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## Axiomatic quantum theory and resonances

C S Sharma and E O Ogunsulire<sup>†</sup>

Department of Mathematics, Birkbeck College, Malet Street, London WC1E 7HX, UK

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**Abstract.** The mathematical models of resonances in quantum mechanics are examined and it is shown that the subject is full of unresolved difficulties of the most fundamental kind. The results in the theory are often proved by methods which not only lack elegance but also rigour and lead to ill-defined (non-unique) definitions and solutions. It remains a difficult task to establish contact between the rigorous quantum theory built on sound foundations by Birkhoff and von Neumann and others and the models usually used to describe resonances. A theorem is proved which gives a set of necessary and sufficient conditions for the existence of solutions of formal perturbation and kindred equations in atomic physics and establishes certain uniqueness properties of solutions which exist. In another theorem it is proved that whenever a state vector belonging to a point eigenvalue of the Hamiltonian is perturbed, one has the phenomenon of spectral concentration and it is possible that in cases where the resulting spectral concentration does not constitute a point eigenvalue of the perturbed Hamiltonian, one has the phenomenon which probably corresponds to a resonance. It is shown that in the autoionising  $2s2p\ ^1\text{P}$  states of helium, a solution of the formal perturbation equations exists in the underlying Hilbert space only in the zero order, though a formal solution which is outside the underlying Hilbert space exists and belongs to the space of distributions on a subset of the Hilbert space. It is also shown that in cases where a complex eigenvalue is obtained by interfering with a self-adjoint operator, the phenomenon is not related to deficiency indices. The mathematical background of the work of Sharma and Bowtell has been examined and some progress has been made towards finding the rigorous mathematical framework in which the theory should find a proper formulation.

### 1. Introduction

Quantum theory as universally practised by physicists uses a mathematical model based on a complex and separable Hilbert space which is a sophisticated mathematical object and is difficult to comprehend purely intuitively. The mathematical foundations of the Hilbert space formalism of quantum theory were laid down by Birkhoff and von Neumann (1936) and considerable further work on the subject has been done by Gleason (1957), Mackey (1963) and Varadarajan (1968). A recent account by Sharma (1972) brings out the physical assumptions from which such a quantum theory can be deduced.

An alternative foundation for quantum theory in Hilbert space is provided by the work of Segal (1947) which leads to a more general theory based on  $C^*$ -algebras now much used in the quantum theory of fields. Both axiomatic theories agree that an observable in quantum mechanics corresponds to a self-adjoint (or essentially self-adjoint) operator on a complex and separable Hilbert space.

<sup>†</sup> Present address: Department of Mathematics, University of Ilorin, Ilorin, Nigeria.

In quantum theory the requirement that the operator which describes an observable is a self-adjoint one is a very fundamental one which cannot be easily abandoned or even relaxed. On the other hand it is quite usual to exploit complex analysis in hydrodynamics and electrodynamics in the study of phenomena which are essentially real. In hydrodynamics, for example, it so happens that the velocity potential and the stream function are mutually related in the same way as are the real and imaginary parts of an analytic complex-valued function, consequently the two can be conveniently combined together to form a complex potential. Thus the reason why one can exploit complex analysis in hydrodynamics is quite transparent. The situation in classical electrodynamics also is quite similar. Unless something equally fortuitous enables us to use non-self-adjoint operators and the basis of the use of such operators is not in contradiction with the considerations which provide the foundations of quantum theory, the use of non-self-adjoint operators for the study of the measurement of values of observables of a quantum system must remain suspect.

It is a matter of the greatest satisfaction to quantum theorists that properties of bound states of isolated quantum systems and particularly of atoms, at any rate in the non-relativistic case, can be calculated with remarkable precision by methods which conform with the requirements of axiomatic quantum theory with the greatest rigour. In fact the ability to predict the energy levels of the low-lying bound states of helium with considerable accuracy has always been regarded as among the finest achievements of quantum theory. Isolated quantum systems are often found in states which are quasi-stationary in the sense that these states decay, perhaps in accordance with the exponential law, into fragments; in isolated atoms this phenomenon is illustrated by the so called autoionising states. Such states are considered to be responsible also for certain peaks of the cross sections in some scattering experiments and are often described as *resonances*. The literature on the quantum theory of resonances is rich in volume; perhaps more has been written on this particular topic than any other in quantum theory. Unfortunately, however, no one so far has succeeded in proposing a mathematical model of resonance which is even approximately consistent with the foundations of axiomatic quantum theory. It is our main purpose in this work to look into the present status of various theories of resonances from the point of view of axiomatic quantum theory and to try to discover the difficulties which are obstructing the construction of a satisfactory model.

