Perturbation theory and atomic resonances since Schrödinger’s time

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Simonfest

Cal Tech

28 March 2006

(as rescheduled)

theory, functional analysis, and nonrelativistic quantum mechanics (particularly Schrödinger operators), including the connections to atomic and molecular physics. More particularly, his work has focused on broad areas of mathematical physics and analysis covering: quantum field theory, statistical mechanics, Brownian motion, random matrix theory, general nonrelativistic quantum mechanics (including N-body systems and resonances), nonrelativistic quantum mechanics in electric and magnetic fields, the semi-classical limit, the singular continuous spectrum, random and ergodic Schrödinger operators, orthogonal polynomials, and non-selfadjoint spectral theory.

Professor Simon has authored more than 300 publications on mathematics and physics. A brilliant student, Simon became a Putnam Fellow in 1965 at 19 years old. He received his A.B. in 1966 from Harvard College and his Ph.D. in Physics at Princeton University in 1970. Following his doctoral studies, Dr. Simon took professorship at Princeton for many years, often working with colleague Elliott H. Lieb on the Thomas-Fermi Theory and Hartree-Fock Theory of atoms in addition to phase transitions and mentoring many of the same students as Lieb. He eventually was persuaded to take a post at Caltech, a post he currently holds. His status is legendary in mathematical physics and he is renowned for his ability to write scientific manuscripts "in five percent of the time ordinary mortals need to write such papers."

A colleague of his, in a tale revealing of his brilliance, once stated:

> Barry has always been remarkable for his vast knowledge of mathematics, so it was many years before I can recall ever telling him a published theorem he didn't already know. One day I saw Barry in Princeton shortly after a meeting and told him about an old inequality for PDEs, which, as I could tell from his intent look, was new to him. I said, "It seems to be useful. Do you want to see the proof?" His response "No, that's OK." Then he went to the board and wrote down a flawless proof on the spot.

There is a similar account of how the mathematical physics seminars at Princeton were conducted while Simon was in residence.

> There was an outside speaker most of the time. Wigner would usually show up and ask his typical "Wignerian" questions. Barry would sit in the audience and write a paper. From time to time he would look up from his notes and ask a question that would unsettle most speakers: Someone in the audience seemed to know more about what he was talking about than himself. Sometimes, at the end of the talk, Barry would go to the board and give his version of the proof, which was always slick.

Quotes

"To first approximation, the human brain is a harmonic oscillator."

Danke vielmals, danke schön, Fritz!

Peter in healthier times. Get well soon!

An article that synthesized much that went before and inspired much afterwards:

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Title: RESONANCES IN BODY QUANTUM SYSTEMS WITH DILATATION ANALYTIC POTENTIALS AND FOUNDATIONS OF TIME-DEPENDENT PERTURBATION-THEORY

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MR0353896 (50 #6378)

Simon, Barry

Resonances in n-body quantum systems with dilatation analytic potentials and the foundations of time-dependent perturbation theory.

Ann. of Math. (2) **97** (1973), 247--274.
81.47

The time-independent perturbation theory in non-relativistic quantum theory has been on a firm mathematical footing since the well-known work of Rellich and Kato. The corresponding time-dependent perturbation theory is not so well founded. There are questions even about the precise nature of the quantity whose calculation the theory should permit. In a substantial introduction the author reviews various approaches to the theory, with references to the physics literature. The scope of the theory is described with reference to a "physically realistic" model of the helium atom and includes the theory of resonances, scattering and autoionising states. The author identifies two main approaches to the problem: the Friedrichs-Howland approach, in which the resonance energy is viewed as a pole of a certain resolvent, and a second approach, associated with the names of Livs\u\i c and Grossmann (see the review of the paper by C. L. Dolph [Bull. Amer. Math. Soc. **67** (1961), 1--69; MR0142219 (25 \#5612)]), in which the resonance energies are viewed as eigenvalues of a non-self-adjoint operator associated in some way with the self-adjoint operator (the Hamiltonian) of interest. A synthesis of these two approaches is proposed to provide a rigorous time-dependent theory for the restricted class of systems mentioned in the title. The potentials considered here are, however, sufficiently general to include certain power-law potentials [$\gamma^{-\alpha}(0<\alpha<{\textstyle\frac 3{2}})$, including the Coulomb potentials], Yukawa potentials $[\gamma^{-1}e^{-μr}(μ>0)]$, and Yukawian potentials $[\gamma^{-1}\int_{m_0}^\infty e^{-mr}\,dμ(m) (m_0>0)$, $\int\,dμ<\infty]$, and are more precisely characterised in an appendix.

1. Schlagheck P, Paul T
Complex-scaling approach to the decay of Bose-Einstein condensates
PHYSICAL REVIEW A 73 (2): Art. No. 023619 FEB 2006
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2. Prodan E, Garcia SR, Putinar M
Norm estimates of complex symmetric operators applied to quantum systems
JOURNAL OF PHYSICS A-MATHEMATICAL AND GENERAL 39 (2): 389-400 JAN 13 2006
Times Cited: 0
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3. Jensen A, Nenciu G
The Fermi Golden Rule and its form at thresholds in odd dimensions
COMMUNICATIONS IN MATHEMATICAL PHYSICS 261 (3): 693-727 FEB 2006
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4. Lefebvre R, Sindelka M, Moiseyev N
Resonance positions and lifetimes for flexible complex absorbing potentials
PHYSICAL REVIEW A 72 (5): Art. No. 052704 NOV 2005
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5. Sajeev Y, Santra R, Pal S
Correlated complex independent particle potential for calculating electronic resonances
JOURNAL OF CHEMICAL PHYSICS 123 (20): Art. No. 204110 NOV 22 2005
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6. Moiseyev N, Cederbaum LS
Resonance solutions of the nonlinear Schrodinger equation: Tunneling lifetime and fragmentation of trapped
PHYSICAL REVIEW A 72 (3): Art. No. 033605 SEP 2005
Times Cited: 1
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7. Yeager DL, Mishra MK
Algebraic modifications to second quantization for non-Hermitian complex scaled Hamiltonians with applicat
INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY 104 (6): 871-879 SEP 20 2005
Times Cited: 0

Physical mechanisms for quantum resonance

- Shape resonance (Alpha emission)/Stark effect - confinement of a particle by a barrier, through which tunneling occurs.
- Dissolving of embedded eigenvalues by a small perturbation. Auger effect.

From Simon 1973:

"The goals of the time-dependent theory are much more ambitious than merely proving certain eigenvalues dissolve. The time--dependent theory is supposed to compute a characteristic lifetime τ, for the decay of a state … It turns out to be a very hard problem to define the lifetime directly."

1. What is the definition of a resonance energy?
2. Is there a “resonance state,” and how is it defined?
3. How can the resonance energy be calculated?
4. How can the time-decay of a resonance be quantified?

The first resonances defined as complex eigenvalues associated with a radiation condition

Quiz: who and when?

J.J. Thomson, 1884

The evidence: J.J. Thomson, 1884

so that the electrical distribution on the shell gradually dies away. Hence we see that the value of λ will be no longer wholly real.

We see, from equations (36) and (37), that the values of λ are given by the equation

$$E_2(\lambda a) + 2E_0(\lambda a) = 0 \qquad \text{.....................(55),}$$

or

$$\epsilon^{i\lambda a}\left\{\frac{i}{(\lambda a)^3} - \frac{i}{\lambda a} - \frac{1}{\lambda^2 a^2}\right\} = 0;$$

therefore

$$\lambda a = \frac{i}{2} \pm \sqrt{\frac{3}{4}} \qquad \text{.........................(56),}$$

Why did physicicists adopt the Schrödinger theory?

Why did physicists adopt the Schrödinger theory?

PICTURE OF
SCHRÖDINGER EMOVED

Quantisierung als Eigenwertproblem. (Dritte Mitteilung.), Ann. Physik, 1926.

