

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

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1. Introduction

It is our goal in this paper to give a precise mathematical definition of the notion of “resonance” in a class of n -body non-relativistic quantum systems and to begin a systematic development of the theory of such resonances. While this class of n -body systems is rather small when viewed in relation to the class of systems [54] for which most of the standard quantum mechanical lore can be developed, it is large enough to include systems with two-body Coulomb, Yukawa or Yukawian interactions. The class thus includes the systems of greatest importance to physics and, in particular, it includes the standard non-relativistic model of the atom.

The principal line of development in this paper and the major new results which we wish to prove concern the so-called “time-dependent perturbation theory”, one of the two standard perturbation theories developed during the earliest days of quantum mechanics. The other standard theory, known as “time-independent” or Rayleigh-Schrödinger perturbation theory, has been on a firm mathematical footing since the work of Rellich [46]. (Important refinements of Rellich’s theory are due to Kato [35] and Sz-Nagy [59].) The time-dependent theory on the other hand has resisted a general mathematical formulation for over forty years although there has been some partly successful work on the subject which we will review later in this introduction. To avoid the natural confusion between “time-dependent” and “time-independent” we will generally avoid the use of the latter term, employing “Rayleigh-Schrödinger” and “Kato-Rellich” instead.

The lowest order terms in the time-dependent perturbation series were developed in the 1920’s as a means of computing radiative lifetimes of excited states of atoms. The quantity which is supposed to be approximated by this series is the inverse of the lifetime, τ , which was assumed to be

* Research supported in part by AFOSR under Contract No. F44620-71-C-0108

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related to the observed width, Γ , of spectral lines by the uncertainty principle relation $\Gamma = \hbar/\tau$ (if Γ is measured in energy units using the formula $E = \hbar\omega$). The most famous later use of lowest order terms in the series is probably the computations of lifetimes in Fermi's theory of β -decay. The second order term for the width, which is the lowest order non-vanishing term in the power series, is often known as "Fermi's Golden Rule" and is a standard tool in modern physics. It is an often discussed fact in the physics literature that the usual "textbook derivation" of the time-dependent series is internally inconsistent and there is not universal agreement among physicists concerning either the higher order terms in the series or the precise quantity which is being approximated.

We will not discuss either radiative or β -decay lifetimes in this article. The dynamics which control the perturbed systems in these cases are believed to be those of interacting quantum fields: While there has been important recent progress on the mathematical formulation of quantum field models (reviewed in [20]), one is still far from a precise theory of quantum electrodynamics or of weak interactions to which a perturbation series can be compared. Instead we will study a *physically realistic* model which can be phrased completely within the framework of non-relativistic quantum mechanics. In order to describe the mathematical problems and the physical ideas involved in time-dependent perturbation theory, let us briefly describe this model to which we will return in § 5.

Let H_0 be the Hamiltonian of a model helium atom in which we ignore the electron-electron repulsion (and also relativistic corrections, corrections due to the finite mass of the nucleus and corrections due to electron spin). Specifically, H_0 is an operator on $\mathcal{H} = L^2(\mathbf{R}^6, d^6x)$. We write $r \in \mathbf{R}^6$ as $r = \langle r_1, r_2 \rangle$ with $r_1, r_2 \in \mathbf{R}^3$ and write $-\Delta_i$ for the usual operator ($-\Delta_i f = \widehat{k_i^2} \widehat{f}$ on $L^2(\mathbf{R}^6)$, where $\widehat{}$ is the Fourier transform, $\widehat{}$ is the inverse Fourier transform and k_1, k_2 are the variables dual to r_1, r_2). Then (in units with $\hbar^2 = 2m = e^2 = 1$),

$$H_0 = -\Delta_1 - 2/r_1 - \Delta_2 - 2/r_2 .$$

In terms of the natural tensor product decomposition $L^2(\mathbf{R}^6) = L^2(\mathbf{R}^3) \otimes L^2(\mathbf{R}^3)$, H_0 has the form $H_0 = h_0 \otimes 1 + 1 \otimes h_0$ where h_0 is $-\Delta - 2/r$ on $L^2(\mathbf{R}^3)$. The spectrum of h_0 is well known to be $\{-1/n^2\}_{n=1}^\infty \cup [0, \infty)$. Thus the spectrum of H_0 is easy to describe. It has eigenvalues at $\{-1/n^2 - 1/m^2\}_{n,m=1}^\infty$ and continuous spectrum in $[-1, \infty)$. Write $E_{n,m}$ for $-n^{-2} - m^{-2}$ with $m > n$. The eigenvalues $E_{1,m}$ are discrete, but the eigenvalues $\{E_{n,m}\}_{n \geq 2}$ are embedded in the continuum.

Now consider Hamiltonians $H(\beta) = H_0 + \beta W$ where $W = 1/|r_1 - r_2|$ is the electron-electron repulsion and β is small and real. We are interested in the behavior of the eigenvalues $E_{n,m}$ under this perturbation. The Kato-Rellich theory deals with the discrete unperturbed eigenvalues $E_{1,m}$. It assures us that there is a function $E_{1,1}(\beta)$ analytic near $\beta=0$, so that $E_{1,1}(0) = E_{1,1}$ and so that $E_{1,1}(\beta)$ is an eigenvalue of $H_0 + \beta W$ for β small. The Taylor coefficients of $E_{1,1}(\beta)$ are precisely those given by the Rayleigh-Schrödinger series. For $m > 1$, $E_{1,m}$ is a degenerate eigenvalue of H_0 so the situation is more complicated but it is still completely understood [36, pp. 81-83].

The time-dependent perturbation theory is supposed to describe what happened to the eigenvalues $\{E_{n,m}\}_{n \geq 2}$ embedded in the continuum. For physical reasons which we will describe shortly, one expects these eigenvalues to "dissolve"; that is, one expects that for fixed n , $m \geq 2$, there is an $\varepsilon > 0$ and a $B > 0$ so that $H_0 + \beta W$ has no eigenvalues in $(E_{n,m} - \varepsilon, E_{n,m} + \varepsilon)$ if $0 < \beta < B$. Proving this is clearly a fairly subtle problem in the theory of spectra of partial differential operators. The situation is complicated by symmetry considerations which we discuss in § 5, but modulo these considerations, the proof that these eigenvalues do dissolve will be reduced to quadratures, i.e. to proving certain explicit integrals are non-zero (see Theorem V.1).

The goals of the time-dependent theory are much more ambitious than merely proving certain eigenvalues dissolve. Consider what we expect to happen if we try to solve the *perturbed* time-dependent Schrödinger equation $i\dot{\psi}(t) = -iH\psi(t)$ with initial condition $\psi(0) = \phi_{2,2}$ where $\phi_{2,2}$ is one of the continuum embedded eigenfunctions of H_0 with $H_0\phi_{2,2} = E_{2,2}\phi_{2,2}$. $\phi_{2,2}$ describes a state of the Helium atom in which both electrons are in excited states. Because of the repulsion, W , between the electrons, one expects $\psi(t)$ to describe a state as $t \rightarrow \infty$, where asymptotically one of the electrons is moving freely and the other is bound in a Helium ion. For obvious reasons, the states $\{\phi_{n,m}\}_{n \geq 2}$ are called *autoionizing states*. The time-dependent theory is supposed to compute a characteristic lifetime, τ , for the decay of a state like $\phi_{2,2}$ into an ion plus a free electron. It turns out to be a very hard problem to define the lifetime directly. The textbooks usually assume $|\langle \psi(t), \phi_{2,2} \rangle|^2$ has an exponential behavior of the form $\exp(-t/\tau)$ and derive formulae from such an ansatz but it is known that such behavior is impossible in an exact sense and cannot be even approximately accurate for t very small or very large.

A more devious method for defining τ goes back to a fundamental paper of Weisskopf and Wigner [65]. Their idea involves the notion of

resonance. Suppose we consider the scattering of electrons off Helium ions in their ground state at a total energy near $E_{2,2}$. We expect that one possible occurrence will involve "capture" of the electron into the almost bound state $\psi_{2,2}$ which will then decay. Therefore we expect that as a function of total energy, the scattering, σ , of electrons off Helium ions (written $e + \text{He}^+ \rightarrow e + \text{He}^+$) will have a "bump" near $E_{2,2}$. Such bumps are actually observed in this process and in the related electromagnetic processes of photoemission: $e + \text{He}^+ \rightarrow \text{He} + \text{photon}$ (called an Auger process) and photoionization: $\text{photon} + \text{He} \rightarrow e + \text{He}^+$ (some recent experimental data on autoionizing states may be found in [18, 40, 48, 49, 58]). The width, Γ , of the bump (or "resonance") is heuristically just "the uncertainty in the energy of the autoionizing state" which should be related to the lifetime, τ , by $\Gamma = \hbar/\tau$. The bumps are actually well approximated by a "Lorentzian line shape", $\sigma(E) \sim c^2[(E - E_0)^2 + (1/4)\Gamma^2]^{-1}$. The factor of 1/4 is included so that Γ is the width of the bump at half its maximum height, i.e. so that $\sigma(E_0 \pm \Gamma/2) = (1/2)\sigma(E_0)$. Differential cross-sections also exhibit such Lorentzian line shapes. It is known that $d\sigma/d\Omega$ is the square of a complex transition amplitude (the scattering amplitude), f , so Weisskopf and Wigner suggest that a resonance might correspond to a term $c[(E - E_0) + (i/2)\Gamma]^{-1}$ in f , i.e. to a pole in an analytic continuation of f to complex energies. Thus up to a factor of 2, we expect the time-dependent series to give the imaginary part of the position of a pole in the scattering amplitude. Since the real part of the position of the pole also shifts, one would expect there to be a perturbation series for this real part also. Physicists often lump the series for E_0 and $(1/2)\Gamma$ together as natural real and imaginary parts of a single series, also called the time-dependent series.