Before we look into individual models, it should be pointed out that the subject is bedevilled by the belief that these quasi-stationary states or resonances decay according to the exponential law. As mathematicians, we are, of course, unable to evaluate the experimental evidence in support of this belief. However, it is possible to assert quite categorically that the exponential law of decay is older than quantum theory and has been used by chemists for the study of rates of reactions in which compounds undergo spontaneous decomposition—the so called monomolecular reactions. Since under the conditions of reaction the substance decomposes, in the simplest model it is natural to assume that every molecule has a constant probability, say  $k$ , of being decomposed in a given interval of, say unit, time. Thus if there are  $N$  molecules, where  $N$  is large, in unit interval of time probably  $kN$  of them will actually decompose and the rate of decomposition of the substance can be described by

$$dN/dt = -kN$$

or

$$\ln(N/N_0) = -k(t - t_0)$$

or

$$N = N_0 \exp[-k(t - t_0)]$$

where  $N_0$  is the number of molecules at some initial time  $t_0$ . This is the original exponential law of decay. It assumes nothing about the internal structure of the molecule except that it has a well defined and constant probability of being decomposed in unit time. This probabilistic law is realised as a concrete observable law because of the very large number of molecules present. The exponential law of decay in chemistry is thus the property of a large collection of molecules rather than that of individual ones. The result is one in statistical mechanics rather than in particle mechanics. An individual molecule at any particular time is either undecomposed or decomposed, it does not undergo exponential decay.

In quantum theory exponential decay has come to mean such a decay of an individual system, or more precisely, that the probability that such a system is undecomposed decreases exponentially to zero with time. The bound states are stationary because the time evolution of the system in such a state changes only the phase of its wavefunction, which, of course, does not change the probability distributions associated with the system. If the system has a complex energy, say  $E - i\gamma$ , with  $E$  and  $\gamma$  real and with  $\gamma > 0$ , then substitution in the formal Schrödinger time-dependent equation

$$i \frac{d\psi}{dt} = H\psi = (E - i\gamma)\psi$$

or

$$\psi(t) = e^{-iHt} \psi(t_0) = e^{-\gamma t} e^{-iEt} \psi(t_0)$$

gives an exponentially decaying factor to the wavefunction. The proposition that the decaying states corresponds to such complex eigenvalues of the Hamiltonian is indeed very attractive. This remarkable theory is originally due to Gamow (1928) and is nearly as old as the quantum theory itself. Gamow, however, was working purely formally and the requirement that a quantum Hamiltonian of an isolated system is a self-adjoint operator on a complex and separable Hilbert space did not particularly bother him. Self-adjoint operators cannot have complex eigenvalues. The theory, therefore, needs careful reformulation. This has been tried by a large variety of authors with, in our opinion, little real success.

## 2. The complex eigenvalue theory

Probably as a consequence of interaction with mathematical logic, the necessity of having absolutely precise definitions is very well appreciated in the framework in which mathematicians work and the rules of the game are rigidly established by the axioms and the definitions. Any proposition in accord with the axioms and the definitions is true while any proposition which contradicts them is false. In mathematical physics, however, there is a long tradition of using mathematics of the intuitive kind; this has its advantages particularly as a great deal of what is studied in mathematical physics is exploratory and heuristic. Nevertheless one would ultimately like to have a rigorous mathematical model and a little lack of precision in rigorous mathematics can cause a lot of obfuscation. Nonetheless the lack of precision is colossal

when it comes to the description of the theory of complex eigenvalues. The language is often more akin to that of oriental mystics rather than of a precise and exact science. In this particular branch of quantum theory unsubstantiated conjectures, in the course of time, turn into 'established truths'. We have collected some examples.