Stark effect

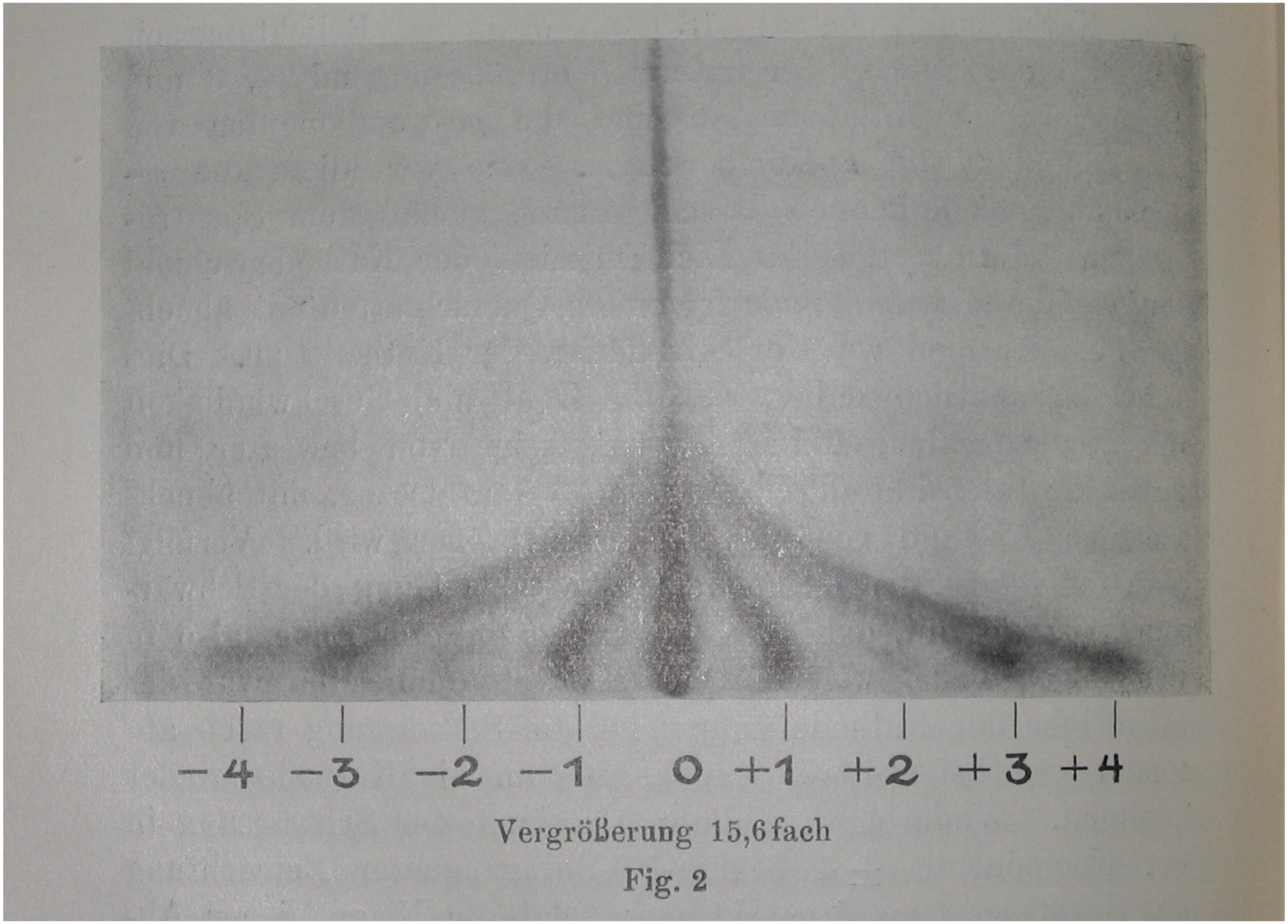
PICTURE OF STARK REMOVED,
(PERMISSION REFUSED BY
DEUTSCHES MUSEUM)

$$-\nabla^2 - \frac{1}{r} + \kappa x_1.$$

Stark (-Lo Surdo?) effect

PICTURE OF STARK REMOVED, (PERMISSION REFUSED BY DEUTSCHES MUSEUM)

Both published in 1913, different experimental techniques.



Vergrößerung 15,6 fach

Fig. 2

One of Stark's measurements. *Ann. der Phys*. **5** (1929), p. 1016.

Proper Values (Part III)

Perturbation Theory, with Application to the Stark Effect of the Balmer Lines

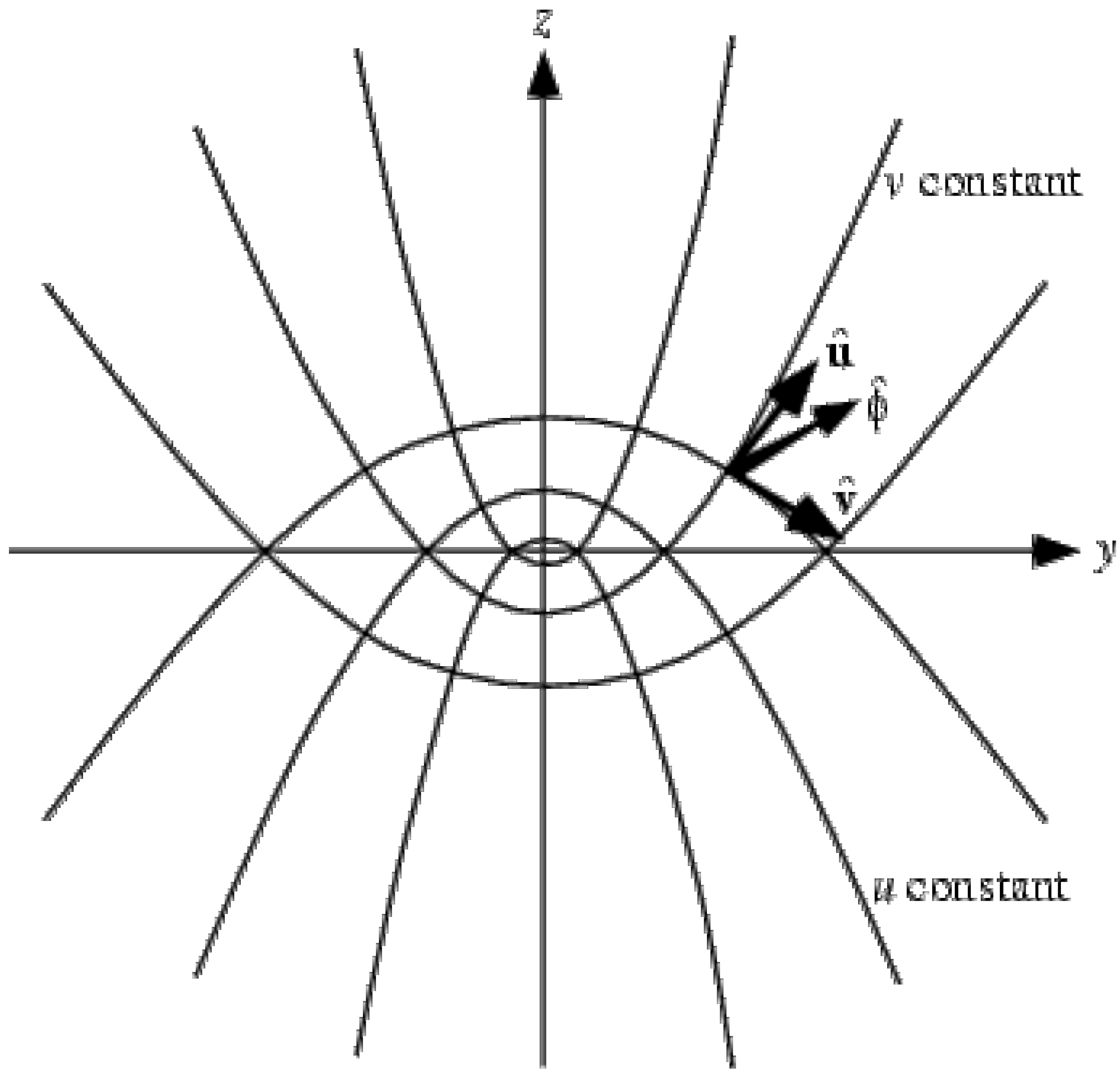
(*Annalen der Physik* (4), vol. 80, 1926)

Introduction. Abstract

As has already been mentioned at the end of the preceding paper,[1] the available range of application of the proper value theory can by comparatively elementary methods be considerably increased beyond the "directly soluble problems"; for proper values and functions can readily be approximately determined for *such* boundary value problems as are sufficiently closely related to a directly soluble problem. In analogy with ordinary mechanics, let us call the method in question the *perturbation* method. It is based upon the important *property of continuity* possessed by proper values and functions,[2] principally, for our purpose, upon their *continuous* dependence on the *coefficients* of the differential equation, and less upon the extent of the domain and on the boundary conditions, since in our case the domain ("entire q-space") and the boundary conditions ("remaining finite") are generally the same for the unperturbed and perturbed problems.

