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Resonances and Complex Scaling: A Rigorous Overview*

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Abstract

We review certain aspects of the theory of resonances and give a comprehensive review of the rigorous aspects of complex scaling.

1. Introduction

As the proceedings of this workshop amply demonstrate, complex scaling has become a powerful tool in the numerical study of resonances in few electron systems. It is also a technique which has had a firm rigorous footing since the work of Agiular, Balslev, and Combes. It seems worthwhile to state as carefully as possible exactly what is or is not known rigorously from a viewpoint that attempts to bridge the language gap between the rigorous types like me and the atomic theorists. I will generally avoid encumbering this review with proofs and I will occasionally avoid giving the most general definition but concentrate rather on giving examples that obey the definition and include all (or most) cases of practical interest.

In Sec. 2, I will discuss some aspects of the definition of resonance, especially those involving a fundamental principle that is often neglected in the literature: I call the principle Howland's Razor since it was emphasized emphatically by Howland [1] and since its cutting significance is somewhat reminiscent of Ockham's razor. The general literature on resonance is enormous and absolutely no attempt is made to summarize it; see Fonda [2] for a recent review.

In Sec. 3, I attempt to review what is rigorously known about complex scaling. In Sec. 4, I raise certain open questions; this is intended mainly as a plea to my fellow mathematical physicists. Finally, in Sec. 5, I briefly discuss other complex canonical transformations (a term coined by Combes); this section should be viewed partly as an advertisement aimed at those who have already been beguiled by complex scaling to consider the charms of some of the other complex beasts.

I should like to thank P-O. Löwdin for organizing a most stimulating conference.

2. What Is a Resonance?

Let me begin with three possible "definitions" of a resonance state that represent the main trends used to study resonances. These definitions are delib-

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erately caricatured. Moreover, they are deliberately stated in a way that makes them absolutely unsuitable because of Howland's Razor, which rips them to shreds! Throughout, H denotes a (Hamiltonian) self-adjoint operator on a Hilbert space, $\mathscr{H}$.

Time Decay. φ is a resonant state of H with width Γ, if

$$|(\varphi, e^{-itH}\varphi)|^2 = e^{-\Gamma t} \tag{1}$$

for all $t>0$.

Gel'fand Triple. Suppose that $\mathscr{H}$ contains a nuclear space (whatever that is!) X (the ket vectors) that is continuously embedded in $\mathscr{H}$ (i.e., for $\varphi \in X$, $\|\varphi\|_{\mathscr{H}} \leq$ (const) $\|\varphi\|_X$, with $\|\cdot\|_X$ a continuous norm on X) and which is left "invariant" by H (i.e., $Hx \in X$ if $x \in X$). Then X^* (the bra vectors) contains $\mathscr{H}$ in a natural way ($\varphi \in \mathscr{H}$ acts as a functional on X via $x \to (\varphi, x)_{\mathscr{H}}$) and $X \subset \mathscr{H} \subset X^*$ will be called a Gel'fand triple for H. By duality, H acts on X^*. We say that $E_r - i\Gamma/2$ is a resonance energy of H if there is *some* Gel'fand triple for H and some $\varphi \in X^*$ with $H\varphi = (E_r - i\Gamma/2)\varphi$.

Resolvent Poles. We say that $E = E_r - i\Gamma/2$ is a resonant energy for H if there is some dense set $\mathscr{D}$ in $\mathscr{H}$, so that for all $\varphi \in \mathscr{D}$, $(\varphi, (H-z)^{-1}\varphi)$ has a meromorphic continuation from $\operatorname{Im} z > 0$ to a region including E, and so that E is a pole of this continuation.

We note that while the complex scaling type of resonance is usually stated in terms of the third notion, it can be rephrased in terms of the first two notions (see, e.g., Ref. 3).

There are several conventional criticisms of these caricatures, among them.

(a) Short-time complaint. If φ has finite energy (i.e., $(\varphi, H\varphi) < \infty$), then $F(t) = |(\varphi, e^{-iHt}\varphi)|^2$ is differentiable and must have zero derivative at $t=0$ (since $F(t) \leq F(0)$ for *all* real t). Since $F(t) = F(-t)$, $F(t) = e^{-\Gamma|t|}$ is impossible unless φ is to have infinite energy.