Landau and Lifshitz (1958) say: 'In discussing the quasi-stationary states, we can use the following somewhat unusual method. Until now we have always considered solutions of Schrödinger's equation with a boundary condition requiring the finiteness of the wavefunction at infinity. Instead of this, we shall now look for solutions which represent an outgoing spherical wave at infinity: this corresponds to the particle finally leaving the system when it disintegrates. Since such a boundary condition is complex, we cannot assert that the eigenvalues of energy must be real.'

It would be interesting to construct a precise mathematical definition of a *complex boundary condition*. It is possible, even likely, that when the Schrödinger Hamiltonian is viewed as a differential operator on the vector space of complex-valued  $C^\infty$  functions on  $\mathbb{R}^n$  ( $n$  depending on the particular problem) which is not a Hilbert space, it has complex eigenvalues. The eigenfunction belonging to a complex eigenvalue cannot be one of the generalised eigenfunctions: these do not necessarily belong to the Hilbert space of square integrable functions but can always be regarded as distributions on such a Hilbert space. Another fundamental difficulty in the approach used by Landau and Lifshitz (1958) (as a matter of historical fact this approach is originally due to Breit and Wigner (1936), but see also Weisskopf and Wigner (1930) and Gamow (1928)) concerns the normalisation of an exponentially decaying wavefunction. Though Landau and Lifshitz (1958) resolve this difficulty up to a point, their approach does not seem to make much sense when looked at from the axiomatic point of view.

We next look at an account of the theory given in a well known text by Newton (1966). Newton starts with a Hamiltonian  $H$  of the form

$$H = H_0 + H'.$$

He then defines an operator  $K$  by

$$K = \frac{1}{E - H_0} H'.$$

He then assumes that  $K$  is compact, but does not put any restrictions on the value of the parameter  $E$  for which this assumption could be correct. He then takes an eigenvector  $\Phi(E)$  of  $K$  belonging to the eigenvalue  $\alpha(E)$  and differentiates

$$\langle \Phi(E), [(E - H_0)\alpha(E) - H']\Phi(E) \rangle = 0 \quad (\text{N.1})$$

to get

$$\frac{1}{\alpha} \frac{d\alpha}{dE} = \frac{1}{\langle \Phi(E), (H_0 - E)\Phi(E) \rangle}. \quad (\text{N.2})$$

Equation (N.1) can be rearranged to yield

$$\langle \Phi(E), (H_0 - E)\Phi(E) \rangle = \frac{1}{\alpha} \langle \Phi(E), H'\Phi(E) \rangle$$

from which it follows that  $\langle \Phi(E), (H_0 - E)\Phi(E) \rangle$  is positive definite if either  $\alpha$  is positive and  $H'$  is positive definite or  $\alpha$  is negative and  $H'$  is negative definite. However, according to Newton (1966)  $\langle \Phi(E), (H_0 - E)\Phi(E) \rangle$  is always positive

definite. Predicated on this extraordinary conclusion there follows a most graphic, picturesque and interesting description of what happens to the eigenvalue of  $K$  as  $E$  moves along the real axis: however, we find it difficult to discern a deductive thread connecting the various parts. The reader should study for himself this most interesting account of the complex eigenvalue theory on pages 236 and 237 of the work by Newton (1966).

We next consider an ingenious theory of resonances as enunciated by Howland (1972). Howland considers an operator of the form

$$H(\kappa) = T + \kappa B^* A$$

where  $T$  is a self-adjoint operator on a separable Hilbert space  $\mathcal{H}$  and  $A$  and  $B$  are closed densely defined operators from  $\mathcal{H}$  to another separable Hilbert space  $\mathcal{H}'$ . We use  $\mathcal{D}_T$ ,  $\mathcal{D}_A$  and  $\mathcal{D}_B$  to denote the domains of  $T$ ,  $A$  and  $B$  respectively. It is assumed that

$$\mathcal{D}_T \subset \mathcal{D}_A \cap \mathcal{D}_B$$

and

$$\langle Ax, By \rangle = \langle Bx, Ay \rangle \quad \forall x, y \in \mathcal{D}_A \cap \mathcal{D}_B$$