We will take a still simpler definition of E_0 and Γ which is one step further removed from the physical notion of lifetime. We will follow the suggestion of several authors [22, 39, 51] who propose that one look at poles in an analytically continued resolvent rather than at poles in the scattering operator; that is, we seek poles of $\langle \psi, (H - E)^{-1}\psi \rangle$ in some simple dense set of states. Of course we will have to discuss why these poles should be thought of as "intrinsically" associated to H rather than with the choice of ψ . Physically, the connection between poles in the resolvent and poles in the scattering amplitude is expected on the basis of certain formal expressions relating the two [21]. In any event, an important question, warranting further study, is the development of a scattering theory for the systems which we will study. Such a theory should be developed to the point where

the resonances we will define can be shown to be the only possible poles of the scattering amplitude. For a class of two-body systems, we will accomplish this goal in § 7.

Having concluded our discussion of the basic problem that we wish to consider, let us briefly describe previous approaches to the problem and present the plan of this paper. There seem to be two main lines of approach that have been used. One involves the study of simple models where the perturbation, W , is of finite rank or compact. Such an approach was initiated by Friedrichs [19] and developed by a variety of authors, most notably Howland in a series of papers [24, 25, 26, 28]. The Friedrichs-Howland approach involves viewing the resonance energy, $E_0 - (i/2)\Gamma$ as the pole of a resolvent. The second main approach involves introducing resonance energies as eigenvalues of a non-self-adjoint operator which is associated in some manner with the self-adjoint operator $H_0 + \beta V$ of direct interest. Notable examples of this method are the work of Livsic [38] and Grossman [22]; there is a summary of the literature relevant to this approach in [16].

Our basic attack involves the synthesis of these two approaches. Recently, Balslev and Combes [5] have developed a technique invented in the study of Regge theory [7, 9, 39] to give a rigorous proof of absence of singular continuous spectra in certain n -body Schrödinger systems. Their technique automatically associates a family of non-self-adjoint operators with H_0 and W . Eigenvalues of the associated operators are poles of an analytically continued resolvent. We review the basic definitions and theorems in the Balslev-Combes theory in § 2. Once one has the machinery of Balslev-Combes, the theory of perturbations of resonances will be reduced to the Kato-Rellich theory and in fact our major convergence results in § 3 will be fairly effortless mergings of the ideas of Balslev-Combes and those of Kato-Rellich. In § 4, we will verify that the lowest order terms in our convergent series are precisely those of the Fermi Golden Rule. We return to the example of autoionizing states in § 5, thereby presenting explicit examples of certain phenomena left open by Balslev and Combes. In § 6, we use ideas of Howland [26] to relate the phenomena of an embedded eigenvalue dissolving to the notion of spectral concentration [36, pp. 471-476]. Finally, in § 7, we discuss some special aspects of the theory in the two-body case.

After the appearance of an announcement of our major results [56] and the preparation of an earlier version of this manuscript, Howland [29, 30] independently arrived at some of our results by extending his earlier work. While his theory does not appear to be able to control Coulomb forces (and

thus autoionizing states), he answered one question left open in the original version of this manuscript. We have decided in this revised version to point out to the reader the analogues of our results in [30] and to rewrite those sections which involve the question answered in [30]. We have also incorporated some new work of our own [57] on extending the Balslev-Combes techniques.

It is a pleasure to thank E. Nelson and A. S. Wightman for a careful reading of the manuscript, and J. Howland for useful correspondence and for making his work available to me before publication.

2. The Balslev-Combes theorems and the definition of resonance

In this section we will review Combes' definition [12] of dilatation analytic potentials and the major technical results of Balslev and Combes [5]. This will enable us to standardize notation and also to present the main results of their theory unencumbered by the proofs which tend to be a little complicated.

Let T_0 be the free Hamiltonian, $-\Delta$, on $L^2(\mathbf{R}^3)$. Introduce, in the standard way, the Sobolev spaces, $\mathcal{H}_{+m} = \{\psi \in D(T_0^m) \mid \|\psi\|_{+m} = \|(T_0 + 1)^{m/2}\psi\|\}$ if $m = 0, 1, 2, \dots$ and \mathcal{H}_{-m} as the completion of \mathcal{H} in the norm $\|\psi\|_{-m} = \|(T_0 + 1)^{-m/2}\psi\|$. We will use $u(\theta)$ to stand for the one parameter family of unitary dilatations on $L^2(\mathbf{R}^3)$:

$$(u(\theta)f)(\vec{r}) = e^{3\theta/2}f(e^\theta\vec{r}).$$

We will primarily discuss the following class of operators on $L^2(\mathbf{R}^3)$ introduced by Combes and which we denote by C_α :

Definition. Let α be a positive real number. An unbounded operator V on $L^2(\mathbf{R}^3)$ is said to be in C_α if and only if:

- (i) $D(V) = D(T_0)$ and V is symmetric.
- (ii) The induced operator $V: \mathcal{H}_{+2} \equiv D(T_0) \rightarrow \mathcal{H}$ is (bounded and) compact.
- (iii) The operators $V(\theta): \mathcal{H}_{+2} \rightarrow \mathcal{H}$ given by $V(\theta) = u(\theta)Vu(\theta)^{-1}$ for θ real have an analytic continuation (with values in $\mathcal{B}(\mathcal{H}_{+2}, \mathcal{H})$, the bounded operators from \mathcal{H}_{+2} to \mathcal{H}) to the strip $\{\theta \mid |\operatorname{Im} \theta| < \alpha\}$.

In [57] Simon introduced a "form analogue" \mathcal{F}_α of C_α . Condition (i) was replaced with the requirement that V be a symmetric quadratic form with $Q(V) = Q(T_0)$, and $\mathcal{B}(\mathcal{H}_{+2}, \mathcal{H})$ in conditions (ii) and (iii) was replaced with $\mathcal{B}(\mathcal{H}_{+1}, \mathcal{H}_{-1})$. C_α is a subset of \mathcal{F}_α , by a "duality and interpolation argument". We will state all our results below for potentials in C_α . If one replaces operator sums by form sums and "perturbation theory of type (A)" by

“perturbation theory of type (B)”, all our results extend to \mathcal{F}_α .

We note that C_α contains power potentials, $[r^{-\alpha}(0 < \alpha < 3/2)$ including the Coulomb potential], Yukawa potentials $[r^{-1}e^{-\mu r}(\mu > 0)]$, and Yukawian potentials $\left[r^{-1} \int_{m_0}^{\infty} e^{-mr} d\mu(m)(m_0 > 0); \int d\mu < \infty \right]$. In Appendix 1, we precisely characterize those operators $V \in C_\alpha$ which are multiplication by some spherically symmetric function $v(r)$.

By (ii), any $V \in C_\alpha$ is a small perturbation of T_0 in the sense of Kato and Rellich [36], so $T_0 + V$ is self-adjoint on $D(T_0)$. More generally, let T_0 be the free Hamiltonian of an n -body system with center of mass, removed, i.e. $T_0 = -\sum_{i=1}^{n-1} \Delta_i$ on $L^2(\mathbf{R}^{3n-3})$. Let $V = \sum_{0 \leq i < j \leq n-1} V_{ij}(r_{ij})$ where $r_{ij} = \vec{r}_i - \vec{r}_j$ with $r_0 = 0$. Suppose that when viewed as an operator on $L^2(\mathbf{R}^3, d^3r_{ij})$ each V_{ij} is in some fixed C_α . Then $H = T_0 + V$ is a self-adjoint operator on $D(T_0)$. Balslev and Combes have found a beautiful way of continuing certain matrix elements of $(H - E)^{-1}$ onto second sheets.

Let $U(\theta)$ be the group of dilatations on \mathbf{R}^{3n-3}

$$(U(\theta)f)(r) = e^{(3n-3)\theta/2} f(e^\theta r) .$$

By the hypothesis that each $V_{ij} \in C_\alpha$, $V(\theta) \equiv U(\theta)VU(\theta)^{-1} = \sum_{i < j} V_{ij}(\theta)$ has a continuation into a strip $\{ \theta \mid |\text{Im } \theta| < \alpha \}$ and thus

$$H(\theta) \equiv U(\theta)HU(\theta)^{-1} = e^{-2\theta} T_0 + V(\theta)$$

has a continuation from the real axis to the strip $|\text{Im } \theta| < \alpha$. In this strip, $H(\theta)$ is an analytic family of type (A).