The method is essentially the same as that used by Lord Rayleigh in investigating[3] the vibrations of a string with *small inhomogeneities* in his *Theory of Sound* (2nd edit., vol. i., pp. 115-118, London, 1894). This was a particularly simple case, as the differential equation of the unperturbed problem had *constant* coefficients, and only the perturbing terms were arbitrary functions along the string. A complete generalisation is possible not merely with regard to these points, but also for the specially important case of *several* independent variables, *i.e.* for *partial* differential equations, in which *multiple proper values* appear in the unperturbed problem, and where the addition of a

[1] Last two paragraphs of Part II.
[2] Courant-Hilbert, chap. vi, §§ 2, 4, p. 337.



z
ν constant
û
φ̂
v̂
y
μ constant

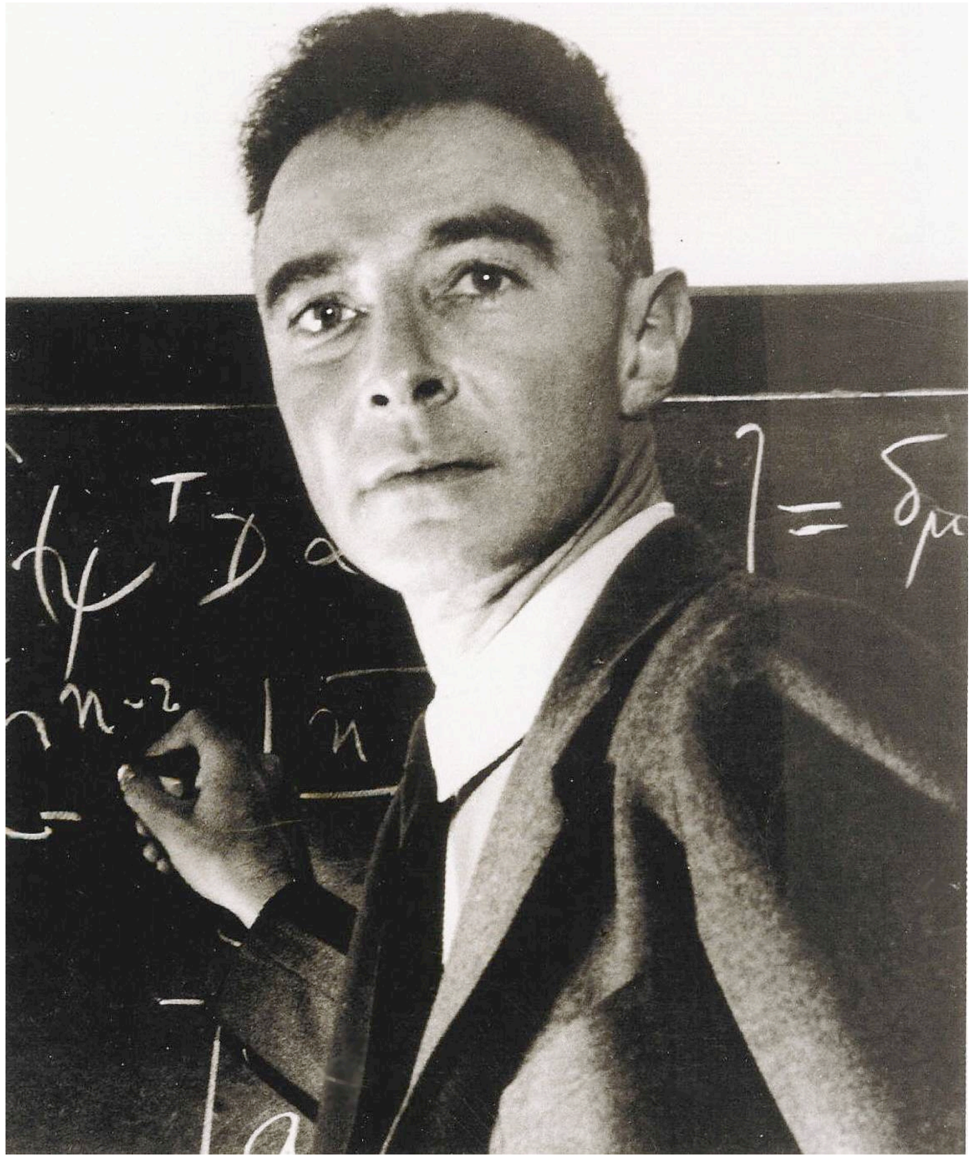
Some little problems with Schrödinger's analysis

Some little problems with Schrödinger’s analysis

- The Stark Hamiltonian has no eigenvalues at all, as soon as $k > 0$ (Titchmarsh 1951; Avron-Herbst 1977).

Some little problems with Schrödinger's analysis

- The Stark Hamiltonian has no eigenvalues at all, as soon as $k > 0$ (Titchmarsh 1951; Avron-Herbst 1977).
- The series coefficients follow a precise asymptotic law, and the radius of convergence is 0 (Graffi-Grecchi 1978, Harrell-Simon 1980).



J. Robert Oppenheimer

THREE NOTES ON THE QUANTUM THEORY OF APERIODIC EFFECTS

By J. R. Oppenheimer*

Abstract

In Section 1 it is shown that the normalization of the characteristic functions corresponding to a continuous spectrum, which has been introduced by Hellinger and Weyl, satisfies the requirements of the δ-normalization of the Dirac-Jordan transformation theory. It is further shown that this normalization makes the flux to and from infinity of systems for which an integral of motion β lies in the little range $\Delta\beta'$ equal to

$$(\partial E/h\partial\beta')\Delta\beta'.$$

In Section 2 the condition for the validity of classical mechanics in the form grad $\lambda << 1$, where λ is the instantaneous wave length $\lambda = (h/2\pi)[2M(E-U)]^{-1/2}$, is applied to establish Rutherford's formula for the scattering of α-particles.

In Section 3 a method is developed for computing the transition probabilities between states of the same energy, and which are represented by almost orthogonal eigenfunctions. The theory is applied to the ionization of hydrogen atoms in a constant electric field. The period of ionization in a field of 1 volt per cm is $10^{10^{10}}$ sec. The bearing of such transitions on the problem of metallic conduction is discussed.

THE normalization of continuous spectra has been formulated mathematically by Hellinger and Weyl; and it has been shown that this may be applied to a large class of quantum-mechanical problems without inconsistency.[1] The problem can, however, be treated a good deal more simply and generally. It may be formulated as follows: The δ-normalization where $\varepsilon \to 0$. For the wave function drops off exponentially within a sphere of radius proportional to ε^{-2}, whereas (4) is not satisfied within a sphere of radius proportional to $\varepsilon^{-3/2}$. Setting $\varepsilon = 0$ within this latter sphere does not, therefore, in the limit $\varepsilon \to 0$, affect the scattering. There is, however, no reason to suppose that for intermediate ε the classical formulae hold.

3. If one separates the wave equation for a hydrogen atom in an homogeneous electric field in parabolic coordinates, one finds that one of the equations has a potential energy which becomes negatively infinite for infinite values of the coordinate. Such an equation has no quadratically integrable solutions, and no point spectrum.[15] There are thus no stable stationary states possible for a hydrogen atom in such a field.

If one encloses the atom in a large box, periodic motions, of course, become possible. If the field is now made very small, the solutions of the wave equation are very much like those for the unperturbed atom; but if the drop in potential across the box is comparable with the resonance potential of the atom this is no longer the case. We must, therefore, conclude that, under the customary experimental conditions the characteristic functions found by the perturbation method, which yield the Stark effect, are not the stationary solutions of the wave equation, and that they do not completely describe the effect of the field.

