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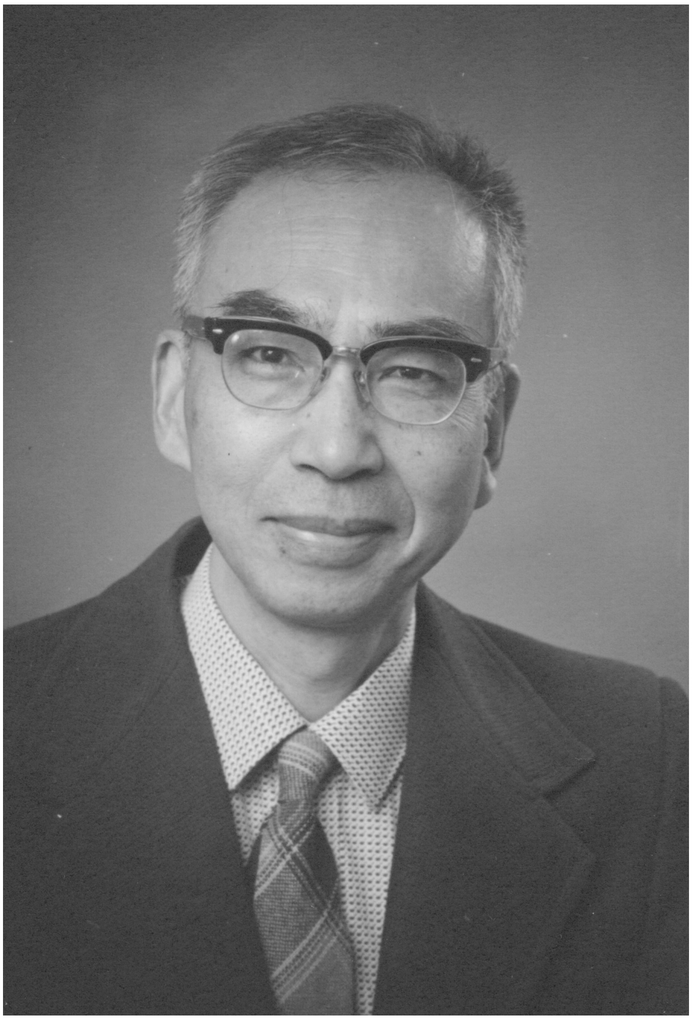

International Association of Mathematical Physics

Tosio Kato's Work on Non–Relativistic Quantum Mechanics: A Brief Report

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1 Introduction

In 2017, we celebrated the 100$^{\text{th}}$ anniversary of the birth of Tosio Kato (August 25, 1917–October 2, 1999), the founding father of the theory of Schrödinger operators. There was a centennial held in Tokyo in his memory and honor in September. I decided to write a review article on his work in nonrelativistic quantum mechanics (NRQM), which, as we'll see, was only part of his opus. I originally guessed it would be about 80 pages but it turned out to be more than 210! It will appear in *Bull. Math. Sci.* Our intrepid newsletter editor asked if I could produce a *Reader's Digest* version for the newsletter and that is what this is. A version of this will appear in *Analysis and Operator Theory – In Honor of Tosio Kato's 100 th Birthday*, a volume edited by Th. M. Rassias and V. Zagrebnov to be published by Springer. Since the longer article has an over 600 item bibliography, I will not provide any detailed references here but refer the reader to the full article. The rest of this introduction will say a little about Kato's life while the next will summarize some major themes in his work. I will then describe in some depth (but less detail than in my *Bull. Math. Sci.* article) five topics that were among the most important of Kato's contributions to NRQM.

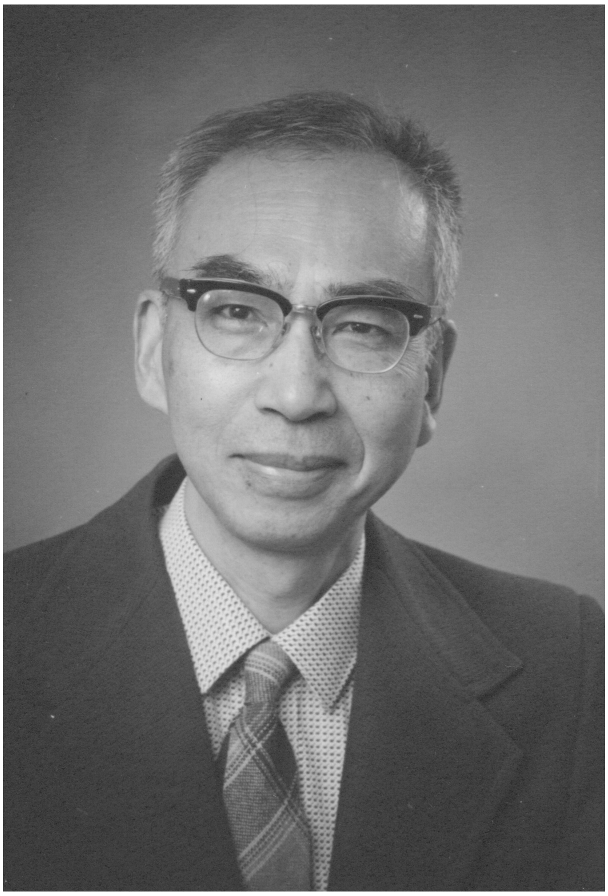
Kato's most significant paper was on self–adjointness of atomic Hamiltonians and was published in 1951 in *Trans. A.M.S.* (See Section 3.) I note that he was 34 when it was published (it was submitted a few years earlier as we'll discuss in Section 3). Before it, his most important work was his thesis, awarded in 1951 and published in 1949-51. One might be surprised at his age when this work was published but not if one understands the impact of the war. Kato got his BS from the University of Tokyo in 1941, a year in which he published two (not mathematical) papers in theoretical physics. But during the war he was evacuated to the countryside. We were at a conference together one evening and Kato described rather harrowing experiences in the camp he was assigned to, especially an evacuation of the camp down a steep wet hill. He contracted tuberculosis in the camp. In his acceptance of the Wiener Prize, Kato says that his work on essential self-adjointness and on perturbation theory were essentially complete by the end of the war.

Kato as a student

In 1946, Kato returned to the University of Tokyo as an Assistant (a position common for students progressing towards their degrees) in physics, was appointed Assistant Professor of

Physics in 1951 and full professor in 1958. I've sometimes wondered what his colleagues in physics made of him. He was perhaps influenced by the distinguished Japanese algebraic geometer, Kunihiko Kodaira (1915-1997) two years his senior and a 1954 Fields medalist. Kodaira got a BS in physics after his BA in mathematics and was given a joint appointment in 1944, so there was clearly some sympathy towards pure mathematics in the physics department.

Beginning in 1954, Kato started visiting the United States. This bland statement masks some drama. In 1954, Kato was invited to visit Berkeley for a year, I presume arranged by F. Wolf. Of course, Kato needed a visa, and it is likely it would have been denied due to his history of TB. Fortunately, just at the time (and only for a period of about a year), the scientific attaché at the US embassy in Tokyo was Otto Laporte (1902-1971) on leave from a Professorship in Physics at the University of Michigan. Charles Dolph (1919-1994), a mathematician at Michigan, learned of the problem and contacted Laporte, who intervened to get Kato a visa. Dolph once told me that he thought his most important contribution to American mathematics was his helping Kato to come to the US. In 1987, in honor of Kato's 70th birthday, there was a special issue of the *Journal of Mathematical Analysis and Applications* and the issue was jointly dedicated to Laporte (passed away in 1971) and Kato and edited by Dolph and Kato's student Jim Howland.



Kato at Berkeley

František Wolf (1904–1989) was important in bringing Kato to Berkeley both as a visitor and later, a regular faculty member. He was a Czech mathematician who had a junior position at Charles University in Prague. Wolf had spent time in Cambridge and did some significant work on trigonometric series under the influence of Littlewood. When the Germans invaded Czechoslovakia in March, 1938, he was able to get an invitation to Mittag–Leffler. He got permission from the Germans for a three week visa but stayed in Sweden! He was then able to get an instructorship at Macalester College in Minnesota. He made what turned out to be a fateful decision in terms of later developments. Because travel across the Atlantic was difficult, he took the trans–Siberian railroad across the Soviet Union and then through Japan and across the Pacific to the US. This was mid–1941 before the US entered the war and made travel across the Pacific difficult.