Balslev and Combes first of all study the spectrum of $H(\theta)$. Let $D = \{D_1, \dots, D_k\}$ be a decomposition of $\{0, \dots, n - 1\}$ into $k \geq 2$ clusters, i.e. $D_i \cap D_j = \emptyset$ if $i \neq j$; $\bigcup_{i=1}^k D_i = \{0, \dots, n - 1\}$. Let H_{D_i} be the Hamiltonian for the cluster D_i i.e. $H_{D_i} = T_{0,D_i} + V_{D_i}$ where T_{0,D_i} is the kinetic energy of the particles in D_i with center of mass removed and V_{D_i} is the set of interactions between particles in D_i . A bound state energy of $\sum H_{D_i}$, i.e. a sum of energies $E_{D_1} + \dots + E_{D_k}$ with E_{D_i} an eigenenergy of H_{D_i} , is called a k -body threshold. The family of all these is denoted Σ . Similarly we define thresholds of $H(\theta)$ and denote them as $\Sigma(\theta)$. Then:

THE FIRST BALSLEV-COMBES THEOREM [5]. *Under the assumptions that all the two-body potentials V_{ij} are in C_α , the spectrum of $H(\theta)[0 < \text{Im } \theta < \alpha]$ is explicitly given as (see Figure 1):*

(a) $\{z + e^{-2\theta} r \mid \text{all } z \in \Sigma(\theta); r \in \mathbf{R}^+\}$,

(b) *A set $\sigma_i(\theta)$ of isolated points of the spectrum which are eigenvalues of finite (geometric and algebraic) multiplicity. Moreover:*

(1) *The real eigenvalues and thresholds of $H(\theta)$ are precisely those of H .*

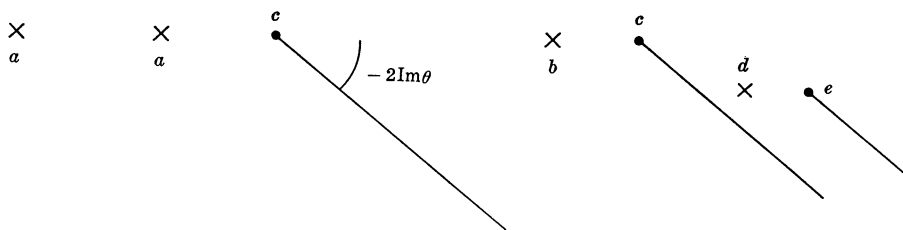


FIGURE 1. The Spectrum of $H(\theta)$

- (a) Discrete eigenvalue of H
- (b) Continuum-embedded eigenvalues
- (c) Thresholds of H
- (d) Resonance eigenvalues
- (e) Complex thresholds

(2) All non-real eigenvalues and thresholds (henceforth called resonance eigenvalues and complex thresholds) of $H(\theta)$ lie in the sector

$$\{z \mid 0 > \arg(z - \Sigma_{\min}) > -2 \operatorname{Im} \theta\},$$

where

$$\Sigma_{\min} = \inf \{x \mid x \in \Sigma \cap \mathbf{R}\},$$

and are only dependent on $\operatorname{Im} \theta$ (i.e. they are independent of $\operatorname{Re} \theta$).

(3) Complex thresholds and eigenvalues of $H(\theta)$ which are isolated from other parts of the essential spectrum of $H(\theta)$ are in $\sigma(H(\theta'))$ if $\operatorname{Im} \theta'$ is sufficiently near $\operatorname{Im} \theta$.

Remarks 1. Balslev and Combes only proved the above theorem for $\alpha < \pi/4$. In [57], the result was extended to arbitrary α .

2. There is an interesting mathematical problem associated with the proof of this theorem. One needs to know that $\sigma(A \otimes I + I \otimes B) = \sigma(A) + \sigma(B)$ for certain unbounded non-normal operators A, B . This is not easy to prove even when A and B are bounded [8, 50] and has only recently been proven for large classes of unbounded operators [32, 43].

Thus, one has the following picture of what happens to $\operatorname{spec}(H)$ as $\operatorname{Im} \theta$ increases. For $\operatorname{Im} \theta = 0$, there is essential spectrum beginning at the lowest threshold of H [31, 67] and a set of bound states some below the continuum, some that may be imbedded in the continuum. It is useful to think of the continuous spectrum, not merely as a half line emanating from the lowest threshold, but as a union of half lines, $[\lambda, \infty)$ for each $\lambda \in \Sigma$.

As $\operatorname{Im} \theta$ “turned up” from 0, the bound states stay fixed but the continuous spectrum swings out into the lower half plane. As it swings out, it can “uncover” some complex eigenvalues and thresholds which stay fixed

unless they happen to get covered again (see Figure 3). In particular, eigenvalues imbedded in the continuum become isolated points of the spectrum of $H(\theta)$.

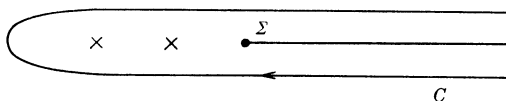


FIGURE 2a

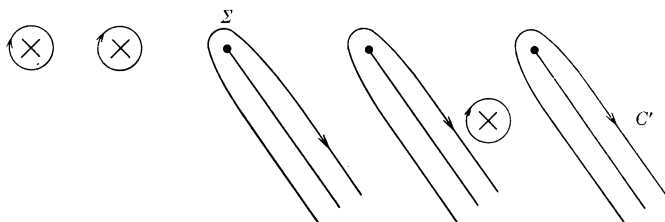


FIGURE 2b

FIGURE 2. Behavior of $\langle \psi, e^{-iHt}\psi \rangle$

Combes original discussion of dilatation analytic potentials in the two-body case [12, 2] included the idea of analytically continuing matrix elements of the resolvent between dilatation analytic vectors onto the second sheet. This idea was extended by Balslev and Combes to the n -body case. A dilatation analytic vector is a vector, ψ , for which $U(\theta)\psi$ has an analytic continuation into a strip $|\text{Im } \theta| < \alpha$. These are precisely the analytic vectors (in the language of Nelson [42]) for the generator $D = (1/2)(\vec{r} \cdot \vec{\nabla} + \vec{\nabla} \cdot \vec{r})$ of the dilations. Any vector $\psi = e^{-|D|\alpha}\phi$ (with $\phi \in L^2$) has an analytic continuation to the strip so the dilatation analytic vectors are dense. Let N_α be the vector space of all vectors, ϕ , for which $\sum_{n=0}^\infty ((i\theta)^n/n!)D^n\phi$ has radius of convergence α or more (these are precisely the vectors for which $U(\theta)\phi$ has a continuation to the strip [42]).

The second main theorem of Balslev and Combes (which follows easily from the first!) is:

THE SECOND BALSLEV-COMBES THEOREM. *Let $\psi \in N_\alpha$. Let H be an n -body system with two-body potentials in C_α . Then $(\psi, (H-z)^{-1}\psi) = f(z)$ originally defined for $z \in \mathbb{C} \setminus \text{spec}(H)$ has a (many-sheeted) continuation onto the union of the complements of the spectra of all $H(\theta)$ with $|\text{Im } \theta| < \alpha$.*

Thus on a dense set, the resolvent has an analytic continuation with singularities only at real (or complex) eigenvalues (poles) and thresholds (branch points). We define a resonance energy as a complex eigenvalue, E ,

of $H(\theta)$ for some θ in the strip $\{\theta \mid |\operatorname{Im} \theta| < \alpha\}$. The width, Γ , of the resonance is defined by $\Gamma = 2 |\operatorname{Im} E|$.

Remarks 1. In the two-body case, this definition was already suggested by Aguilar and Combes [2].

2. $\bigcap_{\beta > \alpha} N_\beta$ with the norm $\|\psi\|_\alpha^2 = \|\psi\|^2 + \|e^{\alpha D}\psi\|^2$ is a pre-Hilbert space, whose completion N_α^- , is a subset of L^2 . If all the potentials are in $\bigcup_{\beta > \alpha} C_\beta$, then $T_0 + V$ is a densely defined operator on N_α^- and the resonance theory of Grossman [22] based on the scale of spaces $N_\alpha^- \subset L^2 \subset N_\alpha^*$ is applicable. His definition of resonance energy is identical to ours, although our choices of “eigenvector” differ from his.

Our definition of resonance seems to associate certain complex eigenvalues to $H = T_0 + V$; one can ask whether they are intrinsic to H alone. The answer is clearly no; they are associated to the pair $\langle H, U(\theta) \rangle$ of H together with the unitary group. The interesting fact is that these resonance eigenvalues can be associated with a pair $\langle H, H_0 \rangle$ in at least two distinct ways:

(1) Howland [30] has remarked that resonances which arise by the mechanism of §§ 3, 4 are intrinsic to the family of operators $H_0 + \beta V$, where $H_0 = T_0 + W$ has eigenvalues embedded in the continuum and both V and W are sums of C_α potentials. As we will see in § 3, $H_0 + \beta V$ typically has resonances $E(\beta)$ near these embedded eigenvalues which for β real, ($\beta \neq 0$) are complex and thus not eigenvalues of $H_0 + \beta V$. What Howland remarks is that for some β complex $E(\beta)$ will be an actual eigenvalue of $H_0 + \beta V$ and that the resonance eigenvalues $E(\beta)$ (β real) can thus be thought of as analytic continuations of functions which are actual eigenvalues of $H_0 + \beta V$ when β is complex. We return to Howland’s interpretation at the end of § 3.

(2) In the two-body case, we will prove that these resonances are poles of the analytic continuations of a scattering amplitude. Since scattering in the two-body case is associated with the pair $\langle H, T_0 \rangle$, the physical picture of § 1 gives resonance a meaning intrinsic to a pair of operators. A major open question involves extending this “scattering pole interpretation” to the n -body case.