(b) Long-time or Paley–Wiener complaint. This is an argument that has been rediscovered often (with considerable fanfare) by a large number of authors. Suppose that H is bounded from below and that $F(t) = |(\varphi, e^{-itH}\varphi)|^2$ merely obeys $|F(t)| \leq Ce^{-A|t|}$ for some $A, C > 0$. The spectral theorem (see Ref. 4 for the necessary functional analysis) assures us that $(\varphi, e^{-itH}\varphi)$ is the Fourier transform of a measure, i.e.,

$$(\varphi, e^{-itH}\varphi) = \int e^{-i\lambda t}\, d\mu(x)$$

and $d\mu$ lives on the spectrum of H. The The Paley–Wiener theorem (indeed it's easy half) tells us that since $F^{1/2}$ has exponential falloff, $d\mu = g(x)\, dx$ with g analytic in a strip of width $\frac{1}{2}A$ about R (indeed, formally

$$\frac{d\mu(x)}{dx} = (2\pi)^{-1} \int e^{ixt} F^{1/2}(t)$$

by the Fourier inversion formula). Since $g(x) = 0$ for x below the lower bound for H, $g \equiv 0$. Thus $(\varphi, \varphi) = 0$.

The usual way out of the first two complaints is to demand that Eq. (1) hold approximately and only for times neither too short nor too long.

(c) Kitchen Sink complaint. If the space X in the Gel'fand triple is too small, then X^* will be so big that it will contain elephants, kitchen sinks, and "resonance eigenvectors" for *every* complex number E! For example, if $H = -\Delta$, $\mathscr{H} = L^2$, and $X = C_0^\infty$ (the smooth functions of compact support), then X^* (the distributions) will contain $e^{iz\cdot x}$ for any z in C^n and $-\Delta(e^{iz\cdot x}) = z^2(e^{iz\cdot x})$. (For the expert reader, I know that C_0^∞ is not nuclear by the usual Gel'fand definition, but one can modify the above if one insists on nuclearity.)

People fond of the Gel'fand triple method try to get rid of the kitchen sink by demanding that X not be too small.

The above complaints are all legitimate ones and are important but they miss a much more fundamental failure of the characters:

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

To illustrate this, let us consider the Stark effect in hydrogen. Let $H(\varepsilon) = -\Delta - 1/r + \varepsilon x$. We all believe that this has resonance: indeed Reinhardt [5] has told us where they are using dilation analytic methods (see Refs. 6–8 for discussion of related rigorous work). But for any nonzero $\varepsilon, \varepsilon'$ we can find, more or less explicity, a unitary operator $U(\varepsilon, \varepsilon')$ with

$$U(\varepsilon, \varepsilon')\, H(\varepsilon')\, U(\varepsilon, \varepsilon')^* = H(\varepsilon) \tag{2}$$

(For, let $H_0(\varepsilon) = -\Delta + \varepsilon x$.) Then [9]

$$V(\varepsilon)\, H_0(\varepsilon)\, V(\varepsilon)^* = x + p_y^2 + p_z^2$$

where $V(\varepsilon) = W(\varepsilon) \exp(ip_x^3/3\varepsilon)$ and $(W(\varepsilon)f)(x, y, z) = \varepsilon^{-1/2} f(\varepsilon^{-1}x, y, z)$ and [10]

$$\Omega(\varepsilon)\, H(\varepsilon)\, \Omega(\varepsilon)^* = H_0(\varepsilon)$$

where

$$\Omega(\varepsilon) = \operatorname*{s-lim}_{t\to\infty} \exp[iH_0(\varepsilon)t] \exp[-itH(\varepsilon)]$$

To get Eq. (2), let

$$U(\varepsilon, \varepsilon') = \Omega(\varepsilon)^*\, V(\varepsilon)^*\, V(\varepsilon')\, \Omega(\varepsilon')$$

The dilation analytic theory tells us that for suitable ε_0, $E(\varepsilon_0)$, and φ, $(\varphi, (H(\varepsilon_0) - z)^{-1}\varphi)$ has a pole at $E(\varepsilon_0)$ when continued. Equation (2) then implies that for any other ε: $(U(\varepsilon, \varepsilon_0)^*\varphi, (H(\varepsilon) - z)^{-1}\, U(\varepsilon, \varepsilon_0)^*\varphi)$ has a pole at the same point $E(\varepsilon_0)$. Thus in some sense, $(H(\varepsilon) - z)^{-1}$ has a pole at $E(\varepsilon_0)$ no matter what ε is. Of course, we are tempted to think that for $\varepsilon \neq \varepsilon_0$, the pole in

$(U(\varepsilon, \varepsilon_0)^*\varphi, (H(\varepsilon)-z)^{-1}U(\varepsilon, \varepsilon_0)^*\varphi)$ is not in the resolvent but in the vector. But for $\varepsilon = \varepsilon_0$, we think it is really in the resolvent. But why?