Wolf stopped in Berkeley to talk with G. C. Evans (known for his work on potential theory) who was then department chair. Evans knew of Wolf's work and offered him a position on the spot!! After the year he promised to Macalester, Wolf returned to Berkeley and worked his way up the ranks. In 1952, Wolf extended Sz.–Nagy's work to the Banach space case. At about the same time Sz.–Nagy himself did similar work and so did Kato. While Wolf and Kato didn't know of each other's work, Wolf learned of Kato's work and that led to his invitation for Kato to visit Berkeley.

During the mid 1950s, Kato spent close to three years visiting US institutions, mainly Berkeley, but also the Courant Institute, American University, the National Bureau of Standards, and Caltech. In 1962, he accepted a Professorship in Mathematics from Berkeley where he spent the rest of his career and remained after his retirement. One should not underestimate the courage it takes for a 45-year-old to move to a very different culture because of a scientific opportunity. That said, I'm told that when he retired and some of his students urged him to live in Japan, he said he liked the weather in Northern California too much to consider it. The reader can consult the Mathematics Genealogy Project for a list of Kato's students (24 listed there, 3 from Tokyo and 21 from Berkeley; the best known are Ikebe and Kuroda from Tokyo and Balslev and Howland from Berkeley). *Notices A.M.S.* **47** (2000), 650–657 is a memorial article with lots of reminiscences.

The pictures here are all from the estate of Mizue Kato, Tosio's wife who passed away in 2011. Her will gave control of the pictures to H. Fujita, M. Ishiguro and S. T. Kuroda. I thank them for permission to use the pictures and H. Okamoto for providing digital versions.

2 Overview

While this review will cover a huge array of work, it is important to realize it is only a fraction, albeit a substantial fraction, of Kato's opus. I'd classify his work into four broad areas, NRQM, non–linear PDE's, linear semigroup theory, and miscellaneous contributions to functional analysis. We will not give references to all this work. The reader can get an (almost) complete bibliography from *MathSciNet*; for papers up to 1987 the dedication of the special issue of *JMAA* on the occasion of Kato's 70^{th} birthday has a bibliography.

Around 1980, one can detect a clear shift in Kato's interest. Before 1980, the bulk of his papers are on NRQM with a sprinkling in the other three areas while after 1980, the bulk are on nonlinear equations with a sprinkling in the other areas including NRQM. Kato's nonlinear work includes looking at the Euler, Navier–Stokes, KdV and nonlinear Schrödinger equations. He was a pioneer in existence results – we note that his famous 1951 paper can be viewed as a result on existence of solutions for the time-dependent linear Schrödinger equation! It almost seems that when NRQM became too crowded with others drawn by his work, he moved to a new area which took some time to become popular.

The basic results on generators of semigroups on Banach spaces date back to the early 1950s, going under the name Feller-Miyadera-Phillips and Hille-Yosida theorems (with a later 1961 paper of Lumer–Phillips). A basic book with references to this work is by Pazy. This is a subject that Kato returned to often, especially in the 1960s. Pazy lists 19 papers by Kato on the subject. Perhaps the most important of these results are the Trotter–Kato theorems and the definition of fractional powers for generators of (not necessarily self–adjoint) contraction semigroups.

Given this work on the theory on a Banach space, it is interesting to see a quote that his friend Cordes attributes to Kato: "There is no decent Banach space, except Hilbert space." It is likely Kato had in mind the spectral theorem and the theory of quadratic forms of operators, a subject where he made important contributions, especially the monotone convergence theorems for forms.

The fourth area is a catchall for a variety of results that don't fit into the other bins. Among these results is an improvement of the celebrated Calderón-Vaillancourt bounds on pseudo-differential operators. Also, Kato proved that the absolute value for operators is not Lipschitz continuous even restricted to the self–adjoint operators, but for any pair of bounded, even non–self–adjoint, operators, one has that

$$\| |S| - |T| \| \leq \frac{2}{\pi} \|S - T\| \left(2 + \log \frac{\|S\| + \|T\|}{\|S - T\|} \right). \tag{1}$$

He was also a key player in variants of Loewner's result that the square root is a monotone function on positive operators on a Hilbert space, a result rediscovered by Heinz. It and its variants have been called the Heinz–Loewner or Heinz–Kato inequality. Kato returned several times to this subject, most notably finding a version of the Heinz–Loewner inequality (with an extra constant depending on s) for maximal accretive operators on a Hilbert space.

One can get a feel for Kato's impact by considering the number of theorems, theories and inequalities with his name on them. Here are some: Kato's theorem (which usually refers to his result on self–adjointness of atomic Hamiltonians), the Kato–Rellich theorem (which Rellich had first), the Kato-Rosenblum theorem and the Kato–Birman theory (where Kato had the most significant results, although, as we'll see, Rosenblum should get more credit than he does), the Kato projection lemma and Kato dynamics (used in the adiabatic theorem), the Putnam–Kato theorem, the Trotter–Kato theorem, the Kato cusp condition, Kato smoothness theory, the Kato class of potentials and Kato–Kuroda eigenfunction expansions. To me *Kato's inequality* refers to the self–adjointness technique discussed in Section 5, but the term has also been used for the Hardy-like inequality with best constant for r^{-1} in three dimensions, for a result on hyponormal operators that follows from Kato smoothness theory (there is a book with a section called "Kato's inequality" on it), and for the above-mentioned variant of the Heinz–Loewner inequality for maximal accretive operators. There are also Heinz–Kato, Ponce–Kato and Kato–Temple inequalities. Erhard Seiler and I proved that if $f, g \in L^p(\mathbb{R}^\nu)$, $p \geq 2$, then $f(X)g(-i\nabla)$ is in the trace ideal $\mathcal{I}_p$. At the time, Kato and I had correspondence about the issue and about some results for $p < 2$. In Reed–Simon Volume 3, we mentioned that Kato had this result independently. Although Kato never published anything on the subject, in recent times, it has come to be called the Kato–Seiler–Simon inequality.

Of course, when discussing the impact of Kato's work, one must emphasize the importance of his book *Perturbation Theory for Linear Operators*, which has been a bible for several generations of mathematicians. One of its virtues is its comprehensive nature. Percy Deift told me that Peter Lax told him that Friedrichs remarked on the book: "Oh, its easy to write a book when you put everything in it!"

We will not discuss every piece of work that Kato did in NRQM – for example, he wrote several papers on variational bounds on scattering phase shifts whose lasting impact was limited.

Kato was a key figure in eigenvalue perturbation theory the subject of his thesis which was codified in his book. For the regular case, the basic results were by Rellich and later Sz.–Nagy but refined by Kato. He was the pioneer in the asymptotic case, originally using his extension of Temple's inequality but later operator techniques. The full version of this article has 5 sections on eigenvalue perturbation theory but I've chosen other areas for this shorter version.

Ever since the work of von Neumann about 1930, it has been clear that self–adjointness of quantum Hamiltonians is crucial. In this regard, Kato has been a, indeed *the*, key figure. His contributions include:

1. Self–adjointness of atomic Hamiltonians. (See Section 3.)
2. His work with Ikebe on $V(x) > -cx^2 - d$, an area where Weinholtz was the pioneer.
3. Kato's inequality, including his theorem that if $V \in L^2_{loc}(\mathbb{R}^\nu)$ and $V \geq 0$, then $-\Delta + V$ is essentially self–adjoint on $C_0^\infty(\mathbb{R}^\nu)$. (See Section 5.)
4. He was a pioneer on the use of quadratic forms, including his work on perturbations (the KLMN theorem) and monotone convergence for forms.

Scattering and spectral theory formed a major thread in Kato's work from 1955 to 1980, so much so that when he gave a plenary talk at the 1970 ICM, it was on this subject. One can identify four areas:

1. Trace-class scattering. (See Section 6.)
2. Kato Smoothness. (See Section 7.)
3. Eigenfunction expansions (Kato–Kuroda theory).
4. Jensen–Kato on low energy and large times.