Finally, we should mention a few words about resonances in relation to characteristic lifetimes in time decay phenomena. Our discussion will be formal on this point. Let ψ be a state “close” to a resonant state in the sense that (i) $\psi \in N_{\alpha+\varepsilon}$ (ii) $H(i\alpha)$ has an eigenvector ϕ_0 and a resonance energy $E = E_0 - i\Gamma/2$ (iii) $\psi(i\alpha)$, the analytic continuation of $U(\theta)\psi$ to $\theta =$

$i\alpha$, is close to ϕ_0 in norm. If ψ is our state at time $t = 0$, then, $P(t)$, the “probability of still being on ψ ” at time t is the square of

$$a(t) = \langle \psi, e^{-iHt}\psi \rangle .$$

If ψ is a sufficiently nice vector in the sense that $d\langle \psi, E_\lambda \psi \rangle$ falls off exponentially where dE_λ is the spectral measure associated to H , then

$$a(t) = (2\pi i)^{-1} \oint_C \langle \psi, (H - \lambda)^{-1}\psi \rangle e^{-i\lambda t} d\lambda$$

where C is a contour going around $\sigma(H)$ as in Figure 2a. We can now simultaneously rotate C and replace $\langle \psi, (H - \lambda)^{-1}\psi \rangle$ with $\langle U(\theta)\psi, (H(\theta) - \lambda)^{-1}U(\theta)\psi \rangle$ (Figure 2b) to find

$$\begin{aligned} a(t) &= (2\pi i)^{-1} \int \langle \psi(i\alpha), (H(i\alpha) - \lambda)^{-1}\psi(i\alpha) \rangle e^{-i\lambda t} \\ &= \langle \psi(i\alpha), \bar{\phi}_0 \rangle \langle \phi_0, \psi(i\alpha) \rangle e^{-iEt} + r(t) \end{aligned}$$

where $r(t)$ represents contributions from the other poles and the cuts. Thus

$$P(t) = ce^{-\Gamma t} + R(t)$$

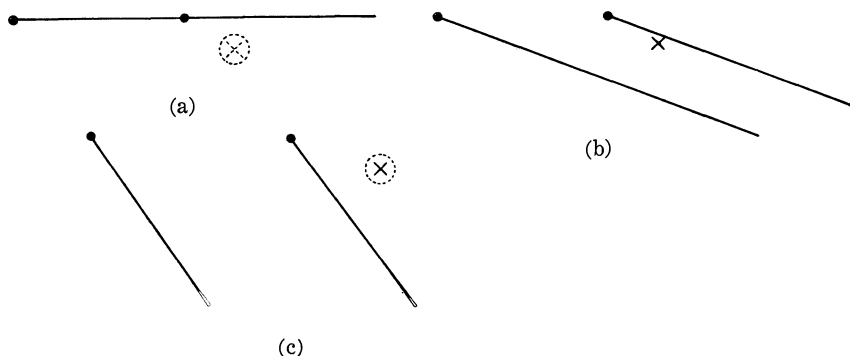
where c is close to 1 and R is “small”. Here we can see explicitly that $P(t)$ is not exponential for large times (because any contribution to $R(t)$ from real energy poles or from the cuts will fall off more slowly than $e^{-\Gamma t}$). And since $\dot{a}(0)$ is purely imaginary and $a(0) = 1$, we see $\dot{P}(0) = 0$, so $P(t)$ is not exponential for small times. But for times neither too small or too large, $P(t)$ falls off with a characteristic lifetime $\tau = \Gamma^{-1}$.

3. Perturbation theory for resonances

Suppose that V is a sum of two-body potentials in C_α for some $\alpha > 0$, and that W is also a sum of two-body potentials in C_α for some $\alpha > 0$. Consider perturbing $T_0 + V$ by adding βW . It is natural to want to know if the position of resonances of $T_0 + V + \beta W$ are analytic in β for β small. That they are is an elementary exercise in Kato’s perturbation theory [36]. First we define:

Definition. Suppose E_0 is a resonance energy for $T_0 + V$, i.e. E_0 is a discrete eigenvalue of $H(\theta)$ for some θ . We say E_0 is a *simple* (or non-degenerate) *resonance* if and only if E_0 is a simple eigenvalue of $H(\theta)$.

By the techniques of Balslev-Combes, this definition is independent of the choice of $\text{Im } \theta$ as long as there isn’t a change of sheet (see Figure 3). Since $W(\theta)$ is a Kato small (type A) perturbation of $H(\theta)$ it follows that [36, pp. 366–379]:

FIGURE 3. Resonance Uncovered and Recovered as $\text{Im } \theta$ Varies

THEOREM 3.1. *Let V and W be sums of two-body potentials in C_α . Let E_0 be a non-degenerate resonance of $T_0 + V$. Then for $|\beta|$ small, there is exactly one resonance of $T_0 + V + \beta W$ near E_0 ; it is simple also, and its position, $E(\beta)$, is analytic near $\beta = 0$. In particular, the width $\Gamma(\beta) = i[E(\beta) - \overline{E(\beta)}]$ is analytic in β also.*

Remark. This theorem remains true if “resonance” is replaced with “resonance or embedded eigenvalue” in both places where “resonance” appears. The interesting phenomenon is that the embedded eigenvalues can become resonances. This is the situation we discuss more fully in §§ 4, 5.

We are now able to describe Howland’s interpretation of “resonance” [30], an interpretation to which we alluded in the last section. Suppose E_0 is a non-degenerate real eigenvalue of H_0 and hence of $H_0(\theta)$, but that $E(\beta)$ is a non-real eigenvalue of $H_0(\theta) + \beta W(\theta)$ when β is real; i.e. $\text{Im } E(\beta) < 0$ for $|\beta|$ small and real. Then for suitable non-real values of β , $\text{Im } E(\beta) > 0$, i.e. $H_0(\theta) + \beta W(\theta)$ has an eigenvalue $E(\beta)$ near E_0 with $\text{Im } \theta > 0$, and $\text{Im } E(\beta) > 0$. Taking $\text{Im } \theta \rightarrow 0$, $E(\beta)$ remains a complex eigenvalue of $H_0 + \beta W$. Thus, E_0 is an embedded real eigenvalue of H_0 . For certain non-real values of β , with $|\beta|$ small, there is a unique (discrete) eigenvalue, $E(\beta)$, of $H_0 + \beta W$ near E_0 . The resonance eigenvalues are just the values of the analytic continuations of $E(\beta)$ to the real β axis. Thus, following Howland, one has a characterization of resonance eigenvalues in terms of the pair (H_0, W) .

Let us return to the general perturbation theory for resonance. In general, E_0 is an eigenvalue of $H(\theta)$ of multiplicity k , there are exactly k eigenvalues of $H(\theta) + \beta W(\theta)$ near E_0 (counting degenerate eigenvalues a number of times equal to their degeneracy) and their positions are all the values of one or more multivalued functions analytic in multisheeted

punctured neighborhoods of $\beta = 0$ with algebraic singularities of order $m \leq k$ at $\beta = 0$.

In a simplified model of the form $H_0 + \beta W$ where H_0 is self-adjoint with a multiplicity two eigenvalue embedded in the continuum and where W is a finite rank self-adjoint (bounded) perturbation, Howland [29, 30] has shown that non-integral powers of β can actually occur in the Puiseux series for the resonance eigenvalue, $E(\beta)$, resulting from the embedded eigenvalue. This is in sharp distinction to the case of perturbation of a discrete eigenvalue (Rayleigh-Schrödinger theory). In the discrete case, it is a theorem of Rellich [46] (see also [11, 66]) that if H_0 and W are self-adjoint and W is a regular perturbation of H_0 , then all discrete eigenvalues of H_0 become eigenvalues, $E(\beta)$, of $H_0 + \beta W$, which are analytic at $\beta = 0$. This result is not applicable to $H_0(\theta) + \beta W(\theta)$ ($\text{Im } \theta \neq 0$) since $H_0(\theta)$ and $W(\theta)$ are not self-adjoint. Howland’s example shows that one can have non-analytic (but algebraic) singularities of $E(\beta)$ at $\beta = 0$ in degenerate time dependent perturbation theory even if H_0 and W are self-adjoint. This interesting distinction between the time-dependent and the time-independent theories seems to have never been noticed in the physics literature. One probable reason for this is that if non-analyticity does occur, it occurs only in a fairly high order:

THEOREM 3.2. *Let E_0 be a non-threshold, non-isolated real eigenvalue of $T_0 + V$ where V is a sum of self-adjoint two-body dilatation analytic potentials. Let W also be a sum of self-adjoint two-body dilatation analytic potentials. Let $E(\beta)$ be any resonance energy of $T_0 + V + \beta W$ going to E_0 as $\beta \rightarrow 0$. Then*

$$E(\beta) = E_0 + a_1\beta + a_2\beta^2 + o(\beta^2); \quad a_1 \text{ real}; \quad \text{Im } a_2 < 0 .$$

Proof. By the general theory, $E(\beta)$ is an eigenvalue of $T_0(\theta) + V(\theta) + \beta W(\theta)$ and is one of several branches $E^{(1)}(\beta), \dots, E^{(p)}(\beta)$ with

$$E^{(k)}(\beta) = \sum_{n=0}^{\infty} a_{n/p} |\beta|^{n/p} e^{ik(\arg \beta)n/p} .$$

The crucial fact is that $\text{Im } E^{(k)}(\beta) \leq 0$ for all real β and all branches (by the first Balslev-Combes theorem). It follows that $a_{p-1}, \dots, a_{p-1(p-1)} = 0$; a_1 is real; $a_{1+p-1}, \dots, a_{1+p-1(p-1)} = 0, \text{Im } a_2 \leq 0$.

Remarks 1. A result of this genre has been proven independently by Howland (Theorem 1.2 of [30]).

2. Howland [30] has examined in detail how the different branches of $E^{(k)}(\beta)$ (dubbed by him a “cluster of resonances”) act in concert to produce

a resolvent $(H(\theta) + \beta V(\theta) - z)^{-1}$ analytic at $\beta = 0$ despite the occurrence of non-analytic polar terms $(E^{(k)}(\beta) - z)^{-1} P^{(k)}(\beta)$.

3. Because of Theorem 3.2, the *generic behavior* at $\beta=0$ of the resonance eigenvalues $E^{(k)}(\beta)$ for self-adjoint H_0 and V with a degenerate unperturbed embedded eigenvalue is quite different from the generic behavior in the case where H_0 and V are non-self-adjoint and the unperturbed eigenvalue is discrete and degenerate (which is the other case where non-analyticity at $\beta = 0$ can occur). In the discrete non-self-adjoint, degenerate case, the generic behavior is non-analyticity at $\beta = 0$; in fact generically fractional powers β^α with $0 < \alpha < 1$ occur. However, if no terms of fractional order β^α , $0 < \alpha < 1$ occur, there is a simple mechanism for "removing the degeneracy in first order" [36, pp. 81-83]. For those non-self-adjoint H_0 and V where no β^α ($0 < \alpha < 1$) terms occur, the generic situation is to have all degeneracies removed to first order. Since Theorem 3.2 prevents fractional powers from appearing before order 1, the generic situation in the degenerate time-dependent theory is to have analyticity at $\beta = 0$. This is illustrated in Howland's example where there is a free parameter ϵ in $(0, 1)$. Non-analyticity only occurs for a single value of ϵ .