and  $\kappa$  is a perturbation parameter. Let

$$G(z) = (T - z)^{-1} \quad z \in \mathbb{C}$$

be the resolvent of  $T$ . Howland (1972) *assumes* that for any  $z \in \rho(T)$  where  $\rho(T)$  is the resolvent set of  $T$ , the operator

$$AG(z)B^*$$

which is defined on  $\mathcal{D}_{B^*}$  has a bounded extension  $Q(z)$  to  $\mathcal{H}'$  and that  $I + Q(z)$  is invertible for some  $z \in \rho(T)$ . Under these conditions  $T + \kappa B^* A$  has a self-adjoint extension  $H(\kappa)$  for sufficiently small  $\kappa$  with the resolvent

$$R(z, \kappa) = G(z) - \kappa [BG(\bar{z})]^* [I + \kappa Q(z)]^{-1} AG(z)$$

where  $z \in \rho(T)$  and  $I + \kappa Q(z)$  has a bounded inverse. An eigenvalue  $\lambda_0$  of  $T$  of multiplicity  $m$  will, of course, be a pole of  $Q(z)$  of rank  $m$ . Howland (1972) then considers a neighbourhood  $\Omega$  of  $\lambda_0$  and defines subregions  $\Omega^\pm$  by

$$\Omega^\pm = \{z \in \Omega: \pm \ln z > 0\}.$$

Howland (1972) then *assumes* that  $Q(z)$  has continuations  $Q^\pm(z)$  from  $\Omega^\pm$  to  $\Omega$  which is analytic on  $\Omega$  except for the single pole at  $\lambda_0$ . This, of course, makes sense only when  $\mathbb{R} \cap \Omega$  is contained in the spectrum of  $T$  so that  $\lambda_0$  is embedded in the continuum. Howland then shows that under these assumptions  $AR(z, \kappa)B^*$  also has a bounded extension  $Q_1(z, \kappa)$  provided  $|z - \lambda_0| < \delta_1$  and  $|\kappa| < \delta_2$  where  $\delta_1$  and  $\delta_2$  are sufficiently small. He then considers the completely meromorphic continuations  $Q_1^\pm(z, \kappa)$  of  $Q_1(z, \kappa)$  from  $\Omega^\pm$  to  $|z - \lambda_0| < \delta_1$ . Howland then *defines* the poles of these continuations  $Q_1^\pm(z, \kappa)$  to be the *resonances* of the perturbation problem. He then proves two theorems, the first of which concerns Puiseux series expansions of the resonances and the second gives a formula for the imaginary part of a resonance (provided certain further assumptions are valid) and this formula can be recognised as Fermi's golden rule. Howland finally proves that under certain additional constraints which ensure that the poles of  $Q_1^\pm(z, \kappa)$  are the complex conjugates of those of  $Q_1^\mp(z, \kappa)$ , there is spectral concentration of  $H(\kappa)$  in the neighbourhood of  $\lambda_0$ .

We now wish to draw attention to the following:

(1) Howland's work is predicated on the assumption that certain operator-valued functions have analytic continuations but he does not tell us the precise conditions under which such continuations exist.

(2) The definition of resonances requires the decomposition of the Hamiltonian in a particular way in which the perturbation can be written as a product of two operators with certain very rigid restrictions on their nature.

(3) Howland's poles, contrary to what Newton (1966) says, correspond to real values of the perturbation parameter.

(4) Contrary to Titchmarsh's (1958) result that the imaginary part of the point where the pole is located is smaller than any positive power of the perturbation parameter, Howland finds that Fermi's golden rule is valid and the lowest term of the imaginary part is proportional to the square of the perturbation parameter.

(5) In the only example he considers, Howland finds: 'The Gold from which the Ruk is made is apparently mixed with Brass.' He has to make an arbitrary alteration in the rule to get a sensible answer.

(6) No attempt has been made to reconcile Howland's definition of a resonance with axiomatic quantum theory.