Three isolated but important contributions:

1. His 1948 paper on the adiabatic theorem. (See Section 4.)
2. His ultimate Trotter product formula: if A and B are arbitrary positive self–adjoint operators, if C is the self–adjoint form sum on $\overline{Q(A) \cap Q(B)} \equiv \mathcal{K}$, and if P is the projection onto $\mathcal{K}$, then
$$\mathrm{s}-\lim_{n\to\infty} \left[e^{-tA/n} e^{-tB/n}\right]^n = e^{-tC} P.$$
3. His 1957 paper on properties of eigenfunctions of general Schrödinger operators and especially of Coulomb Hamiltonians. For the Coulomb case, he proved that eigenfunctions were globally Lipschitz but not generally C^1; instead he found the celebrated Kato cusp condition – at coincidence points, radial averages have well defined jumps (like $e^{-|x|}$ for the hydrogen ground state). Trial function calculations for atoms and molecules use the Kato cusp condition making this paper his most quoted one on Google Scholar (with over 1,700 citations!)

3 Foundations of Atomic Physics

Ever since von Neumann's work around 1930, it has been clear that a fundamental mathematical problem in quantum theory, indeed the fundamental question in atomic physics, is the self–adjointness of atomic Hamiltonians, so Kato's 1951 paper is a pathbreaking contribution of great significance. He considered N–body Hamiltonians on $L^2(\mathbb{R}^{\nu N})$ formally written as

$$H = -\sum_{j=1}^{N} \frac{1}{2m_j}\Delta_j + \sum_{i<j} V_{ij}(x_i - x_j), \tag{2}$$

where $x \in \mathbb{R}^{\nu N}$ is written $\boldsymbol{x} = (x_1, \dots, x_N)$ with $x_j \in \mathbb{R}^\nu$, Δ_j is the ν–dimensional Laplacian in x_j, and each V_{ij} is a real valued function on $\mathbb{R}^\nu$. In 1951, Kato considered only the physically relevant case $\nu = 3$.

If there are $N + k$ particles in the limit where the masses of particles $N + 1, \dots, N + k$ are infinite, one considers an operator like H but adds terms

$$\sum_{j=1}^{N} V_j(x_j), \qquad V_j(x) = \sum_{\ell=N+1}^{N+k} V_{j\ell}(x - x_\ell), \tag{3}$$

where $x_{N+1}, \dots, x_{N+k}$ are fixed points in $\mathbb{R}^\nu$.

More generally, one wants to consider (as Kato did) Hamiltonians with the center of mass removed. We note that the self–adjointness results on the Hamiltonians of the form (2) easily imply results on Hamiltonians (on $L^2(\mathbb{R}^{(N-1)\nu})$) with the center of mass motion removed. Of special interest is the Hamiltonian of the form (3) with $N = 1$, i.e.

$$H = -\Delta + W(x) \tag{4}$$

on $L^2(\mathbb{R}^\nu)$ which we'll call the *reduced two-body Hamiltonian* (since, except for a factor of $(2\mu)^{-1}$ in front of $-\Delta$, it is the two-body Hamiltonian with the center of mass removed).

Kato's big 1951 result was (I will use "esa" as shorthand for essentially self–adjoint and "esaν" for esa on $C_0^\infty(\mathbb{R}^\nu)$):

Theorem 3.1 (Kato's Theorem, First Form)**.** *Let $\nu = 3$. Let each V_{ij} in (2) lie in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then the Hamiltonian (2) is self–adjoint on $D(H) = D(-\Delta)$ and esa–$(3N)$.*

Remarks. *1. The same result holds with the terms in (3) added, so long as each V_j lies in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.*

2. Kato didn't assume that $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, but rather the stronger hypothesis that for some $R < \infty$, one has that $\int_{|x|<R} |V(x)|^2 d^3x < \infty$ and $\sup_{|x|\geq R} |V(x)| < \infty$, but his proof extends to $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.

3. Kato didn't state that $C_0^\infty(\mathbb{R}^{3N})$ is a core, but rather that ψ's of the form $P(x)e^{-\frac{1}{2}x^2}$ with P a polynomial in the coordinates of x form a core (He included the $\frac{1}{2}$ so the set was invariant under the Fourier transform.) His result is now usually stated in terms of C_0^∞.

If $v(x) = 1/|x|$ on $\mathbb{R}^3$, then $v \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, so Theorem 3.1 has an important corollary, which includes the Hamiltonians of atoms and molecules:

Theorem 3.2 (Kato's Theorem, Second Form)**.** *The Hamiltonian, H, of* (2) *with $\nu = 3$ and each*

$$V_{ij}(x) = \frac{z_{ij}}{|x|}, \tag{5}$$

and the Hamiltonian with terms of the form (3)*, where*

$$V_j(x) = \sum_{\ell=N+1}^{N+k} \frac{z_{j\ell}}{|x - x_\ell|}, \tag{6}$$

are self–adjoint on $D(-\Delta)$ and esa–$3N$.

Remark 3.3. *This result ensures that the time-dependent Schrödinger equation $\dot{\psi}_t = -iH\psi_t$ has solutions (since self–adjointness means that e^{-itH} exists as a unitary operator). The analogous problem for Coulomb Newton's equation (i.e. solvability for a.e. initial condition) is open for $N \geq 5$!*

As Kato remarks in his Wiener prize acceptance, "The proof turned out to be rather easy." It has three steps:

(1) The Kato–Rellich theorem, which reduces the proof to showing that each V_{ij} is relatively bounded for Laplacian on $\mathbb{R}^3$ with relative bound 0.

(2) A proof that any function in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, as an operator on $L^2(\mathbb{R}^3)$, is $-\Delta$–bounded with relative bound 0. This relies on the simple Sobolev estimate that on $\mathbb{R}^3$ any function in $D(-\Delta)$ is bounded. Alternatively, for the atomic case, Hardy's inequality (that $(4r^2)^{-1} \leq -\Delta$) implies this fact.

(3) A piece of simple kinematics that says that the two-body estimate in Step 2 extends to one for $v_{ij}(x_i - x_j)$ as an operator on $L^2(\mathbb{R}^{3N})$.

Kato states in the paper that he had found the results by 1944. Kato originally submitted the paper to *Physical Review*. *Physical Review* transferred the manuscript to the *Transactions of the AMS*, where it eventually appeared. They had trouble finding a referee and, in the process, the manuscript was lost (a serious problem in pre-Xerox days!). Eventually, von Neumann got involved and helped get the paper accepted. I've always thought that given how important he knew the paper was, von Neumann should have suggested *Annals of Mathematics* and used his influence to get it published there. The receipt date of October 15, 1948 on the version published in the *Transactions* shows a long lag compared to the other papers in the same issue of the Transactions which have receipt dates of Dec., 1949 through June, 1950. Recently, after Kato's widow died and left his papers to some mathematicians (see the end of Section 1), some fascinating correspondence of Kato with Kemble and von Neumann came to light. There are plans by Kato's students to publish an edited version of these letters.

It is a puzzle why it took so long for this theorem to be found. One factor may have been von Neumann's attitude. Bargmann told me of a conversation several young mathematicians had with von Neumann around 1948 in which von Neumann told them that self–adjointness for atomic Hamiltonians was an impossibly hard problem, and that even for the hydrogen atom the problem was difficult and open. This is a little strange since, using spherical symmetry, hydrogen can be reduced to a direct sum of one-dimensional problems. For such ODEs, there is a powerful limit-point/limit-circle method named after Weyl and Titchmarsh (although it was Stone, in his 1932 book, who first made it explicit). Using this, it is easy to see (there is one subtlety for $\ell = 0$, since the operator then is limit-point at 0) that the hydrogen Hamiltonian is self–adjoint, and this appears at least as early as Rellich in 1944. Of course, this method doesn't work for multielectron atoms. In any event, it is possible that von Neumann's attitude may have discouraged some from working on the problem.

Still it is surprising that neither Friedrichs nor Rellich found this result. Rellich used Hardy's inequality in his perturbation theory papers in a closely related context. Namely he used Hardy's inequality to show that $r^{-1} \leq 4\epsilon(-\Delta) + \frac{1}{4}\epsilon^{-1}$ to note the semiboundedness of the hydrogen Hamiltonian. Since Rellich certainly knew the Kato–Rellich theorem, it appears that he knew steps 1 and 2.