The physical interpretation of this result is very simple. If we imagine the potential energy U of the electron plotted along the direction of the field, we see that it falls from a very high value at one end of the box to a very low value at the other; this uniform fall is broken by a sharp drop due to the nucleus. On the low potential side of the nucleus there is a maximum, sharp inside but gradual outside. If, therefore, we specify the energy of this system, we cannot be certain that the electron is in the neighborhood of the nucleus; it may also be in the low potential part of the field. If we make the box infinite, then it becomes increasingly probable that we shall find the electron in this part of the field, and hence the motion becomes aperiodic. In the classical theory, however, this situation caused no difficulties; for we could specify the other coordinates of the electron (besides the energy), and thus make certain that it was near the nucleus; and it could not leave this region without getting enough energy to clear the maximum in U.

where $v \rightarrow 0$. For the wave function drops off exponentially within a sphere of radius proportional to v^{-2}, whereas (4) is not satisfied within a sphere of radius proportional to $v^{-3/2}$. Setting $v=0$ within this latter sphere does not, therefore, in the limit $v \rightarrow 0$, affect the scattering. There is, however, no reason to suppose that for intermediate v the classical formulae hold.

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The physical interpretation of this result is very simple. If we imagine

[10] H. Weyl, Math. Ann. 68, 220 (1910).

Oppenheimer’s formula (original)

$$\mu_1 \sim a \Gamma e^{-(2/3\alpha)(\lambda_0+\lambda_0)^{3/2}} \cdot (\lambda_0+\lambda_2)^{9/16} \alpha^{-11/8} \tag{17}$$

$$\Gamma = 2^{9/4} e^{-3/4} \Gamma(3/4)/\Gamma(1/2)\Gamma(15/4)$$

Problems with Oppy's formula

$$\mu_1 \sim a\Gamma e^{-(2/3\alpha)(\lambda_0+\lambda_0)^{3/2}} \cdot (\lambda_0+\lambda_2)^{9/16}\alpha^{-11/8} \qquad (17)$$

$$\Gamma = 2^{9/4}e^{-3/4}\Gamma(3/4)/\Gamma(1/2)\Gamma(15/4)$$

- Fishy derivation
- Calculation errors
- Typographic errors


THE WORD
An early example of truthiness?

- And wrong:

Authors	$1/\tau = -2\,\mathrm{Im}E$ (a.u.)
	Ground state
Oppenheimer [a]	$0.1093F^{1/4}e^{-2/3F}$
Oppenheimer (corrected) [b]	$\frac{1}{2}\pi e^{-2/3F}$
Landau and Lifshitz [c]	$(4/F)e^{-2/3F}$
Present work [d]	$(4/F)e^{-2/3F}$
	States with $m^2=1$; $\beta_2^{(0)}=n_2+1$.
Lanczos [e,b]	$(2\pi n^2\beta_2^{(0)})^{-1}\left(\frac{\beta_2^{(0)}}{e}\right)^{-2\beta_2^{(0)}}(\frac{1}{4}n^3F)^{-2\beta_2^{(0)}}\exp\left(3(n_1-n_2)-\frac{2}{3n^3F}\right)$
Lanczos (corrected) [b]	$(2\pi n^3)^{-1}\left(\frac{\beta_2^{(0)}}{e}\right)^{-2\beta_2^{(0)}}(\frac{1}{4}n^3F)^{-2\beta_2^{(0)}}\exp\left(3(n_1-n_2)-\frac{2}{3n^3F}\right)$
Rice and Good [f]	$(nF/\pi)\exp(-2/3n^3F)$
Present work [d]	$[n^3(\beta_2^{(0)}-1)!\,\beta_2^{(0)}!]^{-1}(\frac{1}{4}n^3F)^{-2\beta_2^{(0)}}\exp\left(3(n_1-n_2)-\frac{2}{3n^3F}\right)$
	States with arbitrary n_1, n_2, and m; $\beta_2^{(0)}=n_2+\frac{1}{2}\lvert m\rvert+\frac{1}{2}$.
Present work [d]	$[n^3n_2!\,(n_2+\lvert m\rvert)!]^{-1}(\frac{1}{4}n^3F)^{-2\beta_2^{(0)}}\exp\left(3(n_1-n_2)-\frac{2}{3n^3F}\right)$

[a] Reference 8.
[d] Equation (126).

Yamabe, Tachibana, Silverstone, PRA 1977

Physical mechanisms for quantum resonance

- Shape resonance (Alpha emission)/Stark effect - confinement of a particle by a barrier, through which tunneling occurs.
- Dissolving of embedded eigenvalues by a small perturbation. Auger effect.

PICTURE OF GAMOW REMOVED,
PENDING PERMISSION

Almost every introduction to quantum mechanics has copied Gamow's diagrams:

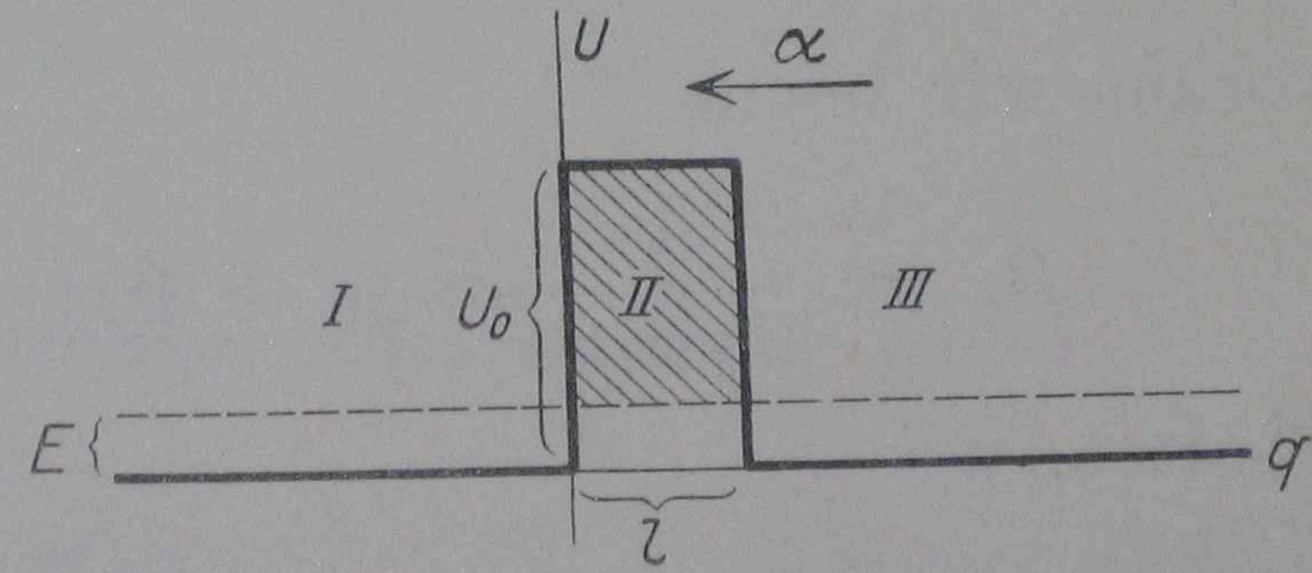

Fig. 2.