The point of the above is that lots of operators in physics are unitarily equivalent to each other so that any notion of resonance that is unitarily invariant (I was careful to state the caricatures in this way; e.g., in Eq. (2), there exists *some* X_0, etc.), is bound to give nonsensical answers. Thus one must have an extra structure around and one must be prepared to defend it!

Why make this big deal about Howland's Razor? It is not intended as a criticism of any explicit way of computing resonances in any explicit problem. The errors come when an attempt is made to abstract a procedure. Since we are brought up to think of abstract quantum mechanics as Hilbert space theoretical, too often the abstraction procedure does violate Howland's Razor. In the end, Howland's Razor is useful in understanding exactly what is involved in any resonance computing procedure.

What possible extra structures are there? One is the structure of configuration space (geometry) and another is consideration of a second operator or a family of operators. Explicit possibilities are the following.

(1) Scattering Theory

To my way of thinking, the only "satisfactory" notion of resonance is one that associates them to poles of the scattering amplitude analytically continued. Here the extra structure can be thought of either as an extra operator (most mathematical treatments of scattering [11] concentrate on the Møller wave operator comparison point of view) or as the geometric structure of space.

(2) Perturbation Problems

One may be able to define a resonance uniquely in terms of a one parameter family. For example, consider a resonance in the Stark problem discussed above obtained by dilation analytic methods; suppose that this "resonance eigenvalue" depends on ε in such a way that as $\varepsilon \to 0$, $E(\varepsilon)$ approaches an eigenvalue of $-\Delta - 1/r$. Then the general theory [6, 8] shows that for $|\varepsilon|$ small, $E(\varepsilon)$ has an analytic continuation from $[0, A)$ to $\{\varepsilon \mid \operatorname{Arg} \varepsilon \in [0, \pi], |\varepsilon| < A\}$ (for example) and for $\arg \varepsilon = \pi/4$ (say), $E(\varepsilon)$ will be an honest to goodness eigenvalue of $-\Delta + \varepsilon x - 1/r$. Thus the "resonance eigenvalue" is a continuation of an honest eigenvalue. This approach was emphasized by Howland [1].

(3) Geometric Structures

We use the geometry of spaces to pick out something distinguished. In the dilation analytic theory, we use the resolvent pole idea but not for any arbitrary dense set, $\mathscr{D}$. Rather $\mathscr{D}$ is the *fixed* set of dilation entire vectors (see Ref. 3). Of course, we need some good reason for thinking that when $(\varphi, (H-z)^{-1}\varphi)$ has a pole under continuation, its pole is "due to H" and not to $\mathscr{D}$. One can have some confidence since for $H_0 = -\Delta$, there are no poles. In the end, one should rely on a connection with scattering; these are partial results along these lines, see Ref. 3. Another example of the use of geometric structure is the classic work of Titchmarsh [12] who studies the x-space Green's function, $G(x, y; E)$, looking for poles in E for fixed x, y.

3. Complex Scaling: What Is Rigorously Known?

In this section, I want to summarize exactly what is known about dilation analytic potentials. There is extensive discussion (including proofs) of many of these things in the recently published fourth volume of Reed and Simon [13].

A. Basic Definitions: Continuation of Matrix Elements ([14]; for Stark [6, 8])

The founding fathers of the subject in their basic papers [14], introduced a basic class of operator perturbations. (We note that van Winter [38] introduced independently a closely related formalism.) This class was extended by Simon [15] with the idea of allowing "complex rotations" 2 Im θ with Im $\theta > \pi/2$. What arises are some basic classes $\mathscr{F}_\alpha$ and $\bar{\mathscr{F}}_\alpha$. Rather than give a precise definition, we give examples which include all those of physical interest.

Example. A central potential $V(r)$ will lie in $\mathscr{F}_\alpha$ if V has an analytic continuation into the sector $|\operatorname{Arg} r| < \alpha$ so that:

$$\text{(i)} \quad \lim_{\substack{r\to\infty \\ |\operatorname{Arg} r|<\beta}} |V(r)| = 0 \quad \text{for all } \beta < \alpha$$

and

$$\text{(ii)} \quad \lim_{\substack{r\to 0 \\ |\operatorname{Arg} r|<\beta}} r^{2-\varepsilon}|V(r)| = 0 \quad \text{for some } \varepsilon > 0 \text{ and all } \beta < \alpha$$

If V is continuous up to $|\operatorname{Arg} r| = \alpha$ and the limit conditions hold for $|\operatorname{Arg} r| \le \alpha$, then we say that V lies in $\bar{\mathscr{F}}_\alpha$. Thus $r^{-\gamma}$ lies in any $\bar{\mathscr{F}}_\alpha$ if $0 < \gamma < 2$, e^{-r}/r is in $\bar{\mathscr{F}}_{\pi/2}$ and e^{-r} is in $\mathscr{F}_{\pi/2}$ (it is not in $\bar{\mathscr{F}}_{\pi/2}$ since e^{-iy} does not go to zero as $y \to \infty$).