In a sense it is pointless to speculate why Rellich didn't find Theorem 3.2, but it is difficult to resist. It is possible that he never considered the problem of esa of atomic Hamiltonians, settling for a presumption that using the Friedrichs extension suffices (as Kato suggests in his Wiener prize acceptance) but I think that unlikely. It is possible that he thought about the problem but dismissed it as too difficult and never thought hard about it. Perhaps the most likely explanation involves Step 3: once you understand it, it is trivial, but until you conceive that it might be true, it might elude you.

Later authors considered the analogues for dimension $\nu \neq 3$ – Stummel was a big hero here. For our discussion in Section 5, we'll need the following: We call p *ν–canonical* if $p = 2$ for $\nu \leq 3$, $p > 2$ if $\nu = 4$ and $p = \nu/2$ if $\nu \geq 5$. The optimal L^p extension of Theorem 3.1 is:

Theorem 3.4. *Let p be ν–canonical. Then $V \in L^p(\mathbb{R}^\nu) + L^\infty(\mathbb{R}^\nu)$ is $-\Delta$–bounded with relative bound zero. If $\nu \geq 5$, then $V \in L^p_w(\mathbb{R}^\nu) + L^\infty(\mathbb{R}^\nu)$ is $-\Delta$–bounded on $L^2(\mathbb{R}^\nu)$.*

It is known that this is optimal since when $\nu > 5$ limit-point/limit-circle methods show that for C sufficiently large $-\Delta - Cr^{-2}$ is not essentially self–adjoint on C_0^∞ and r^{-2} lies in all $L^p + L^\infty$ with $p < \nu/2$. The longer paper includes further discussion of these higher-dimensional analogues and also discusses Kato's application in his 1951 paper to the Coulomb Dirac Hamiltonian.

4 The Adiabatic Theorem

In 1950 Kato published a paper in a physics journal (noted as based on a presentation in 1948) on the quantum adiabatic theorem. It is his only paper on the subject but has strongly impacted virtually all the huge literature on the subject and related subjects ever since. (There are more Google Scholar citations of this paper than of the one on self–adjointness of atomic Hamiltonians.) We will begin by describing his theorem and its proof, which introduced what he called *adiabatic dynamics* and I'll call the *Kato dynamics*. We'll see that the Kato dynamics defines a notion of parallel transport on the natural vector bundle over the manifold of all k–dimensional subspaces of a Hilbert space $\mathcal{H}$, and so a connection. This connection is called the Berry connection and its holonomy is the Berry phase (when $k = 1$). All this Berry stuff was certainly not even hinted at in Kato's work, but it is implicit in the framework. Then I'll say something about the history before Kato.

The adiabatic theorem considers a family of time-dependent Hamiltonians, $H(s)$, $0 \le s \le 1$ and imagines changing them slowly, i.e. looking at $H(s/T)$, $0 \le s \le T$ for T very large. Thus, we look for $\tilde{U}_T(s)$ solving

$$\frac{d}{ds}\tilde{U}_T(s) = -iH(s/T)\tilde{U}_T(s),\ 0 \le s \le T; \qquad \tilde{U}_T(0) = \mathbf{1}. \tag{7}$$

Letting $U_T(s) = \tilde{U}_T(sT)$, $0 \le s \le 1$, we see that $U_T(s)$, $0 \le s \le 1$ solves

$$\frac{d}{ds}U_T(s) = -iTH(s)U_T(s),\ 0 \le s \le 1; \qquad U_T(0) = \mathbf{1}. \tag{8}$$

Here is Kato's adiabatic theorem

Theorem 4.1 (Kato). *Let $H(s)$ be a C^2 family of bounded self–adjoint operators on a (complex, separable) Hilbert space, $\mathcal{H}$. Suppose there is a C^2 function, $\lambda(s)$, so that for all s, $\lambda(s)$ is an isolated point in the spectrum of $H(s)$ and so that*

$$\alpha \equiv \inf_{0\le s\le 1} \text{dist}(\lambda(s), \sigma(H(s)) \setminus \{\lambda(s)\}) > 0. \tag{9}$$

Let $P(s)$ be the projection onto the eigenspace for $\lambda(s)$ as an eigenvalue of $H(s)$. Then

$$\lim_{T\to\infty} (1 - P(s))U_T(s)P(0) = 0 \tag{10}$$

uniformly in s in $[0, 1]$.

Remarks. *1. Thus, if $\varphi_0 \in \text{ran}\, P(0)$, this says that when T is large, $U_T(s)\varphi_0$ is close to lying in $\text{ran}\, P(s)$. That is, as $T \to \infty$, the solution gets very close to the "curve" $\{\text{ran}\, P(s)\}_{0\le s\le 1}$.*

2. If there is an eigenvalue of constant multiplicity near $\lambda(0)$ for s small, it follows from the contour representation of $P(s)$ that $P(s)$ and $\lambda(s)$ are C^2.

3. Kato made no explicit assumptions on regularity in s saying "Our proof given below is rather formal and not faultless from the mathematical point of view. Of course it is possible to retain mathematical rigour by detailed argument based on clearly defined assumptions, but it would take us too far into unnecessary complication and obscure the essentials of the problem." It is hard to imagine the Kato of 1960 using such language! In any event, the proof requires that $P(s)$ be C^2.

4. As we'll see, the size estimate for (10) is $O(1/T)$.

Kato's wonderful realization is that there is an explicit dynamics, $W(s)$ for which (10) is exact, i.e.

$$(1 - P(s))W(s)P(0) = 0. \tag{11}$$

He not only constructs it but proves the theorem by showing that (this formula only holds in case $\lambda(s) \equiv 0$; see (16) below):

$$\lim_{T\to\infty} [U_T(s) - W(s)]P(0) = 0. \tag{12}$$

The $W(s)$ that Kato constructs, he called the *adiabatic dynamics*. It is sometimes called Kato's adiabatic dynamics. We call it the *Kato dynamics*. Here is the basic result:

Theorem 4.2 (Kato dynamics)**.** *Let $W(s)$ solve*

$$\frac{d}{ds}W(s) = iA(s)W(s), 0 \le s \le 1; \qquad W(0) = \mathbf{1}; \tag{13}$$

$$iA(s) \equiv [P'(s), P(s)]. \tag{14}$$

Then $W(s)$ is unitary and obeys

$$W(s)P(0)W(s)^{-1} = P(s). \tag{15}$$

The proof is not hard (see the longer paper for details). Using $P(s)^2 = P(s)$ and its derivative, one shows that $W(s)^{-1}P(s)W(s)$ has zero derivative.

The proof of Theorem 4.1 depends on proving that

$$\|U_T(s)P(0) - e^{-iT\int_0^s \lambda(s)\,ds}W(s)P(0)\| = \mathrm{O}(1/T). \tag{16}$$

(16) says a lot more than (10). (10) says that as $T \to \infty$, $U_T(s)$ maps ran $P(0)$ to ran $P(s)$. (10) actually tells you what the precise limiting map is! One fancy-pants way of describing this is as follows. Fix $k \ge 1$ in $\mathbb{Z}$. Let $\mathcal{M}$ be the manifold of all k–dimensional subspaces of some Hilbert space, $\mathcal{H}$. We want $\dim(\mathcal{H}) \ge k$, but it could be finite. Or $\mathcal{M}$ might be a smooth submanifold of the set of all such subspaces. For each $\omega \in \mathcal{M}$, we have the projection $P(\omega)$. There is a natural vector bundle of k–dimensional spaces over $\mathcal{M}$, namely, we associate to $\omega \in \mathcal{M}$, the space ran $P(\omega)$. If $k = 1$, we get a complex line bundle.