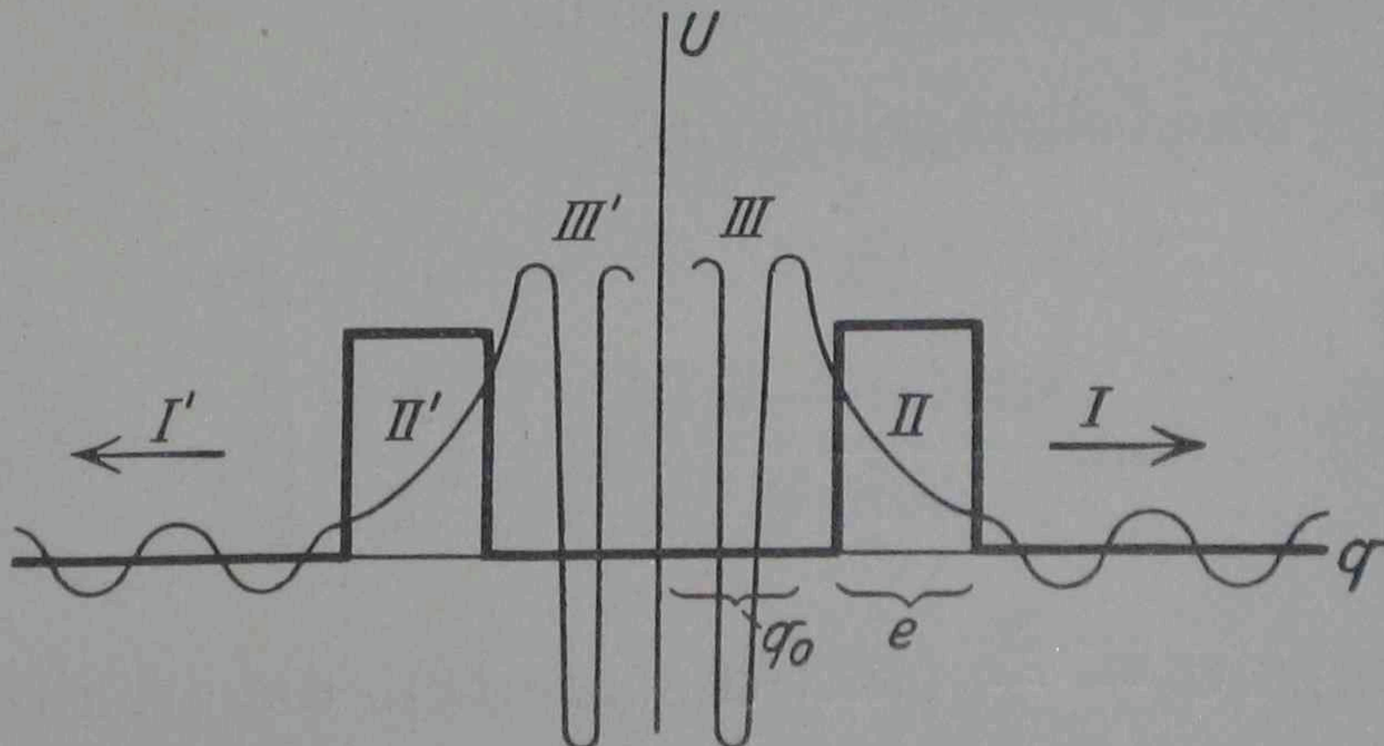

Fig. 3.

And now for completely different textbook diagrams…

And now for completely different textbook diagrams…

see Thaller's *Visual Quantum Mechanics* at

http://www.kfunigraz.ac.at/imawww/vqm/pages/supplementary/107S_resonance-1.html

How to define a quantum resonance?

$$\frac{1}{(\omega - \omega_0)^2 + \frac{\Gamma^2}{4}}$$

Weisskopf-Wigner, 1930. (Breit was later.)

How to define a quantum resonance?

- Bumps in scattering amplitude
- ………..poles in its analytic continuation
- Zeroes in Jost function
- Poles in Green function
- Non-real eigenvalues

How to define a resonance?

Howland’s razor:

No satisfactory definition of a resonance can depend only on the structure of a single operator on an abstract Hilbert space.

PICTURE OF FERMI REMOVED,
PENDING PERMISSION

E. Fermi

Assume $|\langle \Psi_0, \exp(-itH)\Psi_0 \rangle|^2 \sim C \exp(-\Gamma t)$

According to the Fermi Golden Rule, Γ is proportional to the square of a matrix element of the perturbation.

Fermi's golden rule

From Wikipedia, the free encyclopedia

In quantum physics, **Fermi's golden rule** is a way to calculate the transition rate between two eigenstates of a quantum system using time-dependent perturbation theory, which means it's an approximation.

The one-to-many transition probability per unit of time from a state $| i >$ to a set of states $| f >$ is given, to first order in the perturbation, by:

$$T_{i \rightarrow f} = \frac{2\pi}{\hbar} \left| \langle f | H' | i \rangle \right|^2 \rho$$

where ρ is the density of final states, and $< f | H' | i >$ is the matrix element (in bra-ket notation) of the perturbation, H', between the final and initial states.

The most common way to derive the equation is to start with time-dependent perturbation theory and to take the limit for absorption under the assumption that the time of the measurement is much larger than the time needed for the transition.

Although named after Fermi, most of the work leading to the Golden Rule was done by Dirac.

Exponential decay in time is impossible!

- Herbst, 1980: If true as $t \to \infty$, it would imply that the Radon-Nikodym derivative of the spectral measure is analytic in a strip, and by unique analytic continuation, its support must include all of R.

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- For $t \to 0$, clearly quadratic.

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- For t → 0, clearly quadratic.
- Best hope:

$$\langle \Psi_0, \exp(-itH)\Psi_0 \rangle = \exp(-i(E - i\Gamma/2)t) + b(t),$$

Exponential decay impossible!

- Herbst, 1980: If true as t → ∞, it would imply that the Radon-Nikodym derivative of the spectral measure is analytic in a strip, and by unique analytic continuation, its support must include all of R.
- For t → 0, clearly quadratic.
- Best hope:

$$\langle \Psi_0, \exp(-itH)\Psi_0 \rangle = \exp(-i(E - i\Gamma/2)t) + b(t),$$

- How to calculate Γ?

Spectral concentration

- E.C. Titchmarsh, 40s and 50s
- Conley-Rejto, Riddell, Howland, Nenciu

PICTURE OF TITCHMARSH REMOVED PENDING PERMISSION

Spectral concentration

Let H_n be a sequence of self-adjoint operators with spectral projectors $E_n(S)$. Let T and $\{S_n\}$ be subsets of R. Then the part of the spectrum of H_n in T is concentrated on S_n provided that

$$E_n(T - S_n) \to 0$$

in the strong sense.

Spectral concentration

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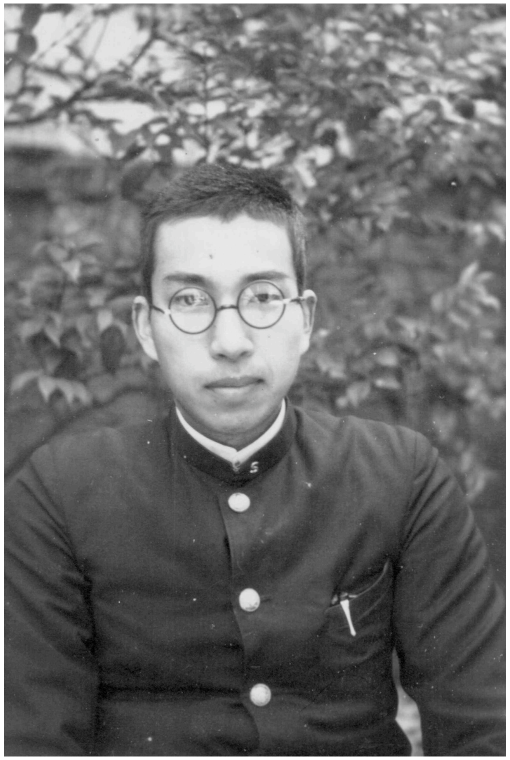
$$En(T - S_n) \rightarrow 0$$

in the strong sense.

Titchmarsh showed that Schrödinger's series for the Stark effect could be used to define shrinking intervals on which the spectrum was concentrated.

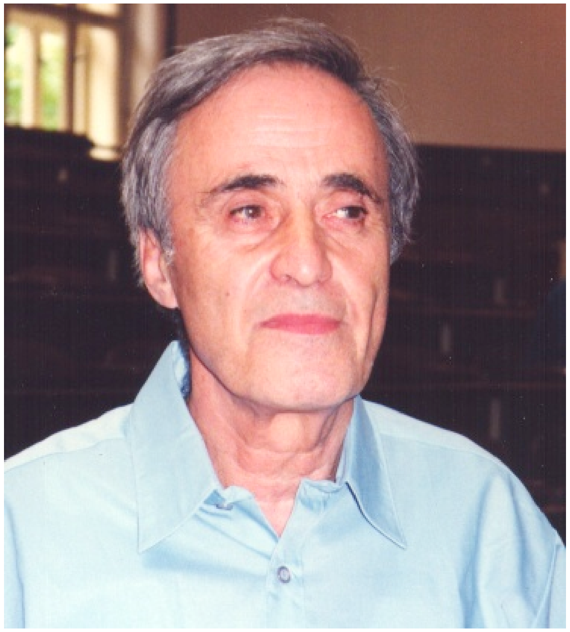
Rigorous perturbation and scattering theory.