4. The Fermi Golden Rule

It has been clear for many years that the Fermi Golden Rule is the right answer; what has been unclear is the right question! In the last section, we showed that an eigenvalue embedded in the continuum can turn into a resonance (Figure 4) when a suitable perturbation is turned on. If the eigenvalue is at non-threshold and is non-degenerate, the width $\Gamma(\beta) = +i[E(\beta) - \overline{E(\beta)}]$ is given by an analytic function. Our goal is to show that the lowest possible non-zero term for $\Gamma(\beta) = b_2\beta^2 + \dots$, is given by the Fermi Golden Rule or more precisely by an exact mathematical formula which is heuristically equal to the (rather imprecisely defined) physics text book version of the Golden Rule.

THEOREM 4.1. *Let V and W be sums of two-body potentials in C_α . Let E_0 be a non-degenerate non-threshold eigenvalue of $T_0 + V$ with eigenvector ψ_0 . For $|\beta|$ small, let $E(\beta)$ be the resonance of $T_0 + V + \beta W$ near E_0 ; $E(\beta) = E_0 + a_1\beta + a_2\beta^2 + \dots$. Let \tilde{P}_Ω be the spectral projection for $T_0 + V$ with the projection onto ψ_0 removed (i.e. $\tilde{P}_\Omega = P_\Omega$ if $E_0 \notin \Omega$; $\tilde{P}_\Omega = P_\Omega - (\psi_0, \cdot)\psi_0$ if $E_0 \in \Omega$). Then*

(a) $f(E) = (W\psi_0, \tilde{P}_{(E_0-\delta, E)} W\psi_0)$ is C^∞ near $E = E_0$.

(b) $\text{Im } a_2 = \pi(df/dE)|_{E=E_0}$.

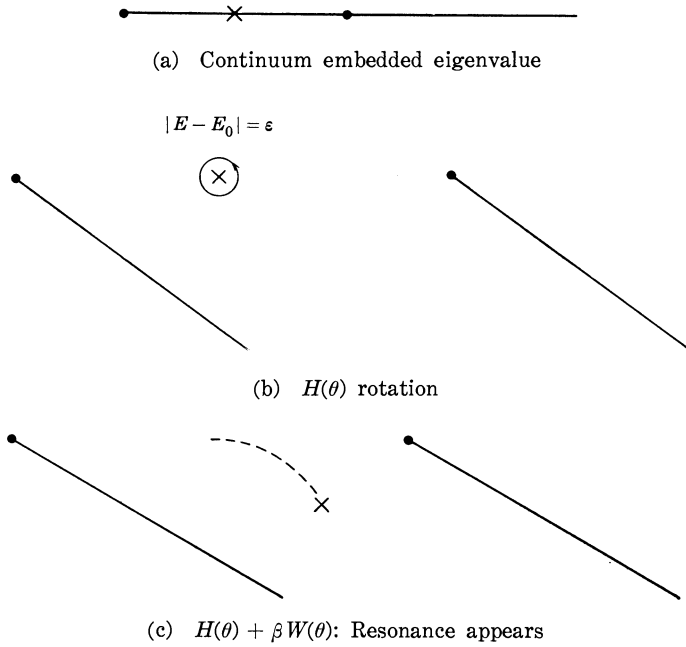


FIGURE 4. A Continuum Eigenvalue Turns into a Resonance

Proof. For $\text{Im } \theta \neq 0$, define

$$P(\theta) = (-2\pi i)^{-1} \int_{|E-E_0|=\epsilon} dE(H(\theta) - E)^{-1}.$$

Let $\psi(\theta) = P(\theta)\psi_0$. By a result of Balslev and Combes [5; see also 2], $\psi(\theta)$ has an analytic continuation to the strip $|\text{Im } \theta| < \alpha$ with $\psi(\theta) = U(\theta)\psi_0$ for θ real, i.e. $\psi_0 \in N_\alpha$. Since $W \in C_\alpha$ and $W: D(T_0) \cap N_\alpha \rightarrow N_\alpha$, $W\psi_0 \in N_\alpha$. $[(W\psi_0)(\theta) = W(\theta)\psi(\theta)]$. By the second Balslev-Combes theorem, $(\overline{W\psi_0}, (H - z)^{-1}W\psi_0)$ has an analytic continuation onto a second sheet neighborhood of E_0 except for a pole term $(\overline{W\psi_0}, P_0 W\psi_0)/(E_0 - z)$ at $E = E_0$. Here $P_0 = (\psi_0, \cdot)\psi_0$. By Stone's formula,

$$f(E) = \lim_{\epsilon \downarrow 0} \int_{E_0-\delta}^E du \text{Im} \left[\frac{1}{\pi} \langle W\psi_0, (H - u - i\epsilon)^{-1} W\psi_0 \rangle - \frac{1}{\pi} \frac{\langle W\psi_0, P_0 W_0 \rangle}{E_0 - z} \right].$$

Thus f is C^∞ as the integral of the imaginary part of an analytic function.

To compute a_2 pick $\text{Im } \theta > 0$ but small. Then (Figure 4b) [36, pp. 77-80]:

$$a_2 = -(2\pi i)^{-1} \oint_{|E-E_0|=\epsilon} \frac{dE}{E_0 - E} (\overline{\psi(\theta)}, W(\theta)(H(\theta) - E)^{-1} W(\theta)\psi(\theta)).$$

Now

$$g_\theta(E) = (\overline{\psi(\theta)}, W(\theta)(H(\theta) - E)^{-1} W(\theta)\psi(\theta))$$

has a pole term $(\overline{\psi}(\theta), W(\theta)P(\theta)W(\theta)\psi(\theta))/(E_0 - E)$ at $E = E_0$, so a_2 , which is the residue of $g_\theta(E)/(E_0 - E)$ at $E = E_0$, is given by

$$\begin{aligned} a_2 &= \lim_{E \rightarrow E_0} [(\overline{\psi}(\theta), W(\theta)(H(\theta) - E)^{-1}W(\theta)\psi(\theta)) - \text{Pole term}] \\ &= \lim_{\varepsilon \downarrow 0} [(\psi_0, W(H - E_0 - i\varepsilon)^{-1}\psi_0) - \text{Pole term}] \end{aligned}$$

where we have used the fact that if $\text{Im } E > 0$, $(\psi(\theta), W(\theta)(H(\theta) - E)^{-1} \times W(\theta)\psi(\theta))$ can be continued to $\theta = 0$. It thus follows that

$$\text{Im } a_2 = \pi \left. \frac{df}{dE} \right|_{E=E_0}.$$

Remarks 1. Howland [29, 30] has proven a similar result for a different class of interactions (which includes Yukawa but not Coulomb potentials). If E_0 is degenerate, but the degeneracy is removed at first order, he has shown that a simple modified Golden Rule holds where ψ_0 in (a) of Theorem 4.1 is replaced with the various eigenvectors of P_0VP_0 . A similar result holds in our situation and can be proved by using the formula for a_2 from degenerate Kato-Rellich theory [36].

2. There is a formal connection between the formula $\text{Im } a_2 = \pi(df/dE)|_{E=E_0}$ and the more usual statements of the Fermi Golden Rule. If $T_0 + V$ has "continuum eigenfunctions" $\psi_n(E)$, then

$$P_{(E_0-\delta, E)} = \sum_n \int_{E_0-\delta}^E (\psi_n(E), \cdot) \psi_n(E)$$

so that formally the second order term for Γ is

$$\begin{aligned} 2\text{Im } a_2 &= 2\pi \sum_n (W\psi_0, \psi_n(E_0))(\psi_n(E_0), W\psi_0) \\ &= 2\pi \sum_n |(\psi_n(E_0), W\psi_0)|^2 \end{aligned}$$

which is the usual statement of the Golden Rule.

3. Since Γ is analytic at $\beta = 0$, we have shown that for small perturbation, the width of the resonance is given by a convergent perturbation series.

4. One would like to say that the higher order terms in our series agree with the "usual" terms in the physicists time-dependent perturbation series. There is unfortunately great confusion in the physics literature concerning the "correct" higher order terms. There seems to be two sources of this confusion: first to lowest order in β^2 , the imaginary part of the position of a pole in the scattering amplitude and the residue of the pole agree in the two-body case; many authors are unclear about the object for which they are finding a series. Secondly the Fermi Golden Rule is so simple that many authors have attempted to guess the correct high order terms to preserve this simplicity; the usual textbook derivation of the Fermi Golden Rule is

unfortunately so vague that if one has one's heart set on particular higher order terms, then one can "justify" them within the vague framework. Of course the higher order terms of the real convergent series are complicated just as the higher order terms in the Rayleigh-Schrödinger series are complicated. Our higher order terms agree with those obtained by the physicists who have found the correct series!

5. Autoionizing states in a Helium atom model

In this section, we apply the general theory of §§ 3, 4 to the case of autoionizing states of the Helium atom in the model discussed in § 1. The additional complication in this Helium model where $\mathcal{H} = L^2(\mathbf{R}^6, d^3r_1, d^3r_2)$ and

$$H_0 = -\Delta_1 - \Delta_2 - 2r_1^{-1} - 2r_2^{-1}$$

$$W = 1/|\vec{r}_1 - \vec{r}_2|$$

is that the embedded eigenvalues of H_0 are degenerate. In fact $E_{n,m} = -n^{-2} - m^{-2}$ has degeneracy $(nm)^2$. There is a venerable technique in the physical literature to reduce a highly degenerate eigenvalue perturbation problem to a set of less degenerate problems: namely the use of symmetries.