The Kato dynamics $W(s)$ tells you how to "parallel transport" a vector $v \in$ ran $P(\gamma(0))$ along a curve $\gamma(s) : 0 \le s \le 1$ in $\mathcal{M}$. In the language of differential geometry, it defines a connection, and such a connection has a holonomy and a curvature. In less fancy terms, consider the case $k = 1$. Suppose γ is a closed curve. Then $W(1)$ is a unitary map of ran $P(0)$ to itself, so multiplication by $e^{i\Gamma_B(\gamma)}$. Returning to U_T, it says that the phase change over a closed curve isn't what one might naively expect, namely $\exp(-i\int_0^T \lambda(s/T)\,ds) = \exp(-iT\int_0^1 \lambda(s)\,ds)$. There is an additional term, $\exp(i\Gamma_B)$. This is the *Berry phase* discovered by Berry in 1983 (it was discovered in 1956 by Pancharatnam, but then forgotten). I realized that this was just the holonomy of a natural bundle connection and that, moreover, this bundle and connection is precisely the one whose Chern integers are the TKN^2 integers of Thouless et al. (as discussed by Avron–Seiler–Simon). Thouless shared in a recent Physics Nobel Prize in part for the discovery of the TKN^2 integers. The holonomy, i.e. Berry's phase, is an integral of the Kato connection $[P, dP]$. As usual, this line integral over a closed curve is the integral of its differential $[dP, dP]$ over a bounding surface. This quantity is the curvature of the bundle and has come to be called the *Berry curvature* (even though Berry did not use the differential geometric language). Naively $[dP, dP]$ would seem to be zero but it is shorthand for the two–form

$$\sum_{i \ne j}\left[\frac{\partial P}{\partial s_i}, \frac{\partial P}{\partial s_j}\right] ds_i \wedge ds_j. \tag{17}$$

This formula of Avron–Seiler–Simon for the Berry curvature is a direct descendant of formulae in Kato's paper, although, of course, he did not consider the questions that lead to Berry's phase.

Finally, a short excursion into the history of adiabatic theorems. “Adiabatic” first entered into physics as a term in thermodynamics meaning a process with no heat exchange. In 1916, Ehrenfest discussed the “adiabatic principle” in classical mechanics. The basic example is the realization (earlier than Ehrenfest) that while the energy of a harmonic oscillator is not conserved under time-dependent change of the underlying parameters, the action (energy divided by frequency) is fixed in the limit that the parameters are slowly changed. (The reader should figure out what Kato’s adiabatic theorem says about a harmonic oscillator with slowly varying frequency.) Interestingly enough, many adiabatic processes in the thermodynamic sense are quite rapid, so the Ehrenfest use has, at best, a very weak connection to the initial meaning of the term!

Ehrenfest used these ideas by asserting that in old quantum theory, the natural quantum numbers were precisely these adiabatic invariants. Once new quantum mechanics was discovered, Born and Fock in 1928 discussed what they called the quantum adiabatic theorem, essentially Theorem 4.1 for simple eigenvalues with a complete set of (normalizable) eigenfunctions. It was 20 years before Kato found his wonderful extension (and then more than 30 years before Berry made the next breakthrough). The longer article has a discussion on the considerable further mathematical literature of the quantum adiabatic theorem.

5 Kato’s Inequality

This section will discuss a self–adjointness method that appeared in a 1972 paper of Kato based on a remarkable distributional inequality. Its consequences are a subject to which Kato returned often with at least seven additional papers. It is also his work that most intersected my own – I motivated his initial paper and it, in turn, motivated several of my later papers.

To explain the background, recall that in Section 3 we defined p to be ν–canonical (ν is dimension) if $p = 2$ for $\nu \le 3$, $p > 2$ for $\nu = 4$, and $p = \nu/2$ for $\nu \ge 5$. For now, we focus on $\nu \ge 5$ so that $p = \nu/2$. As we saw, if $V \in L^p(\mathbb{R}^\nu) + L^\infty(\mathbb{R}^\nu)$, then $-\Delta + V$ is esa–ν. The example $V(x) = -C|x|^{-2}$ for C sufficiently large shows that $p = \nu/2$ is sharp. That is, for any $2 \le q \le \nu/2$, there is a $V \in L^q(\mathbb{R}^\nu) + L^\infty(\mathbb{R}^\nu)$, so that $-\Delta + V$ is defined on but not esa on $C_0^\infty(\mathbb{R}^\nu)$.

In these counterexamples, though, V is negative. It was known since the late 1950s that while the negative part of V requires some global hypothesis for esa–ν, the positive part does not (e.g. $-\Delta - x^4$ is not esa–ν while $-\Delta + x^4$ is esa–ν). But when I started looking at these issues around 1970, there was presumption that for local singularities, there was no difference between the positive and negative parts. In retrospect, this shouldn’t have been the belief! After all, limit-point/limit-circle methods show that if $V(x) = |x|^{-\alpha}$ with $\alpha < \nu/2$ (to make $V \in L^2_{loc}$ so that $-\Delta + V$ is defined on $C_0^\infty(\mathbb{R}^\nu)$) then $-\Delta + V$ is esa–ν although, if $\alpha > 2$, $-\Delta - V$ is not. (Limit-point/limit-circle methods apply for $-\Delta + V$ for any α if we look at $C_0^\infty(\mathbb{R}^\nu \setminus \{0\})$ but then only when $\alpha < \nu/2$ we can extend the conclusion to $C_0^\infty(\mathbb{R}^\nu)$.) This example shows that the conventional wisdom was faulty but people didn’t think about separate local conditions on

$$V_+(x) \equiv \max(V(x), 0); \qquad V_-(x) = \max(-V(x), 0). \tag{18}$$

Kato’s result shattered the then conventional wisdom:

Theorem 5.1 (Kato)**.** *If $V \geq 0$ and $V \in L^2_{loc}(\mathbb{R}^\nu)$, then $-\Delta + V$ is esa–ν.*

Kato's result was actually a conjecture that I made on the basis of a slightly weaker result that I had proven:

Theorem 5.2 (Simon)**.** *If $V \geq 0$ and $V \in L^2(\mathbb{R}^\nu, e^{-cx^2}\, d^\nu x)$ for some $c > 0$, then $-\Delta + V$ is esa–ν.*

Of course this covers pretty wild growth at infinity but Theorem 5.1 is the definitive result since one needs that $V \in L^2_{loc}(\mathbb{R}^\nu)$ for $-\Delta + V$ to be defined on all functions in $C_0^\infty(\mathbb{R}^\nu)$. I found Theorem 5.2 because I was also working at the time in constructive quantum field theory which was then focused on the simplest interacting field models φ_2^4 and $P(\varphi)_2$. (The subscript 2 means two space–time dimensions.) I was able to use results in the theory of hypercontractive semigroups that seemed very different from what Kato used, although connections were later found as well as a semigroup proof of Theorem 5.1. In my preprint proving Theorem 5.2, I conjectured Theorem 5.1, and Kato's response was sent within a few weeks of my mailing him my preprint. The longer paper describes both my proof and these later developements but I want to focus here on Kato's arguments. Kato proved:

Theorem 5.3 (Kato's inequality)**.** *Let $u \in L^1_{loc}(\mathbb{R}^\nu)$ be such that its distributional Laplacian, Δu is also in $L^1_{loc}(\mathbb{R}^\nu)$. Define*

$$\operatorname{sgn}(u)(x) = \begin{cases} \overline{u(x)}/|u(x)|, & \text{if } u(x) \neq 0 \\ 0, & \text{if } u(x) = 0 \end{cases} \tag{19}$$

(so $u \operatorname{sgn}(u) = |u|$). Then as distributions

$$\Delta|u| \geq \operatorname{Re}\left[\operatorname{sgn}(u)\Delta u\right]. \tag{20}$$

Remarks. *1. What we call $\operatorname{sgn}(u)$, Kato calls $\operatorname{sgn}(\bar{u})$.*

2. We should pause to emphasize what a surprise this was. Kato was a long established master of operator theory. He was 55 years old. He simply pulled a distributional inequality out of his hat. It is true, like other analysts, that he'd been introduced to distributional ideas in the study of PDEs, but no one had ever used them in this way. Truly a remarkable discovery.