Definition. A vector η is said to be dilation analytic in the strip $|\operatorname{Im} \theta| < \alpha$ (we write $\eta \in A_\alpha$), if the spherical harmonic expansion $\eta = \sum \eta_{lm}(r) Y_{lm}(\theta, \varphi)$ has each $\eta_{lm}(r)$ analytic in $|\operatorname{Arg} r| < \alpha$ with

$$\sum_{l,m} \int_0^\infty |\eta_{lm}(r e^\theta)|^2 r^2 \, dr < \infty \quad \text{for all } \theta \text{ with } |\operatorname{Im} \theta| < \alpha$$

(This is given in three-dimensions; in multiparticle systems one needs the obvious generalization to $3N-3$ dimensions.)

The point of the above is that if one defines $(U(\theta)\psi)(r) = e^{3\theta/2}\psi(e^\theta r)$ for θ real, then η dilation analytic means that $U(\theta)\eta$ has a vector valued analytic continuation into the strip $|\operatorname{Im} \theta| < \alpha$. Moreover, $V \in \mathscr{F}$ means that if $H = -\Delta + V$, then $H(\theta) = U(\theta)\, HU(\theta) \equiv -e^{-2\theta}\Delta + V(\theta)$ has a continuation into the strip also (for a suitable sense of unbounded operator continuation; actually $(1-\Delta)^{-1/2} H(\theta)(1-\Delta)^{-1/2}$ has an operator norm convergent Taylor series).

By general principles, for any fixed vector ψ and *fixed* θ, $(\psi, (H(\theta)-z)^{-1}\psi) \equiv R_\psi(z)$, is an analytic function for z outside the spectrum of $H(\theta)$, $\sigma(H(\theta))$. $\sigma(H(\theta))$ breaks up into two parts σ_d and σ_e (for *discrete* and *essential*) so that $R_\psi(z)$ is meromorphic outside σ_e; i.e., has its worst poles at $\sigma_d(\theta)$. Now suppose that $V \in \mathscr{F}_\alpha$ and $\eta \in A_\alpha$ and consider

$$R_\eta(\theta, z) \equiv (U(\theta)\eta, (H(\theta)-z)^{-1}U(\theta)\eta)$$

which is analytic (respectively meromorphic) in $\{(\theta, z) | \operatorname{Im}\theta < \alpha; z \notin \sigma(H(\theta))\}$ (respectively, $z \notin \sigma_e(H(\theta))$). But for ϕ real

$$R_\eta(\theta, z) = R_\eta(\theta+\phi, z)$$

since $\theta \to \theta + \phi$ is unitarily implementable on both the vectors and the operators and matrix elements are unitarily invariant.

The spectrum of $H(\theta)$ moves "continuously," so that we can obtain multisheeted continuations of $(\eta, (H\text{-}z)^{-1}\eta)$ onto "$\cup$" $\{z | z \notin \sigma(H)\}$ (where "$\cup$" is in quotes since it is a multisheeted union) as follows: as $z \to \lambda + i0$, $\lambda \geq 0$, we begin to change θ so that the spectrum of $H(\theta)$ moves out of the way. One basic point is that $\sigma_d(\theta)$ is independent of θ (so long as points don't get "covered" by essential spectrum) while $\sigma_e(\theta)$ moves as $\operatorname{Im}\theta$ is changed. In a real sense, $\sigma_e(\theta)$ acts as "cuts" (which can move), while $\sigma_d(\theta)$ as "poles", which are invariant so long as we don't swing a branch cut over them. New eigenvalues "uncovered" by essential spectrum are *defined* to be resonances (see Fig. 1).

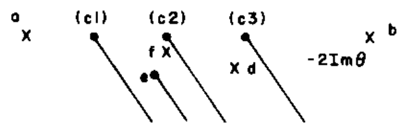

Figure 1. Typical $\sigma(H(\theta))$. (a) Discrete eigenvalue of $H(\theta=0)$. (b) Embedded eigenvalue of $H(0)$ becomes discrete. (c) Real thresholds. (d) "Resonance" eigenvalues. (e) "Resonance" thresholds. (f) "Resonance" uncovered by cut (c1) about to be recovered by cut (c2).