In abstraction, suppose A and B are self-adjoint operators on some Hilbert space \mathcal{H} . Let G be a compact topological group represented by unitary operators $\{U(g)\}_{g \in G}$. Suppose A commutes with $U(g)$ (in the sense that $e^{iAt}U(g) = U(g)e^{iAt}$ for all $t \in R, g \in G$) and that similarly B commutes with $U(g)$. Let R_G be an index set labeling all the irreducible representations of G . For each $\alpha \in R_G$ let $\mathcal{H}_\alpha \subset \mathcal{H}$ be the maximal subspace of \mathcal{H} which is left invariant by $U(g)$ and on which $U(g)|_{\mathcal{H}_\alpha}$ is a direct sum of representations equivalent to the representation, D_α , indexed by α . Then $\mathcal{H} = \bigoplus_{\alpha \in R} \mathcal{H}_\alpha$ and both A and B leave each \mathcal{H}_α invariant by Schur's lemma. Pick a maximal commutative subgroup $M \subset G$. For each $\alpha \in R$, let $m_1^{(\alpha)}, \dots, m_k^{(\alpha)}$ denote the sets of distinct sets of eigenvalues of the operators $\{D_\alpha(g)\}_{g \in M}$. Let $\mathcal{H}_{\alpha,i} = \{\psi \in \mathcal{H}_\alpha \mid U(g)\psi = m_i^{(\alpha)}(g)\psi\}$. A and B leave each $\mathcal{H}_{\alpha,i}$ invariant and the families $A + \beta B|_{\mathcal{H}_{\alpha,i}}$ are unitarily equivalent for $i = 1, \dots, k(\alpha)$. Notice if G is a connected semi-simple Lie group, we can replace M with a Cartan subalgebra of the Lie algebra of G , and that since elements of the center of G are constant on \mathcal{H}_α , we can look at $M/\text{cent}(G)$ rather than M .

In the concrete situation $G = O(3) \times Z_2$ where $(R, +1)$ acts on $L^2(\mathbf{R}^6)$ by $(U_R f)(r_1, r_2) = f(R^{-1}r_1, R^{-1}r_2)$; and $(U_{(1,-1)} f)(r_1, r_2) = f(r_2, r_1)$. Irreducible representations of $O(3)$ are specified by the eigenvalue, $p = \pm 1$, of the

inversion and a non-negative integer j with $\dim D_\alpha = 2j + 1$. Thus $\alpha \in R_g$ is specified by a triple (j, p, π) where $j = 0, 1, \dots$ is called the *total angular momenta*, $p = \pm 1$ is called the *parity*, and $\pi = \pm 1$ is the eigenvalue of $r_1 \leftrightarrow r_2$ symmetry. For reasons connected with the total electron spin when both electron spin and the Pauli principle are taken into account, vectors $\psi \in \mathcal{K}_t = \bigoplus_{j,p} \mathcal{K}_{(j,p,-1)}$ are called *triplet states* and $\psi \in \mathcal{K}_s = \mathcal{K}_t^\perp = \bigoplus_{j,p} \mathcal{K}_{(j,p,+1)}$ are called *singlet states*. The maximal abelian group, M , modulo the center of G can be chosen to be rotation about the z -axis. The Lie algebra of M is just the single operator J_z and the eigenvalues of J_z on $\mathcal{K}_{(j,p,\pi)}$ are $m^{(j)} = -j, -j + 1, \dots, j - 1, j$. The spaces $\mathcal{K}_{(j,p,\pi,m^{(j)})}$, and the associated indices $(\alpha, m^{(\alpha)})$ are called *channels* and the eigenvalues $E_{n,m}$ are said to appear in a channel, $(\alpha, m^{(\alpha)})$ if $E_{n,m}$ is an eigenvalue of $H_0 \upharpoonright \mathcal{K}_{(\alpha,m)}$. To study the behavior of $E_{n,m}$ under perturbation it is sufficient to study the eigenvalue on each channel in which it appears. Since the behavior is independent of the eigenvalue of J_z , it is customary to use α alone as shorthand. Channels fall into three classes:

(i) *Non-degenerate resonant channels*. While $E_{n,m}$ is a degenerate eigenvalue, it will be non-degenerate and embedded in certain channels. This always occurs for example when $j = n + m - 2$. The simple theory of § 3 applies here. To prove that $E_{n,m}$ “dissolves” in such a channel one need only prove that the Fermi Golden Rule term is non-zero. Since H_0 is known to have an eigenfunction expansion, this is equivalent to proving certain integrals of hypergeometric functions are non-vanishing (see Theorem 5.1 below).

(ii) *Non-resonant channels*. It can happen that E is an embedded eigenvalue of H_0 , i.e. $\sigma_{\text{cont}}(H_0) = [\Sigma, \infty)$ with $E > \Sigma$, but that E is not embedded in certain channels i.e. that $\sigma_{\text{cont}}(H_0 \upharpoonright \mathcal{K}_\alpha) = [\Sigma_\alpha, \infty)$ with $\Sigma < E < \Sigma_\alpha$. This actually happens in this autoionizing model. If $\alpha = (j, (-1)^{j+1}, \pm 1)$, then $\Sigma_\alpha = -1/4$, $\Sigma = -1$ and eigenvalues $E_{n,m}$ with $2 = n \leq m$ are discrete eigenvalues of $H_0 \upharpoonright \mathcal{K}_\alpha$ in those channels α in which they occur. These channels with $p(-1)^j = -1$ are called channels of *unnatural parity*. It is known [68, 4] that even at the physical value $\beta = 1$, there are infinitely many eigenvalues with $\Sigma = -1/4$ as limit point in these unnatural parity channels.

(iii) *Degenerate resonant channels*. Finally, there are channels in which $E_{n,m}$ is still an embedded degenerate eigenvalue after the reduction due to symmetry. In this context, let us be more specific about our claim (in Remark 3 following Theorem 3.2) that analyticity at $\beta = 0$ is the generic

situation even for degenerate eigenvalues. Let us fix n, m and some channel $(\alpha, m^{(\alpha)})$ in which $E_{n,m}$ appears as a degenerate embedded eigenvalue. Let P be the projection (in \mathcal{H}_α) onto the eigenspace of H_0 associated with the eigenvalue $E_{n,m}$. Since $D(H_0) \subset D(W)$; $W_P \equiv PWP$ is an everywhere defined self-adjoint operator on the finite dimensional space $\text{Ran } P$. If W_P has distinct eigenvalues, then the resonance energies $E_i(\beta)$ will all be analytic at $\beta = 0$. In fact, if ψ_1, \dots, ψ_k are the eigenvectors of W_P , then the lowest order terms in $-2 \text{Im } E_i(\beta)$ will be $\Gamma_i = 2\pi(df_i/dE)|_{E=E_{n,m}}$ with

$$f_i(E) = (W\psi_i, \tilde{P}_{(E_{n,m}-\delta, E)} W\psi_i) .$$

Even in the non-generic situation where W_P has a degenerate eigenvalue, there is a well-defined reduction procedure [36, pp. 81-83] whereby the degeneracy can still be removed in order 2.

As an example, consider $n = m = 2$. There are five channels:

$$(j, p, \pi) = (2, 1, 1); (1, 1, -1); (1, -1, 1); (1, -1, -1); (0, 1, 1) .$$

The channel $(1, 1, -1)$ is non-resonant since $(-1)^j p = -1$, $E_{2,2} = -1/2$ and

$$\sigma(H_0 + \beta V \upharpoonright \bigoplus_{\alpha=(j, (-1)^{j+1}, \pi)} \mathcal{H}_\alpha) = [-1/4, \infty) .$$

The channels $(2, 1, 1)$ and $(1, -1, \pm 1)$ are non-degenerate. Finally $(0, 1, 1)$ is doubly degenerate (this comes from coupling either two p -electrons or two s -electrons to $j = 0$). We expect that this degeneracy is broken in lowest order and that $\text{Im } a_2 > 0$ in all channels other than the non-resonant $(1, 1, -1)$ channel.

Let us summarize the arguments we have just given in an explicit theorem which is one of a class of results:

THEOREM 5.1. *Let \hat{H} be the Hamiltonian $-\Delta_1 - \Delta_2 - 2/r_1 - 2/r_2$ on $L^2(\mathbf{R}^6)$ restricted to the invariant subspace $\mathcal{H}_{(2,1,1)}$ of functions $f \in L^2$ obeying:*

(i) *The orbit of f under rotations $(U_R f)(r_1, r_2) = f(R^{-1}r_1, R^{-1}r_2)$ generates a subspace on which $SO(3)$ is represented by its five-dimensional irreducible representation.*

(ii) *$f(-\vec{r}_1, -\vec{r}_2) = f(\vec{r}_2, \vec{r}_1) = f(\vec{r}_1, \vec{r}_2)$. Let \hat{V} be the operator $|\vec{r}_1 - \vec{r}_2|^{-1}$ also restricted to $\mathcal{H}_{(2,1,1)}$. Let $\psi(\vec{r}_1)$ be an eigenfunction of $h_0 = -\Delta_1 - 2/r_1$ with $h_0\psi = (-1/4)\psi$ and with $\psi(\vec{r}_1) = R(\vec{r}_1) Y_1^1(\theta, \phi)$ [R is a Laguerre function, Y_1^1 is a spherical harmonic]. Let $\phi(\vec{r}_1)$ be the eigenfunction of h_0 with $h_0\phi = -\phi$ and let η be a continuum eigenfunction of h with energy $1/2$ (η is a confluent hypergeometric function, see e.g. [14, 15]). Let*

$$I = \int d^3r_1 d^3r_2 \widehat{V}(\vec{r}_1, \vec{r}_2) \overline{\psi(\vec{r}_1)} \overline{\psi(\vec{r}_2)} \phi(\vec{r}_1) \eta(\vec{r}_2).$$

If $I \neq 0$, then for all real β sufficiently near but not equal to 0, the eigenvalue of \widehat{H}_0 at $-1/2$ “dissolves”, i.e. for some ε , $\widehat{H}_0 + \beta \widehat{V}$ has no eigenvalue in the interval $(-1/2 - \varepsilon, -1/2 + \varepsilon)$.