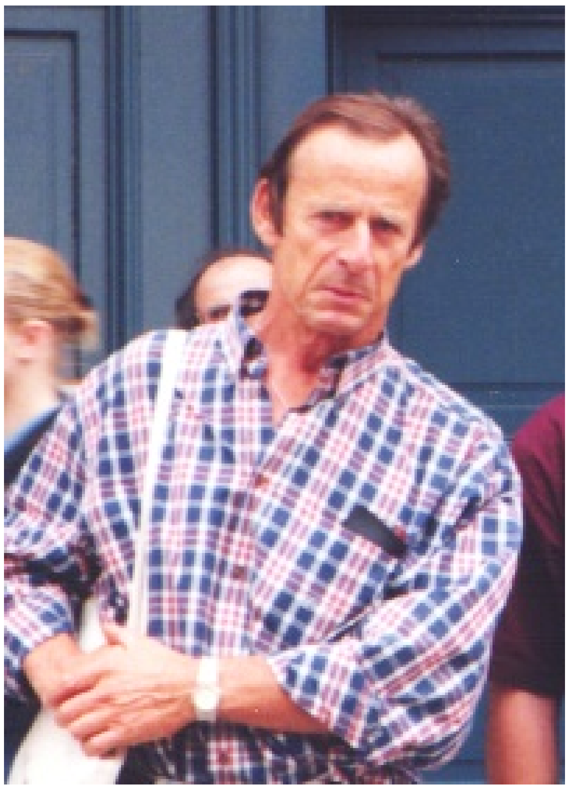
T. Kato

F. Rellich

M. Sh. Birman



Early 1970’s



J.-M. Combes

S. Graffi

Complex scaling

The unitary group of dilatations depends on a real parameter Θ such that $x \to \exp(\Theta)\, x$, hence

$$[U(\Theta) f](x) := \exp(\nu\Theta/2)\, f(\exp(\Theta)\, x)$$

is a unitary group.

For suitable potentials one can treat Θ as a complex variable and regard $H_\Theta := U^*(\Theta)\, H\, U(\Theta)$ as an analytic family.

Complex eigenvalues may arise, but are constant so long as isolated. Therefore they are inherent to H.

Complex scaling

Since

$$-\nabla^2_\Theta := -e^{2\Theta}\nabla^2,$$

the (purely essential) spectrum of H0 is simply rotated into the complex plane, to $e^{2\,\mathrm{Im}(\Theta)}\mathbf{R}$.


KRAFT
100% GRATED
PARMESAN
Cheese
100% REAL
GRATED PARMESAN
NO FILLERS

Many variants of complex scaling

- Translation analyticity (Avron-Herbst 1977)
- Exterior scaling (Simon, 1979)
- Distortion scaling (Hunziker, 1986)

Summing divergent series

- Padé approximation
- Borel summation

  – Anharmonic oscillator - Analysis by Bender-Wu , Banks-Bender-Wu, Simon, and Graffi-Grecchi-Simon related high-order perturbation theory, analytic continuation, tunneling.

Simon's 1973 *Annals* paper

- Connected various notions of resonance
- With complex scaling, reduced questions of resonances to Kato-Rellich perturbation theory
- Interpretation of Fermi Golden Rule as leading-order non-real perturbation correction to eigenvalue
- Spectral concentration for Auger-like resonances

Simon's 1973 *Annals* paper

Simon identified a suitable interpretation of the Fermi Golden Rule for Γ in (3) and as an estimate of the imaginary part of the Taylor coefficient a_2 of a resonance eigenv associated with a bound state at $\kappa = 0$. (The coefficient a_1 is real by first–order perturba theory.) Using Stone's formula and second–order perturbation theory, one can express resonance width for a perturbed non–degenerate discrete bound state as

$$\frac{\Gamma}{2} = 2\pi \frac{d}{d\lambda} \left\langle \Phi_0, W\tilde{P}(\lambda)W\Phi_0 \right\rangle \Big|_{\lambda=\lambda_0},$$

where Φ_0 is the unperturbed eigenfunction and $\tilde{P}(\lambda)$ is the spectral projector for $(-\infty,$ $\{\lambda_0\}$, cf. [147].

The menagerie of canonical models in the 70s-80s

The menagerie of canonical models in the 70s-80s

(Some with physical resonances, some without)

- Anharmonic oscillator $-d^2/dx^2 + x^2 + \kappa\, x^4$
- Double well $-d^2/dx^2 - x^2 + \kappa\, x^4$
- Stark effect $-\nabla^2 - 1/r + \kappa\, x_1$
- Hydrogen mol. ion $-\nabla^2 - 1/|x| - 1/|x - R\, e_1|$

Somewhat different:

- Zeeman Hydrogen + cst. Mag field
- Stark Wannier $-d^2/dx^2 + \cos x + \kappa\, x$
- Shape resonance $-d^2/dx^2 + R\, \chi_{[1,2]}$

Common features for models 1-4 and somewhat for 5-6

- High symmetry - mostly one-dimensional or separable.
- Eigenvalue perturbation series can be calculated based on an H_0 with discrete eigenvalues.

Common features for models 1-4 and somewhat for 5-6

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Common features for models 1-4 and somewhat for 5-6

- They are boundary values of analytic functions of κ, in sufficiently large regions for summability methods to be valid, if Taylor coefficients have controlled growth.

  The typical region is a cut plane.

Common features for models 1-4 and somewhat for 5-6

- They are boundary values of analytic functions of κ, in sufficiently large regions for summability methods to be valid, if Taylor coefficients have controlled growth.
Note: In the models with continuous spectra, we need complex scaling to define these analytic functions as eigenvalues.

Common features for models 1-4 and somewhat for 5-6

- They are boundary values of analytic functions of κ, in sufficiently large regions for summability methods to be valid, if Taylor coefficients have controlled growth.
Note: Standard dilatation analyticity might not be the right kind of complex scaling.

Common features for models 1-4 and somewhat for 5-6

- They are boundary values of analytic functions of κ….
- An exponentially small quantity related to the eigenvalues can be identified. (Imaginary part of a resonance eigenvalue, imaginary part of continuation of eigenvalue on the cut, gap from broken symmetry…)

Common features for models 1-4 and somewhat for 5-6

- They are boundary values of analytic functions of κ….
- With Cauchy's formula the Taylor coefficients can be written as moments of the discontinuity on the cut plane.

  Hence high-order pert. series asymptotics $\Leftrightarrow$ *asymptotics of the exponentially small quantity as* $\kappa \rightarrow 0$.

Common features for models 1-4 and somewhat for 5-6

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- *Hence high-order pert. series asymptotics $\Leftrightarrow$ asymptotics of the exponentially small quantity as $\kappa \to 0$.*
- Since an exponentially small quantity would be swamped by any finite-order correction in perturbation theory, non-perturbative methods are needed.
- *With integration by parts, the exponentially small quantity can be related back to the solutions of the Schrödinger equation.*

Example: Stark effect

The dispersion relation:

$$a_{2n} = -\frac{1}{\pi}\int_0^R \kappa^{-2n-1}\Gamma(\kappa)d\kappa + O(R^{-2n})$$

For Stark, or any other Schrödinger equations with real potential but non-real eigenvalue parameter, as a consequence of Green's identity:

$$\Gamma \int_S |\Phi_r|^2 d^\nu x = 2\int_{\partial S} \mathrm{Im}\left(\overline{\Phi_r}\Phi_r\right) d^{\nu-1}x.$$

Shape resonance

- Perturbation theory with large barriers

  $H_0 + \lambda W$, W a nonnegative bump
- Ashbaugh thesis, Ashbaugh-Harrell 1982
  - Fractional powers of $1/\lambda$
  - Calculation of resonance width Γ