For Stark problems, the situation is much more complicated. $H(\theta)$ is very nonanalytic as $\operatorname{Im}\theta$ moves from 0, but there is still enough continuity to get some analyticity, "second sheet poles," etc. Moreover, there is the striking discovery of Herbst [6] that for $\operatorname{Im}\theta$ nonzero and small (actually $0 < \operatorname{Im}\theta < \pi/3$ will do), $\sigma(\theta)$ is purely discrete! I cannot describe the situation in this brief space; see Refs. 6–8 for details. I note that the class of allowable potentials is defined differently but includes those in the example above.

B. Thresholds as Branch Points [14]

Balslev and Combes [14] precisely described $\sigma_e(\theta)$ in terms of the spectrum of subsystems. Consider a potential V, which is a sum of $V_{ij}(r_i - r_j)$ with $V_{ij} \in \mathscr{F}_\alpha$. For each subcluster $C \subset \{1, \ldots, N\}$, let $H_C(\theta)$ denote the scaled Hamiltonian for

C with its center of mass motion removed. Let D denote a decomposition of $\{1, \ldots, N\}$ into disjoint clusters $C_1, \ldots, C_k$. Let

$$\Sigma(\theta) = \bigcup_D \{E_1 + \cdots + E_k \,|\, E_i \in \sigma_i(H_{C_i}(\theta))\}$$

For $\theta = 0$, these are precisely the scattering thresholds and, for arbitrary θ, we think of them as "complex thresholds." Then (see Fig. 1):

Theorem (Balslev and Combes [14]).

$$\sigma_{\text{ess}}(\theta) = \bigcup_{\lambda \in \Sigma(\theta), \mu \in (0,\infty)} \lambda + \mu\, e^{-2\theta}$$

This says that $\cup\Sigma(\theta)$ acts as the branch points for $(\eta, (H(\theta)-z)^{-1}\eta)$ under continuation and that the branch cuts come out at an angle $-2\operatorname{Im}\theta$.

A and B together lead to a technical result of interest to us rigorous types called the absence of singular continuous spectrum.

C. Information on $\sigma_{\text{disc}}(\theta)$

(a) Analytically of eigenvectors [14]. It follows from the general theory [14] that if ψ is an eigenvector for $H(\theta)$ and remains one for $H(\theta+\phi)$ with $|\operatorname{Im}\phi| < \beta$, then $\psi \in A_\beta$. Thus, $(U(\phi)\psi)(r)$ is a function of $re^{i\phi}$. This remark [16] is the basis of some techniques of numerical analysis by Ho and Junker.

(b) Real points of $\sigma_d(\theta)$ [14]. **Theorem** [14]. Let $0 < |\operatorname{Im}\theta| < \frac{1}{2}\pi$. Then $\sigma_d(\theta) \cap (-\infty, \infty) = \sigma_{pp}(H)/\Sigma(0)$ where $\sigma_{pp}(H)$ = eigenvalue of H.

This result says that eigenvalues of H, even those embedded in the continuous spectrum, remain under complex scaling. It implies an important distinction between eigenvalues of H and those of $H(\theta)$ (resonances). When a cut sweeps over a resonance, the resonance may disappear; indeed, it *must* if we sweep over the last cut before reaching $\theta = 0$. Eigenvalues of H persist. The intuition is simple: if θ_0 is a critical value at which a cut is just sweeping over a resonance, the resolvent may only have a pole as the cut is approached from one side. But at $\theta = 0$, self-adjointness implies that all poles must appear on *both* sides.

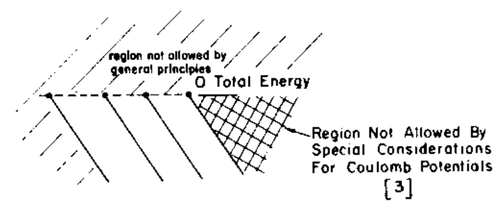

Figure 2. No resonance region for atoms.

(c) General limitation on $\sigma_d(\theta)$ [14]. (See Fig. 2.) **Theorem** [14]. Let $0 < \operatorname{Im}\theta < \frac{1}{2}\pi$. Let Σ_0 = bottom of the spectrum of H. Then *all* complex thresholds and resonances occur in the region $\{E | -2\operatorname{Im}\theta < \arg(E - \Sigma_0) < 0\}$.