The proof is not hard. By replacing u by $u * h_n$ with h_n a smooth approximate identity and taking limits (using $\operatorname{sgn}(u * h_n)(x) \to \operatorname{sgn}(u)(x)$ for a.e. x and using a suitable dominated convergence theorem), we can suppose that u is a C^∞ function. In that case, for $\epsilon > 0$, let $u_\epsilon = (\bar{u}u + \epsilon^2)^{1/2}$. From $u_\epsilon^2 = \bar{u}u + \epsilon^2$, we get that

$$2u_\epsilon \vec{\nabla} u_\epsilon = 2\operatorname{Re}(\bar{u}\vec{\nabla} u), \tag{21}$$

which implies (since $|\bar{u}| \leq u_\epsilon$) that

$$|\vec{\nabla} u_\epsilon| \leq |\vec{\nabla} u|. \tag{22}$$

Applying $\frac{1}{2}\overrightarrow{\nabla}\cdot$ to (21), we get that

$$u_\epsilon \Delta u_\epsilon + |\overrightarrow{\nabla} u_\epsilon|^2 = \text{Re}(\bar{u}\Delta(u)) + |\overrightarrow{\nabla} u|^2. \tag{23}$$

Using (22) and letting $\text{sgn}_\epsilon(u) = \bar{u}/u_\epsilon$, we get that

$$\Delta u_\epsilon \geq \text{Re}(\text{sgn}_\epsilon(u)\Delta u). \tag{24}$$

Taking $\epsilon \downarrow 0$ yields (20).

Once we have (20), here is Kato's proof of Theorem 5.1. Consider T, the operator closure of $-\Delta + V$ on $C_0^\infty(\mathbb{R}^\nu)$. $T \geq 0$, so, by a simple argument, it suffices to show that $\text{ran}(T + \mathbf{1}) = \mathcal{H}$ or, equivalently, that $T^* u = -u \Rightarrow u = 0$. So suppose that $u \in L^2(\mathbb{R}^\nu)$ and that

$$T^* u = -u. \tag{25}$$

Since T^* is defined via distributions, (20) implies that

$$\Delta u = (V + 1)u. \tag{26}$$

Since u and $V + 1$ are both in L^2_{loc}, we conclude that $\Delta u \in L^1_{loc}$, so by Kato's inequality,

$$\Delta|u| \geq (\text{sgn}(u))(V + 1)u = |u|(V + 1) \geq |u|. \tag{27}$$

Convolution with non–negative functions preserves positivity of distributions, so for any non-negative $h \in C_0^\infty(\mathbb{R}^\nu)$, we have that

$$\Delta(h * |u|) = h * \Delta|u| \geq h * |u|. \tag{28}$$

Since $u \in L^2$, $h * |u|$ is a C^∞ function with classical Laplacian in L^2, so $h * |u| \in D(-\Delta)$. $(-\Delta + 1)^{-1}$ has a positive integral kernel, so (28)$\Rightarrow (-\Delta + 1)(h * |u|) \leq 0 \Rightarrow h * |u| \leq 0 \Rightarrow h * |u| = 0$. Taking h_n to be an approximate identity, we have that $h_n * u \to u$ in L^2, so $u = 0$, completing the proof.

At first sight, Kato's proof seems to have nothing to do with the semigroup ideas used in the proof of Theorem 5.2 and the proof of Theorem 5.1 that I found using semigroup methods. But in trying to understand Kato's work, I found the following abstract result:

Theorem 5.4 (Simon). *Let A be a positive self–adjoint operator on $L^2(M, d\mu)$ for a σ–finite, separable measure space $(M, \Sigma, d\mu)$. Then the following are equivalent:*

(a) (e^{-tA} is positivity preserving)

$$\forall u \in L^2,\ u \geq 0, t \geq 0 \Rightarrow e^{-tA}u \geq 0.$$

(b) (Beurling–Deny criterion) $u \in Q(A) \Rightarrow |u| \in Q(A)$ and

$$q_A(|u|) \leq q_A(u). \tag{29}$$

(c) (Abstract Kato Inequality) $u \in D(A) \Rightarrow |u| \in Q(A)$ and for all $\varphi \in Q(A)$ with $\varphi \geq 0$, one has that

$$\left\langle A^{1/2}\varphi, A^{1/2}|u|\right\rangle \geq \text{Re}\left\langle \varphi, \text{sgn}(u)Au\right\rangle. \tag{30}$$

In his original paper, Kato proved more than (20). He showed that

$$\Delta|u| \geq \mathrm{Re}\left[\mathrm{sgn}(u)(\overrightarrow{\nabla} - i\overrightarrow{a})^2 u\right]. \tag{31}$$

In his initial paper, he required that $\overrightarrow{a}$ to be $C^1(\mathbb{R}^\nu)$ and he then followed his arguments to get Theorem 5.1 with $-\Delta+V$ replaced by $-(\nabla-ia)^2+V$ when $a \in C^1(\mathbb{R}^\nu), V \in L^2_{loc}(\mathbb{R}^\nu), V \geq 0$. But there was a more important consequence of (31) than a self–adjointness result. I noted that (31) implies, by approximating $|u|$ by positive $\varphi \in C_0^\infty(\mathbb{R}^\nu)$, that

$$\langle |u|, \Delta|u| \rangle \geq \left\langle u, D^2 u \right\rangle$$

where $D = \overrightarrow{\nabla} - i\overrightarrow{a}$, which implies that

$$\left\langle u, (-D^2 + V)u \right\rangle \geq \langle |u|, (-\Delta + V)|u| \rangle. \tag{32}$$

This, in turn, implies that turning on any, even non–constant, magnetic field always increases the ground state energy (for spinless bosons), something I called *universal diamagnetism*.

If one thinks of this as a zero-temperature result, it is natural to expect a finite-temperature result. (That is, for, say, finite matrices, one has that $\lim_{\beta\to\infty} -\beta^{-1}\mathrm{Tr}(e^{-\beta A}) = \inf \sigma(A)$ which in statistical mechanical terms is saying that as the temperature goes to zero, the free energy approaches a ground state energy.)

$$\mathrm{Tr}(e^{-tH(a,V)}) \leq \mathrm{Tr}(e^{-tH(a=0,V)}), \tag{33}$$

where

$$H(a,V) = -(\nabla - ia)^2 + V. \tag{34}$$

This suggested to me the inequality

$$|e^{-tH(a,V)}\varphi| \leq e^{-tH(a=0,V)}|\varphi|. \tag{35}$$

I mentioned this conjecture at a brown bag lunch seminar when I was in Princeton. Ed Nelson remarked that formally, it followed from the Feynman–Kac–Ito formula for semigroups in magnetic fields which says that adding a magnetic field with gauge $\overrightarrow{a}$ adds a factor $\exp(i\int \overrightarrow{a}(\omega(s))\cdot d\omega)$ to the Feynman–Kac formula. (The integral is an Ito stochastic integral.) Eq. (35) is immediate from $|\exp(i\int \overrightarrow{a}(\omega(s))\cdot d\omega)| = 1$ and the positivity of the rest of the Feynman–Kac integrand. Some have called (35) the Nelson–Simon inequality but the name I gave it, namely *diamagnetic inequality*, has stuck.

The issue with Nelson's proof is that, at the time, the Feynman–Kac–Ito formula was only known for smooth a's. One can obtain the Feynman–Kac–Ito formula for more general a's by independently proving a suitable core result. After sucessive improvements by me and then Kato, I proved that

Theorem 5.5 (Simon)**.** *Equation* (35) *holds for* $V \geq 0$*,* $V \in L^1_{loc}(\mathbb{R}^\nu)$ *and* $\overrightarrow{a} \in L^2_{loc}$*.*

The optimal self-adjointness result ($V \geq 0, V \in L^2_{loc}, a \in L^4_{loc}, \operatorname{div} a \in L^2_{loc}$) was proven by Leinfelder–Simader.

As with Theorem 5.4, there is an abstract two-operator Kato inequality result (originally conjectured by Simon) which was proven by Hess–Schader-Uhlenbrock and Simon. For more details as well as a discussion of the Kato class which Kato introduced in his original Kato inequality note, see the longer paper.

6 Kato–Rosenblum and Kato–Birman

Starting with Rutherford's 1911 discovery of the atomic nucleus, scattering has been a central tool in fundamental physics, so it isn't surprising that one of the first papers in the new quantum theory was by Born in 1926 on scattering. While scattering is at a deep level a time-dependent phenomenon, Born used eigenfunctions and time–independent ideas. In the early 1940s, the theoretical physics community first considered time-dependent approaches to scattering. Wheeler and Heisenberg defined the S–matrix and Møller introduced wave operators as limits (with no precision as to what kind of limit).