Remark. In physics parlance, ψ is a $2p$ state and ϕ is a $1s$ state.

Proof. \widehat{H}_0 has an explicit eigenfunction expansion since H_0 does [14]. A simple argument proves that if we look at the subspace $\mathcal{K}_{(2,1,1;2)}$ of $\mathcal{K}_{(2,1,1)}$ on which $J_z = +2$, \widehat{H}_0 has continuous spectrum of multiplicity 1 in the interval $[-1, -1/4)$ and an unnormalized continuum eigenfunction at energy, E , is $P(\phi \otimes \eta)$ where P is the projection onto $\mathcal{K}_{(2,1,1;2)}$ and η has energy $E + 1$. Since $I = \langle \psi \otimes \psi, V(\phi\eta) \rangle$ and $\psi \otimes \psi \in \mathcal{K}_{(2,1,1;2)}$ the result follows from Theorem 4.1.

Remark. One might expect that I had been calculated in the physics literature but a search of the relevant literature has not yielded an explicit calculation showing that $I \neq 0$. This is because the physical value $\beta = 1$ is sufficiently far from $\beta = 0$ that various ad hoc attempts of estimating higher order corrections are included (see [10] for a recent theoretical calculation). In [37], an integral similar to I is calculated (in place of η , $\tilde{\eta}$ a continuum eigenfunction of $-\Delta - 1/r_1$ is used; the replacement of η by $\tilde{\eta}$ is an attempt to estimate “in a physical way” the higher order terms in the perturbation series which can be interpreted physical as “corrections” due to the electron-electron repulsion). This similar integral is non-zero. The methods of [37] could be used to compute I .

Our analysis in this section can be carried over to atoms with more than two electrons. The symmetry group $O(3) \times Z_2$ is then replaced with $O(3) \times S_n$ where S_n is the permutation group on the number of electrons. Channels are labeled by (j, p, π) where π is now a Young tableau. Only those tableaux with two or one rows are relevant to physics since only those channels persist when electron spin together with the demand of total antisymmetry are added to the problem.

6. Spectral concentration

The theory of spectral concentration was originally formulated [60] to discuss the Stark effect where isolated levels dissolve in a continuum. The theory was further developed by various authors [13, 35, 36, 44, 45, 47, 61, 62]. Applications to a case where an eigenvalue embedded in the continuum is removed by a finite rank perturbation have been made by Howland

[25, 26, 30]. Our Theorem 6.1 is of the genre of his results on spectral concentration and such a result appears in [30]. We state Theorem 6.1 in terms of non-degenerate unperturbed eigenvalues but it generalizes easily to the degenerate case.

THEOREM 6.1. *Let V and W be sums of dilatation analytic potentials. Let E_0 be a non-threshold, non-degenerate eigenvalue of $T_0 + V$ embedded in the continuum. For β small, and real, let $E(\beta) = E_r(\beta) - i\Gamma(\beta)/2$ be the resonance energy of $H_0 + V + \beta W$ near E . Let $P^\beta(\Omega)$ be the spectral projections of $H_0 + V + \beta W$ (β real). Suppose $\Gamma(\beta) = \Gamma_{2n}\beta^{2n} + o(\beta^{2n+1})$; $\Gamma_{2n} \neq 0$. Let $|J_\beta|$ be a family of intervals centered about $E_r(\beta)$ so that $|J_\beta| \rightarrow 0$ and $\lim_{\beta \rightarrow 0} |J_\beta|/\Gamma_{2n}\beta^{2n}$ exists and equals a (a may be infinite). Let $P_0 = P^0(\{E_0\})$. Then*

$$\text{w-}\lim_{\beta \rightarrow 0} P^\beta(J_\beta) = [(2/\pi) \text{Arctan}(a)]P_0.$$

In particular, if $a = \infty$, $P^\beta(J_\beta) \rightarrow P_0$ strongly as $\beta \rightarrow 0$.

Proof. Let $\phi \in N_\alpha$. We will show that

$$\lim_{\beta \rightarrow 0} \langle \psi, P^\beta(J_\beta)\phi \rangle = [(2/\pi) \text{Arctan}(a)]\langle \psi, P_0\phi \rangle$$

and conclude the theorem by the density of N_α in $L^2(\mathbf{R}^{3n-3})$. Let θ be chosen purely imaginary with $0 < \text{Im } \theta < \alpha$. Then $(H_0(\theta) + V(\theta) + \beta W(\theta) - z)^{-1}$ is norm analytic near $z = E_0$ except for a pole at $E(\beta)$. Thus $A(\theta; \beta; z) = (H_0(\theta) + V(\theta) + \beta W(\theta) - z)^{-1} - (E(\beta) - z)^{-1}P(\theta; \beta)$ is analytic in β and z at $\beta = 0$, $z = E_0$, and in particular bounded near $z = E_0$, $\beta = 0$. Writing

$$\langle \phi, P^\beta(J_\beta)\phi \rangle = (1/\pi) \text{Im} \int_{J_\beta} dz \left[\langle \phi(\theta), A(\theta; \beta, z)\phi(\theta) \rangle + \frac{\langle \phi(\theta), P(\theta, \beta)\phi(\theta) \rangle}{E(\beta) - z} \right]$$

using $|J_\beta| \rightarrow 0$ and the boundedness of $A(\theta; \beta, z)$ we see that

$$\langle \psi, P^\beta(J_\beta)\phi \rangle = (1/\pi) \text{Im} \left[\langle \phi(\theta), P(\theta, \beta)\phi(\theta) \rangle \int_{J_\beta} \frac{dz}{E(\beta) - z} \right] + o(1).$$

But

$$\int_{J_\beta} \frac{dz}{E(\beta) - z} \int_{E_r - |J_\beta|/2}^{E_r + |J_\beta|/2} dz \frac{E_r - z + i\Gamma(\beta)/2}{(E_r - z)^2 + \Gamma(\beta)^2/4} = i2 \text{Arctan} \left[\frac{|J_\beta|}{\Gamma(\beta)} \right].$$

Thus

$$\lim_{\beta \rightarrow 0} \langle \phi, P^\beta(J_\beta)\phi \rangle = (2/\pi)[\text{Arctan}(a)] \text{Re} \langle \phi(\theta), P(\theta; 0)\phi(\theta) \rangle.$$

Finally $\langle \phi(\theta), P(\theta, 0)\phi(\theta) \rangle = \langle \phi, P_0\phi \rangle$. This proves the theorem.

In the language of spectral concentration $H_0 + V + \beta W$ has spectrum concentrated to order $2n - 1$ if $\Gamma(\beta) = o(\beta^{2n})$ and to no higher (integral) order. In a natural extension of the language $H_0 + V + \beta W$ has spectrum

concentrated to order $\beta^{2n-\alpha}$ for any $\alpha > 0$. This agrees with one's intuition viz-a-viz the relation of width and concentration.

7. The two-body case

In this final section we wish to establish three facts about two-body systems with dilatation analytic potentials: (i) If the potentials are "local", we wish to prove embedded eigenvalues are not possible. (ii) We wish to point out that there still exist local systems with resonances. (iii) For the case of local potentials which fall off exponentially, we establish the connection between resonances and poles in the scattering amplitude.

A multiplication operator, V , is called a *local* potential. An operator $V\psi(x) = \int v(x, y)\psi(y)dy$ with some Hilbert Schmidt kernel, V , is called a *non-local* potential. This terminology is borrowed from the physics literature.

THEOREM 7.1. *Let V be a central, local potential in some $C_\alpha(\alpha > 0)$. Then $-\Delta + V$ has no eigenvalues in $(0, \infty)$.*

Proof. By a result we prove in the Appendix, V is multiplication by a function, v , analytic in a sector $\{z \mid 0 < |\arg z| < \alpha\}$ with

$$\lim_{\substack{|z| \rightarrow \infty \\ |\arg z| < \alpha - \epsilon}} |v(z)| = 0.$$

Let $\gamma < \cos \alpha$. Then for z real $v(w)$ is analytic in $\{w \mid |w - z| < \gamma|z|\}$. Thus

$$\begin{aligned} \left| r \frac{\partial v}{\partial r} \right|_{r=z} &= \frac{1}{|2\pi|} |z| \left| \oint_{|w-z|=\gamma|z|} \frac{dw v(w)}{(w-z)^{-2}} \right| \\ &\leq \frac{1}{2\pi\gamma^2} \sup_{|w-z|=\gamma|z|} |v(w)| \rightarrow 0 \end{aligned}$$

as $|z| \rightarrow \infty$. We conclude $r(\partial v/\partial r)$ and $v \rightarrow 0$ at ∞ . The result then follows from a theorem of Agmon and Simon [1, 53].

Remarks 1. Since $\sigma_{\text{cont}}(-\Delta + V) = [0, \infty)$, $-\Delta + V$ has no non-threshold eigenvalues in the continuum.

2. For non-local C_α potentials, the analogue of Theorem 7.1 is false. For pick $\psi \in N_\alpha \cap D(H_0)$ with $\|\psi\| = 1$. Let $E = \langle \psi, (-\Delta)\psi \rangle$. Let $V = -\langle \psi, \cdot \rangle (-\Delta - E)\psi + \langle (-\Delta - E)\psi, \cdot \rangle \psi$. Then $V \in C_\alpha$ and $(-\Delta + V)\psi = E\psi$.