This result comes from taking $\mathrm{Im}\,\theta$ back to zero and noting that it must happen that all complex resonances are hit by $\sigma_e(\theta)$ since they have to be hidden away before we reach a self-adjoint H.

(d) Absence of "positive" eigenvalues and resonance in atoms [3]. (See Fig. 2.) **Theorem** [3]. If each $V^{ij}=e_{ij}|r_i-r_j|^{-1}$, then for $0<\mathrm{Im}\,\theta<\frac{1}{2}$, $H(\theta)$ has no eigenvalues or thresholds in $\{E|-2\,\mathrm{Im}\,\theta<\arg E<0\}$.

This result has been extended to certain other homogeneous potentials by Balslev [17]; for the region $0<\mathrm{Im}\,\theta<\frac{1}{4}\pi$, a beautiful proof has been supplied by Hunziker [18], which we now give. We break our no-proof rule for two reasons: first, this is probably the one rigorous theoretical result that might be somewhat unexpected. Second, modulo the connection with scattering (see Sec. 3 F), this result has real experimental significance; indeed, it calls into doubt some experiments [19].

Proof [18]. Let $(\cdot,\cdot)$ denote the *usual* L^2 inner product (*not* the inner product $\int fg$ popular in calculations and in the variational principle for $H(\theta)$, but $\int \bar{f}g$). Then

$$E=(\psi, H(\theta)\psi)/(\psi,\psi)=e^{-2\theta}a+e^{-\theta}b$$

where E is an eigenvalue with eigenvector ψ. Here

$$a=\int|\nabla\psi|^2\Big/\int\psi^2>0 \quad\text{and}\quad b=\int V|\psi|^2\Big/\int|\psi|^2$$

is real, so E must have an argument between $-\mathrm{Im}\,\theta$ and $-\pi-\mathrm{Im}\,\theta$ (see Fig. 3). QED

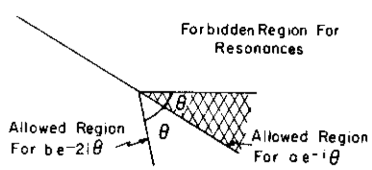

Figure 3. Hunziker's proof.

(e) Absence of positive eigenvalues [20]. **Theorem** [20]. If each V_{ij} lies in $\bar{\mathscr{F}}_{\pi/2}$, then H has no positive eigenvalues or real thresholds.

I emphasize that *no* assertion is made about resonances in the sector $-2\,\mathrm{Im}\,\theta<\arg E<0$; indeed, this theorem includes suitable Bargmann potentials [21] and some examples of Doolen [22] where resonances are known to occur. Moreover, note the overbar in $\bar{\mathscr{F}}_{\pi/2}$. We are in the absurd situation of having information on e^{-r}/r but not e^{-r}!

(f) Nonzero widths in the Stark problem. By using methods related to those in Ref. 20, Herbst and Simon [8] have proven that Stark Hamiltonians cannot have real eigenvalues in certain regions. In particular, for all small field, any given discrete eigenvalue of an atom must turn into a resonance.

D. *Perturbation of $\sigma_d(\theta)$*

We recall that by turning embedded eigenvalues into discrete eigenvalues of $H(\theta)$, one is able to study the process whereby a resonance is formed by coupling an eigenvalue to continuum via a perturbation. This is studied in detail in Ref. 3. There are two important results; there is a rigorous proof of the Fermi Golden Rule in a model (and the correct higher-order "time-dependent" theory) and a rigorous proof of convergence of the complete series.

For a beautiful application of dilation analytic methods to a coupling constant questions in atoms, see Ref. 23.

E. *Connection with Two-Body Scattering*

In Ref. 3, it was proven that for potentials falling off exponentially, "resonances" in the dilation analytic sense are the only suitable poles of the scattering amplitude. Balslev [24] has recently extended this to a much larger class of potentials. These results give one some reassurance that "resonances" really are resonances.