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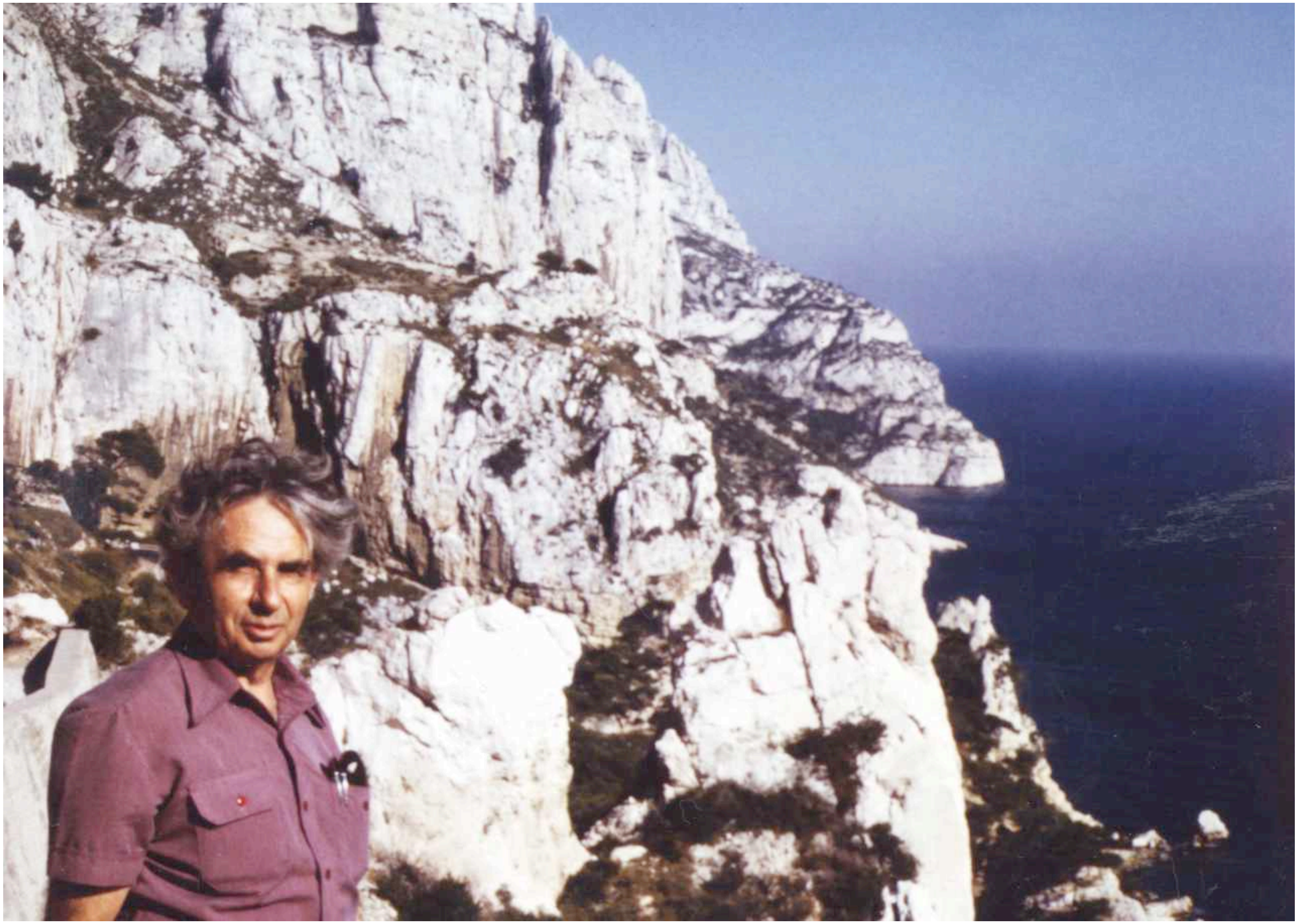
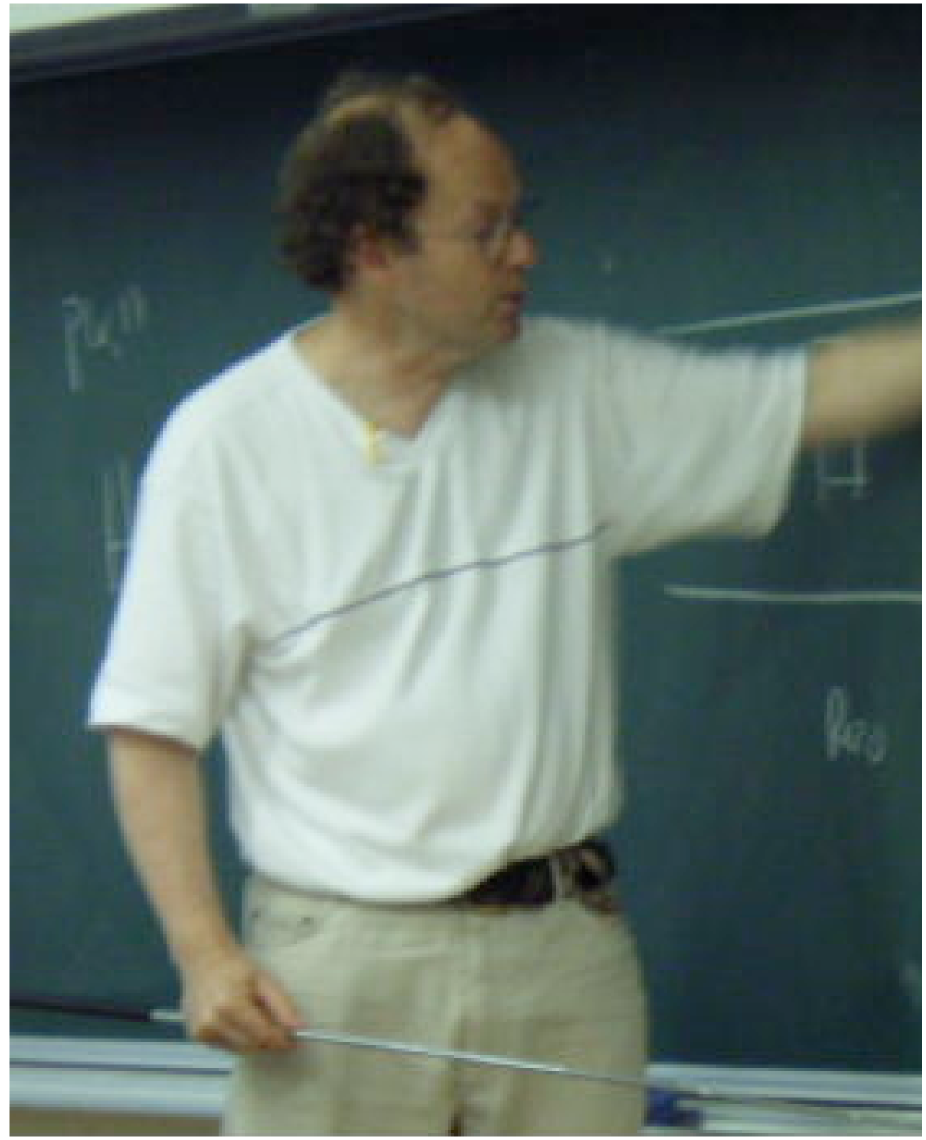
- Not much, only that in the early seventies good pointwise control was available for solutions of ODEs but not for PDEs.
- Solutions of elliptic PDEs were better understood in the 1980's