In order to prove that resonances correspond to spectral concentration Howland (1972) has to make assumptions regarding a certain symmetry between poles of  $Q_1^\pm(z, \kappa)$ . According to folk-lore these *poles* are at complex eigenvalues of the adjoint of a densely defined symmetric operator or, in other words, the complex eigenvalues originate due to the Hamiltonian being a symmetric operator with non-zero deficiency indices. Hamiltonians in quantum theory and particularly in atomic physics are either self-adjoint or essentially self-adjoint and in either case the deficiency indices have to be zero. It is easy to prove that the complex poles in the theory of resonances cannot even correspond to complex eigenvalues of the adjoint of any symmetric restriction of the Hamiltonian. There is a well known theorem in functional analysis (see, for example, Naimark 1968) according to which if the adjoint of a densely defined symmetric operator has a complex eigenvalue in the upper (or lower) half of the complex plane then every complex number in the upper (or lower) half plane is also an eigenvalue of the adjoint operator. We cannot, therefore, get a unique complex eigenvalue by taking a densely defined symmetric restriction of the Hamiltonian and then taking its adjoint and this is what would be necessary to establish some relation between resonance poles and such complex eigenvalues.

We next consider the definition of resonance given by Simon (1973). This is based on certain analytic continuations defined by Balslev and Combes (1971). Balslev and Combes (1971) define a group  $U(\theta)$  of dilatations on  $L^2(\mathbb{R}^{3n})$  by

$$(U(\theta))(r) = \exp(3n\theta/2)f(e^\theta r) \quad \forall f \in L^2(\mathbb{R}^{3n}) \text{ and } \forall \theta \in \mathbb{R}.$$

Assuming that  $L^2(\mathbb{R}^{3n})$  is a concrete realisation of the Hilbert space corresponding to a physical system and  $H$  is a Hamiltonian with a decomposition

$$H = H_0 + V$$

where  $V$  satisfies certain compactness criteria (the details of which we omit here because such details involve technicalities which are of little relevance to our present considerations) and  $H_0$  is an essentially self-adjoint operator corresponding to the

kinetic energy. Balslev and Combes (1971) then use the dilatation group to define an operator

$$H(\theta) = U(\theta)H_0U(\theta)^{-1} = e^{-2\theta}H_0 + V(\theta)$$

where

$$V(\theta) = U(\theta)VU(\theta)^{-1}.$$

They then *assume* that  $H(\theta)$  has an analytic continuation to complex values of  $\theta$  in the strip  $\{\theta: |\text{Im } \theta| < \alpha\}$  for some positive real  $\alpha$ . One of the most remarkable features in the work of Simon (1973) is that the basic *assumption* about the existence of the analytic continuation of  $H(\theta)$  in the work of Balslev and Combes (1971) is throughout referred to as a well established fact.

Balslev and Combes (1971) have studied the spectral properties of  $H(\theta)$  and they claim to have proved that isolated real eigenvalues of  $H$  are also eigenvalues of  $H(\theta)$  but the continuous spectra of  $H(\theta)$  are, in general, a set of lines in the complex plane.  $H(\theta)$  has also isolated eigenvalues in the complex plane: these Simon (1973) defines to be resonances. However, some quotations from his work would demonstrate the strange methodology being used by him. In § 3 of his paper he makes the remark: "This theorem remaining true if 'resonance' is replaced with 'resonance or embedded eigenvalue' in both places where 'resonance' appears. The interesting phenomenon is that embedded eigenvalue can become resonances. This is the situation we discuss more fully in §§ 4, 5." Simon does not give any justification for the assertion in his remark, but in the later section he asserts: 'In the last section we showed that an eigenvalue embedded in the continuum can turn into a resonance when a suitable perturbation is turned on.' Thus an assertion made in § 3 becomes with the greatest ease a demonstration in § 4. Simon in § 4 makes the rather eloquent but absurd remark: 'It has been clear for many years that the Fermi Golden Rule is the right answer; what has been unclear is the right question.'

Simon (1973) goes on to show that in a case where the operator  $H_0 + V$  is perturbed by a third operator  $W$ , the imaginary part of the second-order term in a power series expansion of the complex energy  $E(\beta)$  in powers of  $\beta$  is given by

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

where

$$f = \langle W\psi_0, \tilde{P}_{]E_0-E, E[} W\psi_0 \rangle$$

and  $\tilde{P}_\Omega$  is the spectral projection for  $H_0 + V$  with the projection on to the eigenfunction  $\psi_0$  of  $H_0 + V$  belonging to the eigenfunction  $E_0$  embedded in the continuum removed.