F. *N-Body Scattering*

In the early days of the dilation analytic theory, one hoped the methods would also lead to a solution of the basic asymptotic completeness problem of scattering theory and also to a number of neat formulas for scattering amplitudes. The naïve hope was based on the fact that complex scaling separated the different thresholds in two different ways ($\mathrm{Im}\,\theta>0$ or <0), presumably corresponding to the past and future. One imagined proving completeness by a two-step process. For each scattering channel, α, one has a threshold (we assume

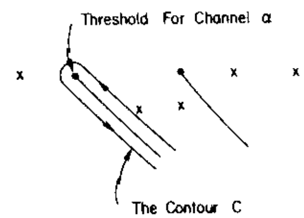

Figure 4. Contour defining of $P_\alpha^\pm(\theta)$.

no degeneracy in threshold). By drawing a contour C around the cut coming from this threshold (see Fig. 4), one tries to define for $\mathrm{Im}\,\theta>0$

$$P_\alpha^-(\theta)=(2\pi i)^{-1}\oint_C (z-H(\theta))^{-1}\,dz$$

The naive hope was that $\lim_{\varepsilon\downarrow 0}P_\alpha^0(i\varepsilon)$ would exist for each α and would be the orthogonal projection onto the out states for channel α. The statement of completeness, $\sum_\alpha P_\alpha^-=1-P_{\mathrm{bound}}$ would then follow from the much easier statement at nonzero θ; i.e., one uses the complex situation to disentangle the scattering channels whose entanglement complicates scattering theory.

Following this scheme turned out to be much harder than anyone had imagined. Just showing the convergence of the contour integral defining $P_\alpha^-(\theta)$ turned out to be nontrivial! This is because there is no norm falloff of the resolvent as infinity is approached parallel to the spectrum. Owing to hard work of van Winter [25] (for certain nonlocal dilation analytic potentials) and Balslev [26], one can define $P_\alpha^-(\theta)$ for suitable potentials.

A second difficulty in this scheme involves the $\varepsilon \downarrow 0$ limit and the following remark of Hagedorn and Simon [27]: $\lim_{\varepsilon\downarrow 0} P_\alpha^-(i\varepsilon)$ cannot be self-adjoint in multichannel systems. For $P_\alpha^-(i\varepsilon)^* = P_\alpha^+(-i\varepsilon)$, so self-adjointness of the limit would imply that the in states for channel α are the same as the out states for channel α, i.e., no scattering between channels. Put differently the separation of channels by complex scaling is too efficient: it completely stops the channels from communicating owing to conservation of energy. Staring at the physical literature [28] convinces one [27] that formally $P_\alpha^-(i0)$ wants to be the non-orthogonal projection onto the out states along the orthogonal complement of the in states. In general, I see no reason for these two subspaces to be complementary (i.e., for the P to be a bounded operator); for this reason I remain skeptical of any claims of controlling these projections on the limit!

Balslev [29] and van Winter [29] have announced substantial progress on following through with the above scheme; indeed for suitable nonlocal dilation analytic potentials, van Winter [29] has claimed asymptotic completeness with these methods.

Hagedorn [30] and Sigal [30] have announced completeness results for suitable local multiparticle dilation analytic potentials (Hagedorn for $N=4$, Sigal for any N) by methods which go beyond the above scheme. Hagedorn uses dilation analytically at only one point and it is far from clear that his methods are capable of establishing the link between scattering and "resonances." Sigal uses a clever refinement of the above projection scheme constructed to avoid the difficulty described. It seems likely that his methods will be able to establish the link between "resonances" and scattering.

Both Hagedorn and Sigal require generic couplings, i.e., they may need to change each coupling constant by a small amount and both require $r^{-2-\varepsilon}$ falloff. Recent exciting developments of Enss [31] appear likely to lead to a proof of completeness of scattering without these restrictions; indeed, he appears likely to be able to control atomic scattering! It is still not clear that his methods will yield the kind of detailed information made available by the resolvent techniques of Hagedorn and Sigal and, in particular, whether they shed any light on the resonance principle.

4. Complex Scalings: What We Would Like to Know

Here we mention three kinds of open mathematical problems connected with complex scaling.

A. *Scattering and Resonances*

In the complex scaling theory, a resonance was *defined* to be a complex eigenvalue of $H(\theta)$. Except for the two-body case, it remains to be shown that the "resonances" are the only possible poles of the analytically continued resolvent. Sigal's work [30] gives us hope that this problem may be solved in the near future.

B. *Rigorous Error Estimates on Eigenvalues of $H(\theta)$*

An especially simple error estimate for eigenvalues of self-adjoint operators is Temple's inequality [32] in the following form:

Theorem. If A is self-adjoint and $\|(A-E)\varphi\|^2 \leq \varepsilon\|\varphi\|^2$, then A has some spectrum in the interval $[E-\varepsilon, E+\varepsilon]$.