The Kato group, late 1950s.
S.T. Kuroda (standing), T. Kato, T. Ikebe, H. Fujita, Y. Nakata

It was Friedrichs in a prescient 1948 paper who first considered the invariance of the absolutely continuous spectrum under sufficiently regular perturbations. Friedrichs was Rellich's slightly older contemporary. Both were students of Courant at Göttingen in the late 1920s (in 1925 and 1929 respectively). By 1948, Friedrichs was a professor at Courant's institute at NYU. He looked at several simple models, and for one with purely a.c. spectrum he could prove that the perturbed models were unitarily equivalent to unperturbed models. While Friedrichs neither quoted Møller nor ever wrote down the explicit formulae

$$\Omega^{\pm}(H, H_0) = \mathrm{s} - \lim_{t\to\mp\infty} e^{itH} e^{-itH_0} \tag{36}$$

(the strange $\pm$ vs. $\mp$ convention that we use is universal in the theoretical physics community, uncommon among mathematicians, and not the convention that Kato used), he did prove something equivalent to showing that the limit Ω^+ existed and was the unitary he constructed with time-independent methods.

Motivated in part by Friedrichs, in 1957 Kato published two papers that set out the basics of the theory we will discuss in this section. In the first, he had the important idea of defining

$$\Omega^{\pm}(A,B) = \text{s} - \lim_{t\to\mp\infty} e^{itA}e^{-itB}P_{ac}(B), \tag{37}$$

where $P_{ac}(B)$ is the projection onto $\mathcal{H}_{ac}(B)$, the set of all $\varphi \in \mathcal{H}$ for which the spectral measure of B and φ is absolutely continuous with respect to Lebesgue measure. If these strong limits exist, we say that the wave operators $\Omega^{\pm}(A,B)$ exist.

By replacing t by $t+s$, one sees that if $\Omega^{\pm}(A,B)$ exist then $e^{isA}\Omega^{\pm} = \Omega^{\pm}e^{isB}$. Since $\Omega^{\pm}$ are unitary maps, $U^{\pm}$, of $\mathcal{H}_{ac}(B)$ to their ranges, we see that $U^{\pm}B \restriction \mathcal{H}_{ac}(B)(U^{\pm})^{-1} = A \restriction \operatorname{ran}\Omega^{\pm}$. In particular, ran $\Omega^{\pm}$ are invariant subspaces for A and lie in $\mathcal{H}_{ac}(A)$. It is thus natural to define: $\Omega^{\pm}(A,B)$ are said to be *complete* if

$$\operatorname{ran}\Omega^{+}(A,B) = \operatorname{ran}\Omega^{-}(A,B) = \mathcal{H}_{ac}(A). \tag{38}$$

In the first of the 1957 papers, Kato proved the following:

Theorem 6.1 (Kato)**.** *Let $\Omega^{\pm}(A,B)$ exist. Then they are complete if and only if $\Omega^{\pm}(B,A)$ exist.*

The proof is almost trivial. It depends on noting that

$$\psi = \lim_{t\to\infty} e^{iAt}e^{-itB}\varphi \iff \varphi = \lim_{t\to\infty} e^{itB}e^{-itA}\psi. \tag{39}$$

That said, it is a critical realization because it reduces a completeness result to an existence theorem. In particular, it implies that symmetric conditions which imply existence also imply completeness. We'll say more about this below.

To show the importance of this idea, motivated by it in 1977, Deift and Simon proved that completeness of multichannel scattering for N–body scattering was equivalent to the existence of geometrically defined "inverse" wave operators. All proofs of asymptotic completeness for N–body systems prove it by showing the existence of these Deift–Simon wave operators, in support of Kato's Theorem 6.1.

One consequence of Theorem 6.1 is that a symmetric condition for existence implies completeness also. Using this idea, in his first 1957 paper, Kato proved:

Theorem 6.2 (Kato)**.** *Let H_0 be a self–adjoint operator and V a (bounded) self–adjoint finite rank operator. Then $H = H_0 + V$ is a self–adjoint operator and the wave operators $\Omega^{\pm}(H,H_0)$ exist and are complete.*

Later in 1957, Kato proved:

Theorem 6.3 (Kato–Rosenblum Theorem)**.** *The conclusions of Theorem 6.2 remain true if V is a (bounded) trace-class operator.*

$$\|\psi - e^{iAt}e^{-itB}\varphi\| = \|e^{itB}e^{-itA}\psi - \varphi\|. \tag{40}$$

In a sense this theorem is optimal. It is a result of Weyl–von Neumann that if A is a self–adjoint operator, one can find a Hilbert–Schmidt operator, C, so that $B = A + C$ has only pure point spectrum. Kato's student, S. T. Kuroda, shortly after Kato proved Theorem 6.3, extended this result of Weyl–von Neumann to any trace ideal strictly bigger than trace class. So within trace-ideal perturbations, one cannot do better than Theorem 6.3.

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The name given to this theorem comes from the fact that before Kato proved Theorem 6.3, Rosenblum proved a special case that motivated Kato: namely, if A and B have purely a.c. spectrum and $A - B$ is trace class, then $\Omega^{\pm}(A, B)$ exist and are unitary (so complete).

I'd always assumed that Rosenblum's paper was a rapid reaction to Kato's finite rank paper, which, in turn, motivated Kato's trace-class paper. But I recently learned that this assumption is not correct. Rosenblum was a graduate student of Wolf at Berkeley who submitted his thesis in March, 1955. It contained his trace-class result under some additional technical hypotheses; a Dec., 1955 Berkeley technical report had the result as eventually published without the extra technical assumption. Rosenblum submitted a paper to the *American Journal of Mathematics* which took a long time refereeing it before rejecting it. In April, 1956, Rosenblum submitted a revised paper to the *Pacific Journal*, in which it eventually appeared. (This version dropped the technical condition; I've no idea what the original journal submission had.)

Kato's finite rank paper was submitted to *J. Math. Soc. Japan* on March 15, 1957, and was published in the issue dated April, 1957(!). The full trace-class result was submitted to *Proc. Japan Acad.* on May 15, 1957. Kato's first paper quotes an abstract of a talk Rosenblum gave at an A.M.S. meeting, but I don't think that abstract contained many details. This finite-rank paper has a note added in proof thanking Rosenblum for sending the technical report to Kato, quoting its main result and saying that Kato had found the full trace-class results. ("Details will be published elsewhere."). That second paper used some technical ideas from Rosenblum's paper.

I've heard that Rosenblum always felt that he'd not received sufficient credit for his trace-class paper. There is some justice to this. The realization that trace class is the natural class is important. As I've discussed, trace class is maximal in a certain sense. Kato was at Berkeley in 1954 when Rosenblum was a student (albeit some time before his thesis was completed) and Kato was in contact with Wolf. However, there is no indication that Kato knew anything about Rosenblum's work until shortly before he wrote up his finite rank paper when he became aware of Rosenblum's abstract. My surmise is that both, motivated by Friedrichs, independently became interested in scattering.

The longer paper describes further developments and some applications of the trace-class theory, some of them due to Kato himself. To me the heroes of this later work are Kuroda, Pearson, and especially Birman.

7 Kato Smoothness

In this final section we discuss the theory of Kato smoothness, which is based primarily on two papers of Kato published in 1966 (when Kato was 49) and 1968. The first is the basic one with four important results: the equivalence of many conditions giving the definition, the connection to spectral analysis, the implications for existence and completeness of wave operators and, finally, a perturbation result. The second paper concerns the Putnam–Kato theorem on positive commutators.

To me, the 1951 self–adjointness paper is Kato's most significant work (with the adiabatic theorem paper a close second), Kato's inequality his deepest, and the subject of this section his most beautiful. One of the things that is so beautiful is that there isn't just a relation between the time–independent and time–dependent objects – there is an equivalence! Part of the equivalence depends on the simple formula that holds when H is a self–adjoint operator on a (complex) Hilbert space $\mathcal{H}$ (where $R(\mu) = (H-\mu)^{-1}$),

$$\int_0^\infty e^{-\epsilon t} e^{it\lambda} e^{-itH} \varphi \, dt = -iR(\lambda + i\epsilon)\varphi \tag{41}$$

for any $\varphi \in \mathcal{H}$, because $\int_0^\infty e^{-\epsilon t} e^{i(\lambda - x)t} \, dt = -i(x - \lambda - i\epsilon)^{-1}$.