The calculation yielding the result is obtained by enclosing the pole corresponding to the resonance in a closed contour which does not intersect the spectrum of  $H_0 + V + \beta W$ . Unfortunately  $[z - (H_0 + V + \beta W)]^{-1}$  does not have a pole corresponding to the resonance for any real value of  $\beta$  and the calculation is valid only for poles of  $(z - H(\theta))^{-1}$  with  $\theta$  complex. Simon (1973) also finds spectral concentration associated with resonances. He does not seem to prove that his conclusions continue to be valid even when the imaginary part of  $\theta$  is allowed to go to zero.

We wish to make a number of remarks on the work of Simon (1973). First Simon finds that resonances are properties of a pair  $(H, H_0)$  and are not intrinsic properties of the Hamiltonian  $H$  and there seems, except in certain two-body problems, no unique



way of choosing  $H_0$ . Thus Simon's resonances are ill defined. Second, the mathematical device by which complex poles and eigenvalues are obtained is so invidious that it does not give any clear idea of what, if anything, the non-self-adjoint Hamiltonian represents in terms of the propositional calculus of quantum mechanics (Birkhoff and von Neumann 1936, Mackey 1963). Third, Simon by heuristic calculations finds that the exponential law can only be approximate and yet he thinks that Fermi's golden rule is the right answer. Fourth, no attempt has been made to reconcile his definitions and results with axiomatic quantum theory.

It is sometimes said that only self-contained physical systems have self-adjoint Hamiltonians (see, for example, Wong 1967). In principle the entire universe is the only self-contained physical system, but in practice many physical systems can be well approximated as completely isolated. It is argued (Nakayama and DeWitt 1964) that for the description of quantum mechanical systems which are intimately coupled to their environments, the energy is not a constant of motion and for such non-conservative systems it is legitimate to use non-self-adjoint operators as models for their Hamiltonians. Unfortunately, in all the examples of actual uses of non-self-adjoint Hamiltonians, the absence of self-adjointness arises neither from the necessity nor from a prescription of taking into account the interaction with the environment; in each case, self-adjointness is abandoned only because it is mathematically convenient so to do, that is, from pure mathematical opportunism. The suggestion, therefore, though worthy of further consideration is at the present time of no value in providing a justification for the actual use of non-self-adjoint operators as models for the Hamiltonians of quantum systems.

### **3. Spectral concentration**

Spectral concentration would be easier to describe if one were an experimentalist. If the emission spectrum of an atom (or a molecule) is viewed through a spectroscope, in the continuous spectrum are seen bands which are brighter than neighbouring parts of the continuum on either side and even in the discrete part of the spectrum are sometimes seen broad bands rather than sharp lines. These bright bands (dark in the case of the absorption spectrum) correspond to the phenomenon of spectral concentration. If the quantum mechanical model provides a good description of the atomic phenomenon described above, then the corresponding structure in the mathematical model is described as a spectral concentration in the mathematical sense. The sharp lines in the experimental spectrum of an atom correspond to discrete points in the mathematical spectrum of the operator corresponding to the Hamiltonian and the continuous part of the experimental spectrum corresponds to the continuous part of the mathematical spectrum of the Hamiltonian. In the experimental situation a spectral concentration is something intermediate between discrete and continuous spectra. At first sight, it might seem that bands in the spectrum should correspond to intervals of the real line with particular properties in the mathematical spectrum of the Hamiltonian, but the situation is rendered extremely difficult by the fact that if an interval is contained in the spectrum then it must be part of the continuous spectrum. It is necessary, therefore, to construct a model which is a little more complicated than one based on simple intervals in the spectrum with particular properties. Before proceeding any further it should be observed that the image of a spectral measure corresponding to any interval, however small, of the continuous spectrum is an