The proof is trivial by the spectral theorem. This result is not especially useful in actually trying to estimate the limit of some series of computer calculations, which will converge much more quickly than the ε above, but since it is rigorous, it will give some absolute bounds. It is especially important if some instabilities in the data make one uneasy. This is the situation occasionally in the calculation of resonance eigenvalues for $H(\theta)$. Alas, $H(\theta)$ is not self-adjoint or normal. This leads to:

Problem. Find some kind of analog of the above theorem for $H(\theta)$; more generally find any rigorous estimate on errors in computing resonance eigenvalues.

We note that one must be prepared to use some special property of the $H(\theta)$ since an arbitrary A may have no spectrum!

C. *Dilation Analyticity and Molecular Dynamics*

We have heard at this conference [33] the suggestion that one try to find "resonance excitation curves" for molecules by trying to complex scale a Born–Oppenheimer Hamiltonian. The problem is that one wants to consider only scaling the electrons but *not* the protons. To see the problem, let

$$V(x, y, z) = [(x-1)^2 + y^2 + z^2]^{-1/2} \equiv f(x, y, z)^{-1/2}$$

(of course, one would be foolish to dilate this about (0, 0, 0) rather than (1, 0, 0), but if one has a sum of Coulomb potentials about several points, one will obtain difficulties of the type described below).

Now fix θ. The condition $f(xe^{i\theta}, ye^{i\theta}, ze^{i\theta}) = 0$ is equivalent to $x = \cos\theta$, $y^2+z^2 = \sin^2\theta$, i.e., a circle for $\theta \neq 0$ (and small). Moreover, it is a "branch cut circle," in that the argument of V only changes by π if one loops around the circle. At first sight, it seems absurb to hope that $H(\theta)$ can be defined in any reasonable way. But the applicability of these methods to the Stark problem also seemed unlikely at first sight.

Question. Is there any notion of complex scaling for Born–Oppenheimer Hamiltonians? See *Note added in proof.*

5. What Other Complex Canonical Transformations Have Been Used

Complex scaling is one example of a real canonical transformation analytically continued in a parameter. Several others have been used in the literature:

A. Simple Complex Boosts

The three-parameter family $(U\psi)(x) = e^{ia \cdot x}\psi(x)$ acts by $x \to x$, $p \to p - a$; thus they are called "boosts." Any local potential is automatically "boost analytic," i.e., $U(a)VU(a)^{-1}$ is analytic in a (it's constant!). Moreover, $H_0(a) \equiv U(a)p^2U(a)^{-1} = (p-a)^2$ is analytic in a. As Im a is turned on, the spectrum of $H_0(a)$ blossoms out into a solid parabola; see Figure 5. The point of all this [34],

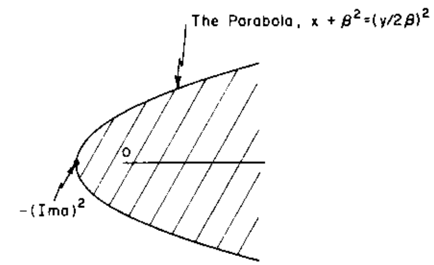

Figure 5. Spectrum of $(p-a)^2$.

is that discrete eigenvalues of $H_0 + V$ will be analytic vector for $U(a)$, i.e., $U(a)\psi$ will be in L^2 for suitable a. But this is just an assertion about exponential falloff of ψ!

B. "Complex" Complex Boosts

Motivated by Combes and Thomas [34], a number of unitary families of the form $(U(a)\psi)(x) = e^{iaf(x)}\psi(x)$ have been studied, i.e., $x \to x$, $p \to p - a(\nabla f)$. Falloff as e^{-x^m} has been studied for potentials V diverging at infinity in 35. Rather subtle falloff of atomic wave functions has been studied in Ref. 36 with f a homogeneous function of degree 1. Finally, in the Stark problem, it is important to have falloff as $\exp(-\delta x_+^{3/2})$ (the potential of the field goes to $+\infty$ as x goes to $+\infty$) and this is obtained by a complex boost argument [8].

C. Translation Analyticity

Avron and Herbst [9] have proposed the use of translation analyticity, i.e., $(U(a)\psi)(x) = \psi(x-a)$ as a way of studying Stark Hamiltonians.

D. Local Distortions

Babbitt and Balslev [37] and Thomas [40] have proposed an interesting technique, which only locally distorts the continuous spectrum. It has not been extensively studied although it may be quite promising; also see Jensen [39].

Note added in proof. One solution of Problem C of Sec. 4 has been given by Simon who calls his new method the method of "Exterior Complex Scaling." (See papers by Simon to be submitted to *Physical Review Letters* and *Annals of Physics.*)

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