addition to dilation analyticity, the proof uses the Combes-Thomas method of proving exponential decay.

3.6 Other $N$-body papers


The paper [9] is an early work on the question of whether an $N$-body Hamiltonian has finitely many or infinitely many bound states. The mechanism for infinitely many bound states discussed here is the presence of longer range intercluster potentials (as opposed to the Efimov effect which may occur for potentials of compact support) and the proof uses trial functions and minimax.

In [96], Simon shows how Cook’s method can be adapted to prove existence of wave operators where the difference is only defined as a quadratic form.

The paper [122] with Klaus is a continuation to the $N$-body setting of the study in [115] of the behaviour of an eigenvalue $e(\lambda)$ as a function of the coupling constant $\lambda$ at the point where the eigenvalue is absorbed into the continuum. The results in in [115] are highly dimension dependent. So, in the $N$-body case, it is important to determine the effective dimension of the bottom of the continuum, since this will give the right asymptotic behaviour of $e(\lambda)$. For example, if the bottom of the continuous spectrum is determined by a two-cluster breakup, the effective dimension is the dimension of the
Laplacian giving the inter-cluster kinetic energy. This is the case treated in this paper.

4 Resonances

[107] The definition of molecular resonance curves by the method of exterior complex scaling, Phys. Lett. 71A (1979), 211-214

A resonant state $\phi$ of a quantum system described by a Schrödinger operator $H$ is a state that behaves almost like a bound state, or eigenvector, but is ultimately unstable. Heuristically, $\phi$ should be an eigenvector with complex eigenvalue $E - i\Gamma/2$ so that $|\langle \phi, e^{-itH} \phi \rangle|^2$ decays like $e^{-\Gamma t}$. But, of course, a self-adjoint operator $H$ cannot have a complex eigenvector, and giving a mathematical definition of resonances was a challenge from the first days of quantum mechanics.

“No satisfactory definition of a resonance can depend only on the structure of a single operator in an abstract Hilbert space.” This remark of Howland was dubbed Howland’s Razor, in reference to Ockham, by Simon in his review article [xv] for quantum chemists. The reason is that it is possible to display two Hamiltonians that are unitarily equivalent, but where one, on physical grounds, should have resonances and the other of which should not. Simon goes on to say that the only “satisfactory” definition of a resonance is as a scattering pole, that is, a pole in the analytic continuation of the scattering amplitude. The extra structure involved is then a reference operator $H_0$ (for a time dependent definition of the scattering operator) or the geometric structure of space.

However, other definitions of resonances are easier to work with, and Simon’s papers on resonances deal mostly with the dilation analyticity def-
inition. In this definition, one starts with the complex dilated Hamiltonian

\[ H(\theta) = -e^{-2\theta} \Delta + V(e^\theta x) \]

defined for \( \theta \) in a strip in the complex plane for suitable \( V \). Aguilar and
Combes (for two-body Hamiltonians) and Balslev and Combes (for \( N \)-body
Hamiltonians) proved that as \( \theta \) moves from the real axis into the com-
plex plane the essential spectrum pivots into the complex plane around the
thresholds. Along the way complex eigenvalues are uncovered which, once
exposed, do not depend on \( \theta \). These complex eigenvalues are the (dilation
analytic) resonances.

Simon’s papers [19] and [20] use the dilation analytic definition of reso-
nance to give a mathematical meaning to perturbation theory for embedded
eigenvalues, and to the Fermi Golden rule. Important physical examples of
this phenomenon are the so-called autoionizing states for helium. Here one
starts with the \( N \)-body Hamiltonian describing a helium atom, but with the
electron-electron interaction turned off. Explicitly,

\[ H_0 = -\Delta_1 - \Delta_2 - 2/|x_1| - 2/|x_2|. \]

Since this Hamiltonian has the form \( h \otimes 1 + 1 \otimes h \) it is easy to compute
the spectrum and one finds there are eigenvalues at \(-n^2 - m^2, n, m \in \mathbb{Z}\)
embedded in the continuous spectrum, which starts at \(-1\). When the
electron-electron interaction, \( \beta/|x_1 - x_2| \) is turned on (that is, \( \beta \) is increased
from zero to some small value) one expects that the embedded eigenvalues
dissolve. The basic idea of these papers is to first perform a complex dilation.
This turns the embedded eigenvalues into isolated discrete eigenvalues, albeit
of a non self-adjoint operator. Nevertheless, regular perturbation can be
applied to these, giving a series expansion for the perturbed eigenvalue.
The leading order for the imaginary part of this series yields Fermi’s Golden
rule for the lifetime of the resonance. It can be used to show that the
eigenvalue really does move into the complex plane to become a resonance.
For the autoionizing states there are additional issues stemming from the
high multiplicity of the eigenvalues, and Simon also addresses these.

Another physically important resonance problem is the hydrogen atom
in a constant electric field, with Hamiltonian given by

\[ H(F) = -\Delta - 1/|x| + Fx_3. \]

When \( F = 0 \) this is the Hamiltonian for the hydrogen atom with negative
eigenvalues accumulating at zero. However, for all non-zero real \( F \) the spec-
trum is purely absolutely continuous and covers the entire real line. Clearly,
this is a very singular perturbation problem. Nevertheless, Herbst succeeded in extending the Balslev-Combes framework to this problem and obtained an expansion $E(F) \sim E_0 + \sum A_{2n} F^{2n}$ for the resonances. The coefficients $A_{2n}$ in this expansion are all real, which implies that the imaginary part $\Re E(F)$ of $E(F)$, which he shows are non-zero, must be very small as $F$ tends to zero. In fact there is a formula proposed by physicists, called the Oppenheimer formula, for the width of the resonance associated with the lowest eigenvalue of $H(0)$. It is given by

$$\Re E(F) \sim \frac{1}{2F} \exp \left( \frac{-1}{6F} \right).$$

The papers [105] (with Harrell) and [156] (with N. Corngold and E. Harrell) deal with this and related situations (including the anharmonic oscillator and the Bender-Wu formula). One of their results is a proof of the Oppenheimer formula. The proofs proceed by reducing the problem to a problem in ODE’s.

Simon’s most recent paper on resonances [276] deals with the one dimensional case. There are two main results in this paper. One is an expansion formula for a Fredholm determinant appearing in my own work on the counting function for resonances. This formula allows Simon to connect my approach with the original approach of Zworski. The second result is a counting result for antibound states.

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