S. Agmon, playing hookey at Luminy, 1984.

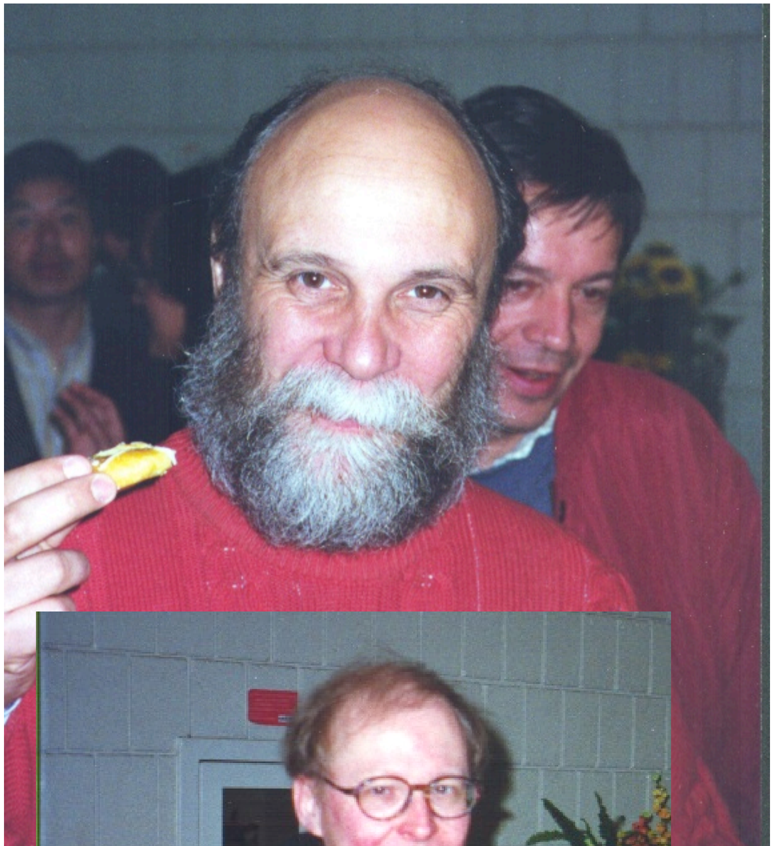


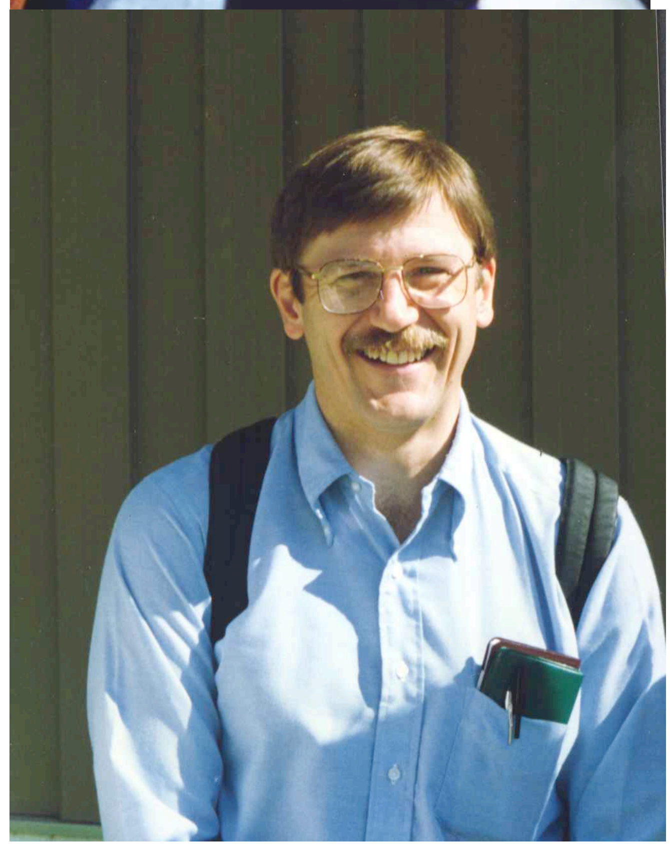
B. Helffer, book, 1998

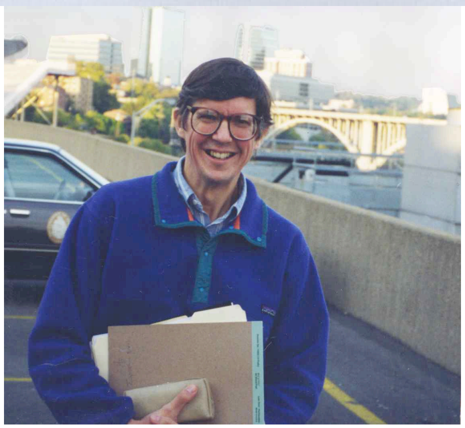
J. Sjöstrand. Lectures on webpage

Many other resonators

Including, but far from limited to, the following selection:







P. Hislop and Sigal, 1996,
Introduction to spectral theory,
state of art at the time.

Quantum resonance in the post-Simon 1973 era

A. Continuing the tradition.

- Simon did some work in the 1980’s, with occasional appearances into this millennium!
- Helffer-Sjöstrand, etc., basically all the canonical models without separability.
- Combes-Duclos-Klein-Seiler, Hislop-Sigal, shape resonances without separability.
- Hunziker, Skibsted, etc. exponential decay in time.

Quantum resonance in the post-Simon era

B. Independent traditions.

- Lavine,“Sojourn time” and time-delay.
- Melrose-Zworski, in the Lax-Phillips tradition, studied the effects of “trapping.”
- Attempts at abstract formalisms by Gesztesy, Holden, more recently Agmon
- Asymptotics and bounds on resonances of various kinds (Ashbaugh, Burq, Froese, Gérard, Harrell, Jensen, Martinez, Melrose, Sjöstrand, Svirsky, Zworski)

Quantum resonance in the post-Simon era

C. Conceptual advances in questions inspired by Simon 1973

- Mourre estimates - Commutator bound implying local a.c. spectrum and decay of Green functions.
- In canonical case, A is symmetrized generator of dilatations, $B = i[H,A]$,

  and a Mourre estimate is of the form

  $P_\Delta B P_\Delta \geq \alpha P_\Delta + K$

Quantum resonance in the post-Simon era

C. Conceptual advances in questions inspired by Simon 1973

- Mourre estimates - Commutator bound implying local a.c. spectrum and decay of Green functions.
  - originally not connected with resonances, but notice the continued presence of the group of dilatations.

Quantum resonance in the post-Simon era

C. Conceptual advances in questions inspired by Simon 1973

- Mourre estimates - Commutator bound implying local a.c. spectrum and decay of Green functions.
- Livshits-Feshbach matrix
  - Howland realized the importance of this already in the 1970s.
  - Thesis and article of Orth

Definition 2 Let H be self–adjoint and let P be a finite–dimensional projector (norm the projector onto the unperturbed eigenvector ψ_0 of a reference operator H_0). The *Liv Feshbach matrix* is the finite–dimensional operator $B(z)$ acting on $\mathcal{K} := \mathrm{Ran}P$ such that

$$(B(z) - z\mathbf{1})^{-1} = P(H - z\mathbf{1})^{-1}P, \quad ($$

when the right side is "compressed" to $\mathcal{K}$.

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Howland showed B(z) meromorphic off the essential spectrum, with only real singularities, & Kato-Rellich methods work.

It follows by a calculation from (12) that, with $\bar{P} := (\mathbf{1} - P)$ and $\bar{H} := \bar{P}H\bar{P}$,

$$B(z) = PHP - PH\bar{P}(\bar{H} - z)^{-1}\bar{P}HP. \tag{13}$$

(Again, this formula is to be interpreted as compressed to $\mathcal{K}$.) Replacing H by $H_0 + \kappa W$ and taking P as the orthogonal projector corresponding to an eigenvalue $\lambda_0 \in \sigma_p(H_0)$ with normalized eigenvector Φ_0 yields the *Feshbach formula*

$$B(z, \kappa) = \lambda_0 \mathbf{1} + \kappa PWP - \kappa^2 F(z, \kappa),$$

where $F(z, \kappa) = PW\bar{P}(\bar{H} - z)^{-1}\bar{P}WP$ [48]. When P is one–dimensional, $B(z, \kappa)$ and F reduce to scalar functions that satisfy

$$B(z, \kappa) = \lambda_0 + \kappa \langle \Phi_0, W\Phi_0 \rangle - \kappa^2 F(z, \kappa). \tag{14}$$

Observe that the first–order term is identical to that of Rayleigh-Schrödinger perturbation theory for the first–order correction to a non–degenerate eigenvalue, and that $-\kappa^2 F(z, \kappa)$ resembles the second–order correction. From (14) the leading–order expression for the resonance width is found to be

$$\frac{\Gamma}{2} = -\mathrm{Im} F(\lambda_0 + i\epsilon, 0). \tag{15}$$

Definition 3 Suppose that there exists a dense subspace $\mathcal{H}_+$ containing $\mathcal{K}$, $W(\mathcal{K})$, and all possible eigenvectors of $H(\kappa)$. If for λ in some neighborhood of λ_0 and κ near 0, $((\mathbf{1} - P)H(\kappa)(\mathbf{1} - P) - \mathbf{1})^{-1}$ can be continued analytically in z to the real axis as a bounded operator from $\mathcal{H}_+$ onto its dual $\mathcal{H}_-$, and that the continuation is Lipschitz continuous with Lipschitz constant $O(\kappa^{-2})$, then $B(z,\kappa)$ can likewise be continued to the real axis, and the *resonance eigenvalue* near λ_0 is the fixed point of the equation

$$\lambda(\kappa) = B(\lambda(\kappa), \lambda).$$

Orth showed spectral concentration

Recent mileposts using Howland-Orth definition

- Soffer-Weinstein, 1998. Assuming the decay implied by a Mourre est., nonvanishing of FGR, nonthreshold, then mod exponential decay in time.
- Jensen-Nenciu, 2006. Nice analysis of Livshits-Feshbach matrix, modified FGR that works at some thresholds
- Cattaneo-Graf-Hunziker, preprint. Lay out very general assumptions (Mourre + existence of some commutators involving A s.t. exi(isA) maps D(H) to itself). Then modified exp. Decay in time for states smoothly projected near an unperturbed eigenvalue.

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The canonical choice of A continues to be the generator of dilatations.

Happy Birthday, Barry!

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