3. We conjecture that n -body systems with two-body central, local, dilatation analytic potentials have no bound states in $(0, \infty)$ for any n . Such results are known in several special cases [3, 63, 64]. The best way of going about proving this conjecture would seem to be to find a proof in the two-body case that depends more directly on the analyticity in scaling.

One can still construct two-body systems with resonances by using

suitable Bargmann potentials [6]. Let V be a central local two-body potential in C_α . Any solution of the radial Schrödinger equation extends to the sector $\{z \mid |\arg z| < \alpha\}$ by Poincaré's theorem. If the Jost function vanishes at some point k with $\text{Im } k^2 < 0$, it is not hard to see that the regular solution, $f(z)$ of energy k^2 has the property that $\int_0^\infty |f(re^{i\beta})|^2 dr < \infty$ so long as $|\arg k^2| < \beta < \alpha$. In particular k^2 is an eigenvalue of $-e^{-2\theta}\Delta + V(\theta)$ if $\alpha > \text{Im } \theta > |\arg k^2|$. In this way, Bargmann's construction yields two-body systems with resonances in the sense defined in § 2.

Finally, let us consider resonances in two-body systems as poles of an analytically continued scattering amplitude. We will suppose our potential falls off exponentially. Under such assumptions, second sheet continuations of the scattering amplitude has been discussed by a variety of authors [17, 23, 27, 41, 52, 54].

We note first that under the condition that $V = e^{-\alpha r} W$ with $W \in L^2$, one can rigorously prove the connection between the "T-matrix" and scattering [33, 34, 54]:

(a) If f, g are in a suitable dense set

$$\langle f, Sg \rangle = \langle f, g \rangle - 2\pi i \int dk dk' T(k, k') \delta(k^2 - k'^2) \bar{f}(k) \hat{g}(k').$$

(b)
$$T(k, k') = (2\pi)^{-3} \left[\int e^{i(k-k') \cdot \vec{r}} V(r) dr - \lim_{\epsilon \downarrow 0} \int e^{ik \cdot \vec{r}} V(r) G(r, r', k^2 + i\epsilon) V(r') e^{-ik' \cdot \vec{r}} \right]$$

where $G(r, r', E)$ is the kernel of the Carleman integral operator $(H - E)^{-1}$. Thus:

THEOREM 7.2. *Suppose $V = e^{-\alpha r} W$ where $W(r)$ is a two-body central dilatation analytic potential in C_β . Then the forward T-matrix $T(k, k) = F(k)$ has a meromorphic continuation into the region*

$$R = \{k \mid \text{Im } k > 0\} \cup \left\{ k \mid |\arg k| < \frac{\beta}{2}, |\text{Im } k| < \alpha \left[1 - 2 \frac{|\text{Im } k|^2}{|k|^2} \right] \right\}.$$

The only possible positions for poles of F in R are at resonance energies as defined in § 2.

Proof. The theorem follows by a simple superposition of the method of Grossman-Wu [23] and the continuation techniques of Balslev-Combes [5].

APPENDIX. Two-body central dilatation analytic potentials

Our goal here is to characterize central, local dilatation analytic two-

body potentials. The possibility of two-body potentials other than those allowed by Theorem A.1 was left open by Balslev and Combes.

THEOREM A.1. *Let v be a function of $|\vec{r}| = r$ so that the operator of multiplication by v on $L^2(\mathbf{R}^3)$ is in C_α for some $\alpha > 0$. Then v is equal, a.e., to the restriction to $[0, \infty)$ of a function, v , analytic in $\{z \mid |\arg z| < \alpha\}$ with $v(z) \rightarrow 0$ as $|z| \rightarrow \infty$ uniformly in any sector $|\arg z| \leq \beta < \alpha$.*

LEMMA A.1. *Let $f \in L^2(\mathbf{R}^3)$ with $f \in D(T_0)$. Suppose f is central and that $(T_0 + 1)U(\theta)f$ has an analytic continuation to $\{\theta \mid |\operatorname{Im} \theta| < \alpha\}$ with $\alpha < \pi/4$. Then f is equal, a.e., to a function, F , analytic in $\{z \mid |\arg z| < \alpha\}$.*

Proof. Let $g_\theta = (T_0 + 1)U(\theta)f$. Then $(T_0 + 1)^{-1}g_\theta \in D(H_0)$ and thus is a bounded continuous function [36, pp. 301–302]. Let

$$F(z) = [(T_0 + 1)^{-1}g_{\ln z}](x_0)$$

where $x_0 = (1, 0, 0) \in \mathbf{R}^3$. F is analytic in $\{z \mid |\arg z| < \alpha\}$ since $F(z) = (2\pi)^{-3/2} \int e^{ip \cdot z_0} (p^2 + 1)^{-1} \hat{g}_\theta(p) d^3p$ where \hat{g}_θ is the Fourier transform of g_θ . Since f is continuous and bounded, $F(z) = (U(\ln z)f)(x_0) = f(zx_0) = f(z)$ for almost all real z .

LEMMA A.2. *Let $h \in L^2(\mathbf{R}^3)$ so that h is central and $h \in N_\alpha$ with $\alpha < \pi/4$. Then h is equal a.e. to a function H analytic in $\{z \mid |\arg z| < \alpha\}$.*

Proof. Let $f = (T_0 + 1)^{-1}h$. Then

$$(T_0 + 1)U(\theta)f = (T_0 + 1)(e^{-2\theta}T_0 + 1)^{-1}U(\theta)h$$

is analytic in $\{\theta \mid |\operatorname{Im} \theta| < \alpha\}$. By Lemma 1, f is analytic in the sector $\{z \mid |\arg z| < \theta\}$. Since f is C^∞ in $\mathbf{R}^3 \setminus \{0\}$, h is given as $z^{-2}(\partial z^2/\partial z)(\partial f/\partial z)$ if $z \neq 0$. Thus h has an analytic continuation into the sector.

LEMMA A.3. *Let v obey the conditions of the theorem. Then v is analytic in $\{z \mid |\arg z| < \alpha\}$.*

Proof. $(r^2 + 1)^{-1} \in L^2$ and in $D(T_0) \subset D(V)$. Let $h(r) = v(r)(r^2 + 1)^{-1}$. $h \in L^2$ and $U(\theta)h = V(\theta)[e^{2\theta}r + 1]^{-1}$ is analytic in $\{\theta \mid |\arg \theta| < \alpha\}$. By Lemma A.2, h has an analytic continuation to $\{r \mid |\arg r| < \alpha\}$ so $v = (r^2 + 1)h$ has a continuation also.

LEMMA A.4. *Let \mathcal{F} be a family of C^∞ functions of compact support with common support and with $\sup_{f \in \mathcal{F}} \|(-\Delta + 1)f\|_2 < \infty$. Then for any $\alpha < \pi/4$, $(T_0 + 1)U(\theta)^{-1}f \rightarrow 0$ **weakly** as $\operatorname{Re} \theta \rightarrow +\infty$ uniformly on \mathcal{F} and uniformly in $\{\theta \mid |\operatorname{Im} \theta| < \alpha\}$.*

Proof. An elementary computation.

LEMMA A.5. Let \mathcal{F} be as in Lemma A.4. Let $V \in C_\alpha$ and let $\beta < \alpha < \pi/4$. Then

$$\lim_{\text{Re } \theta \rightarrow +\infty} \|V(\theta)f\|_2 = 0$$

uniformly for $f \in \mathcal{F}$ and $|\text{Im } \theta| < \alpha$.

Proof. $V(i\gamma)(T_0 + 1)^{-1}$ is compact and uniformly continuous for $\gamma \in [-\beta, \beta]$. Since $(T_0 + 1)U(\theta)^{-1}f \rightarrow 0$ uniformly in f as $\theta \rightarrow \infty$ (θ real),

$$\|V(i\gamma)(T_0 + 1)^{-1}(T_0 + 1)U(\theta)^{-1}f\|,$$

θ , real, goes to 0 uniformly in f and γ . But then since $U(\theta)$ is unitary, $U(\theta)V(i\gamma)U(\theta)^{-1}f \rightarrow 0$ in norm uniformly in f and γ . We conclude that $V(\theta)f \rightarrow 0$ in norm.

Proof of Theorem A.1. Analyticity is proven in Lemma A.3. To prove $v(z) \rightarrow 0$ as $|z| \rightarrow \infty$ uniformly in sectors, let $0 < \beta < \alpha$ be given. Pick a closed disk about $w = 1$ inside the sector $\{w \mid |\arg w| < \alpha - \beta\}$, say of radius r_0 . Then for any function f analytic in the sector

$$f(1) = \frac{1}{2\pi} \int_{r_0/2 < |w-1| < r_0} g(|w-1|)f(w)d^2w$$

where $g^{1/2}$ is positive, C^∞ , with support in $(r_0/2, r)$ obeying $\int g(|w-1|)rdr = 1$. In particular

$$v(z) = \frac{1}{2\pi} \int g(w-1)v(zw)d^2w.$$

Writing $w = re^{i\theta} \mid z \mid = z'e^{i\theta}$

$$v(z) = \frac{1}{2\pi} \int_{-\theta_0}^{\theta_0} d\theta \int r dr g(|w-1|)v(\mid z \mid re^{i(\theta+\phi)}).$$

Thus v is an integral of expectation values of $V(\ln \mid z \mid + i\theta + i\phi)$. By Lemma A.5, $\mid v(z) \mid \rightarrow 0$ uniformly in the sector in question.

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(Received October 15, 1971)

(Revised May 5, 1972)