infinite-dimensional subspace of the underlying Hilbert space and furthermore given any  $\epsilon > 0$  and an interval  $]\lambda - \epsilon, \lambda + \epsilon[$  of the real line contained in the continuous spectrum of a self-adjoint operator  $H$ , there are infinitely many linearly independent vectors  $u$  which satisfy

$$\|(H - \lambda)u\| \leq \epsilon \|u\| \tag{1}$$

and thus given any positive real number  $\epsilon$ , however small, there are infinitely many approximate eigenvectors of  $H$  such that closeness of the approximation is less than  $\epsilon$  in the norm. This is precisely what makes the study of continuous spectra rather uncomfortable, particularly so if one is inclined to use approximate methods. With these remarks in mind we now proceed to define concepts which lead to the definition of a spectral concentration. The approach here is based on the work of Conley and Rejto (1966).

Let

$$H_\epsilon = H_0 + \epsilon H_1 \tag{2}$$

be a family of self-adjoint (or essentially self-adjoint) operators depending on a real parameter  $\epsilon$ . The domains  $\mathcal{D}_{H_\epsilon}$  of the operators depend on  $\epsilon$ , but it is assumed that there is a dense linear set  $\mathcal{D}_H$  such that

$$\mathcal{D}_H \subset \mathcal{D}_{H_\epsilon} \tag{3}$$

for sufficiently small  $\epsilon$ .

Following Rellich (1936) we define

$$\begin{aligned} H_\epsilon &\xrightarrow{s} H_0 && \text{if for } \phi \in \mathcal{D}_H \\ H_\epsilon \phi &\rightarrow H_0 \phi && \text{as } \epsilon \rightarrow 0. \end{aligned}$$

Note that if all the operators are bounded then this reduces to the usual definition of strong convergence. With this definition Rellich (1936) proves the following theorem.

*Theorem 3.1* (Rellich 1936). Let  $H_\epsilon \xrightarrow{s} H_0$  in the above sense and let  $P_\epsilon$  and  $P_0$  be the spectral measures corresponding to  $H_\epsilon$  and  $H_0$  respectively. Let  $\Delta$  be an interval of the reals whose end points are not in the point spectrum of  $H_0$ . Then

$$P_\epsilon(\Delta) \xrightarrow{s} P_0(\Delta). \tag{4}$$

Let  $\lambda_0$  be an isolated point eigenvalue of  $H_0$ : the eigenspace of  $H_0$  belonging to  $\lambda_0$  will be denoted by  $\mathcal{H}_{\lambda_0}$ . Conley and Rejto (1966) then define a spectral concentration at  $\lambda_0$  for the family  $H_\epsilon$  as follows.

*Definition.* The spectrum of  $H_\epsilon$  is concentrated to order  $p$  at  $\lambda_0$  as  $\epsilon \rightarrow 0$  if there is a family of Borel sets  $\Delta_\epsilon$  whose Lebesgue measures  $\nu(\Delta_\epsilon)$  satisfy

$$\nu(\Delta_\epsilon) = O(\epsilon^p) \tag{5}$$

and such that

$$P_\epsilon(\Delta_\epsilon) \xrightarrow{s} P_0(\{\lambda_0\}) \quad \text{as } \epsilon \rightarrow 0. \tag{6}$$

Next Conley and Rejto (1966) define an asymptotic eigenvector family as follows.

*Definition.* An asymptotic eigenvector family of order  $p$  at  $\lambda_0$  is a family  $\phi_\epsilon$  of unit vectors satisfying the following conditions:

(i) there is an open interval  $\Delta$  containing  $\lambda_0$  and a family  $\lambda_\epsilon$  of real numbers such that

$$\|P_\epsilon(\Delta)(H_\epsilon - \lambda_\epsilon)\phi_\epsilon\| = O(\epsilon^p) \quad \text{as } \epsilon \rightarrow 0; \tag{7}$$

and (ii)

$$(I - P_0(\{\lambda_0\}))\phi_\epsilon \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0. \tag{8}$$

From our earlier remark about the continuous spectrum it follows that whenever  $H_\epsilon$  has a continuous spectrum in a neighbourhood of  $\lambda_0$  condition (i) is always satisfied and furthermore even when the operators  $H_\epsilon$  have eigenvalues  $\lambda_\epsilon$  approaching  $\lambda_0$  continuously as  $\epsilon \rightarrow 0$ , then also condition (i) is satisfied. It is the requirement in condition (ii) which is what characterises an asymptotic eigenvector family and hence, in view of the lemma in the next paragraph, a spectral concentration. It should be noted that when  $H_\epsilon$  has eigenvalues approaching  $\lambda_0$  continuously as  $\epsilon \rightarrow 0$  condition (ii) is also satisfied, so that point eigenvalues of a family of perturbed operators are trivial examples of spectral concentration.