Here is the set of equivalent definitions:

Theorem 7.1 (Kato (1966)). *Let H be a self–adjoint operator and A a closed operator. The following are all equal:*

$$\sup_{\substack{\|\varphi\|=1 \\ \epsilon>0}} \frac{1}{4\pi^2} \int_{-\infty}^\infty \left(\|AR(\lambda + i\epsilon)\varphi\|^2 + \|AR(\lambda - i\epsilon)\varphi\|^2 \right) \, d\lambda \tag{42}$$

$$\sup_{\|\varphi\|=1} \frac{1}{2\pi} \int_{-\infty}^\infty \|Ae^{-itH}\varphi\|^2 \, dt \tag{43}$$

$$\sup_{\substack{\|\varphi\|=1,\, \varphi \in D(A^*) \\ -\infty<a<b<\infty}} \frac{\|P_{(a,b)}(H)A^*\varphi\|^2}{b-a} \tag{44}$$

$$\sup_{\substack{\mu \notin \mathbb{R},\, \varphi \in D(A^*) \\ \|\varphi\|=1}} \frac{1}{2\pi} | \langle A^*\varphi, [R(\mu) - R(\bar{\mu})]A^*\varphi \rangle | \tag{45}$$

$$\sup_{\substack{\mu \notin \mathbb{R},\, \varphi \in D(A^*) \\ \|\varphi\|=1}} \frac{1}{\pi} \|R(\mu)A^*\varphi^2 \, |Im\|\mu|. \tag{46}$$

In particular, if one is finite (resp. infinite), then all are.

Remarks. *1. In (42)/(43), we set $\|A\psi\| = \infty$ if $\psi \notin D(A)$, so, for example, to say that (43) is finite implies that for each φ, we have that $e^{-itH}\varphi \in D(A)$ for Lebesgue a.e. $t \in \mathbb{R}$.*

2. If one and so all of the above quantities are finite we say that A is H–smooth. The common value of these quantities is called $\|A\|_H^2$.

3. The proof is not hard. For example, if the integral in (43) has a factor of $e^{-2\epsilon t}$ *put inside it, the equality of the integrals in (42) and (43) follows from (41) and the Plancherel theorem. By monotone convergence, the* $\sup$ *of the time-integral with the* $e^{-2\epsilon t}$ *factor is the integral without that factor.*

Smoothness has an immediate consequence for the spectral type of H:

Theorem 7.2 (Kato)**.** *Let H be a self–adjoint operator and let A be H–smooth. Then* $\text{ran}(A^*) \subset \mathcal{H}_{ac}(H)$*. In particular, if* $\ker(A) = \{0\}$*, then H has purely a.c. spectrum.*

The proof is very easy. If $d\nu$ is the H–spectral measure for $A^*\varphi$, then (44) says that

$$\nu(I) \le \|A\|_H \|\varphi\|^2 |I| \tag{47}$$

(where $|\cdot|$ is Lebesgue measure) for open intervals I. By taking unions and using outer regularity, (47) holds for all sets, so ν is absolutely continuous.

Smoothness also implies existence and completeness of wave operators.

Theorem 7.3 (Kato)**.** *Let H, H_0 be two self–adjoint operators. Let A, B be closed operators so that A is H–smooth and B is H_0–smooth and so that*

$$H - H_0 = A^*B. \tag{48}$$

Then $\Omega^{\pm}(H, H_0)$ *exist and are complete.*

Remark 7.4. *The proof is again easy (indeed, one of the beauties of Kato smoothness theory is how much one gets with simple proofs). The key is to use*

$$\begin{aligned} |\langle \psi, (W(t) - W(s))\varphi \rangle| &= \left| \int_s^t \langle Ae^{-iuH}\psi, Be^{-iuH_0}\varphi \rangle \, du \right| \\ &\le \left(\int_{-\infty}^{\infty} \|Ae^{-iuH}\psi\|^2 \, du \right)^{1/2} \left(\int_{-s}^{t} \|Be^{-iuH_0}\varphi\|^2 \, du \right)^{1/2} \\ &\le \sqrt{2\pi}\|A\|_H \|\psi\| \left(\int_{-s}^{t} \|Be^{-iuH_0}\varphi\|^2 \, du \right)^{1/2}, \end{aligned}$$

which implies that

$$\|(W(t) - W(s))\varphi\| \le \sqrt{2\pi}\|A\|_H \left(\int_{-s}^{t} \|Be^{-iuH_0}\varphi\|^2 \, du \right)^{1/2}. \tag{49}$$

We say that a closed operator, A is H–*supersmooth* if and only if

$$\|A\|_{H,SS}^2 \equiv \sup_{z \in \mathbb{C}\setminus\mathbb{R}} \|A(H - z)^{-1}A^*\| < \infty. \tag{50}$$

The notion is in Kato's basic 1966 paper and the name is from a 1989 paper of Kato–Yajima. The name hasn't stuck but I like it, so I'll use it. The fourth important result in Kato's 1966 paper is:

Theorem 7.5 (Kato). *Let H_0 be a self–adjoint operator. Let A be H_0–supersmooth and C a bounded self-adjoint operator so that*

$$\alpha \equiv \|C\| \|A\|^2_{H_0,SS} < 1. \tag{51}$$

Let $B = A^*CA$. Then B is relatively form bounded with relative form bound at most α. If $H = H_0 + B$, then A is also H–supersmooth with

$$\|A\|_{H,SS} \leq \|A\|_{H_0,SS}(1-\alpha)^{-1/2}. \tag{52}$$

In particular, $\Omega^{\pm}(H, H_0)$ exist and are complete.

Remark 7.6. *Once again, the proofs are simple. The key is a formal geometric series:*

$$\begin{aligned} A(H-z)^{-1}A^* &= A(H_0-z)^{-1}A^* \\ &+ \sum_{j=0}^{\infty} (-1)^{j+1} A(H_0-z)^{-1}A^* \left[CA(H_0-z)^{-1}A^*\right]^j CA(H_0-z)^{-1}A^*. \end{aligned} \tag{53}$$

In his original paper, Kato proved for $\nu \geq 3$, any $V \in L^{\frac{1}{2}\nu-\epsilon} \cap L^{\frac{1}{2}\nu+\epsilon}$ is supersmooth and Kato–Yajima improved that to $L^{\nu/2}$. Iorio–O'Carroll used supersmooth ideas to get a weak coupling result for N–body systems. If one has an N–body system on $\mathbb{R}^\nu$ with two-body potentials in $L^{\nu/2}$ and if $\nu > 2$, then for small coupling H has purely a.c. with spectrum $[0, \infty)$.

In his 1968 paper, Kato used smoothness ideas to prove that if A and B are bounded self–adjoint operators so that $i[A, B] > 0$, then A and B have purely a.c. spectrum (a result proven the year before by very different methods by Putnam). If A is the generator of dilations and B an N-body potential with repulsive potentials one has positivity of the commutator but neither operator is bounded so Kato's argument doesn't apply. In a series of papers, Lavine was able to use smoothness ideas to prove that suitable N-body systems with repulsive potentials have purely a.c. spectrum and, with sufficiently fast decay, have complete wave operators. To do this, he introduced the important notion of local smoothness. For details, the reader can consult the longer paper or, better, the relevant section of Reed–Simon.

The longer paper also discusses a paper of Vakulenko that should be better known. For two-body systems, he proved that if $|V(x)| \leq C(1 + |x|)^{-1-\epsilon} \equiv g(x)^2$, then g is $-\Delta + V$ locally smooth on $[0, \infty)$ which recovers the results of Agmon–Kato–Kuroda on completeness of wave operators and absence of singular continuous spectrum in this case and also the result of Kato on the absence of positive eigenvalues. The longer paper also has references to work of Yafaev on long-range and on N–body systems that uses smoothness as one tool in the analysis of such problems.