*Lemma* (Conley and Rejto 1966). Let  $\mathcal{H}_{\lambda_0}$  have dimension  $n$  and let there be  $n$  asymptotic eigenvector families  $\phi_\epsilon^j$  ( $j = 1, \dots, n$ ) of order at least  $p$  at satisfying

$$\|(\phi_\epsilon^j, \phi_\epsilon^k)\| \leq \delta < \frac{1}{n} \quad \text{whenever } j \neq k. \tag{9}$$

Then the spectrum of  $H_\epsilon$  is concentrated to order  $p$  at  $\lambda_0$ .

In particular when  $\lambda_0$  is a non-degenerate eigenvector, the existence of an asymptotic eigenvector family guarantees the existence of a spectral concentration.

With these results available as tools, in cases where formal solutions of perturbation equations exist up to order, say  $n$ , then by taking

$$\phi_\epsilon = \sum_{i=0}^{n-1} \phi_i \epsilon^i \tag{10}$$

and

$$\lambda_\epsilon = \sum_{i=0}^n \lambda_i \epsilon^i \tag{11}$$

it is easy to prove that

$$\|(I - P_0(\{\lambda_0\}))\phi_\epsilon\| \rightarrow 0 \tag{12}$$

and

$$\|P_\epsilon(\Delta)(H_\epsilon - \lambda_\epsilon)\phi_\epsilon\| \rightarrow O(\epsilon^n), \tag{13}$$

where  $\Delta$  is any open interval containing  $\lambda_0$  but not containing other points in the spectrum of  $H_0$ . Thus whenever formal solutions to the perturbation equations exist to order  $n$ , so does spectral concentration to the same order. We wish to point out that if solutions to the formal perturbation equations exist up to the  $n$ th order, we use solutions only up to  $(n - 1)$ st order to define  $\delta_\epsilon$ . Conley and Rejto (1966) state a somewhat stronger result, for they seem to require the existence of the solutions only

up to  $(n - 1)$ st order to guarantee spectral concentration up to order  $n$ . However, their proof depends on certain properties of  $H_1\phi_{n-1}$  and in cases where the formal perturbation equation for  $\phi_n$  does not have a solution  $\phi_{n-1}$  may not belong to the domain  $\mathcal{D}_{H_1}$  of  $H_1$  and then  $H_1\phi_{n-1}$ , of course, has no meaning. This difficulty would not arise if condition (3) were satisfied and this partly explains the necessity of having this requirement.

The work of Conley and Rejto (1966) defines spectral concentration in the case where an isolated eigenvalue of a self-adjoint operator disappears as a result of a self-adjoint perturbation and a neighbourhood of the isolated eigenvalue becomes part of the continuous spectrum of the perturbed operator. The work also shows how spectral concentration in such cases is related to asymptotic eigenvector families.

In the case where an eigenvalue of the unperturbed operator is embedded in the continuum and dissolves in the continuum as a result of the perturbation, the situation is a little more complicated. However, there seems absolutely no reason why the same definition of spectral concentration cannot be used. It seems that in limiting their definition of spectral concentration to the case of isolated eigenvalues only Conley and Rejto (1966) were being unduly cautious. Indeed Howland (1972) has studied the relation between spectral concentration and formal solutions of perturbation equations even in cases where an eigenvalue of the unperturbed operator is embedded in the continuum and using the same definition of spectral concentration does not seem to present any difficulty whatsoever. In this work we prove that in the simplest example of physical interest of an embedded eigenvalue dissolving into the continuum as a result of a perturbation (such an example is provided by an autoionising state of helium), even the first-order perturbation equation does not have a solution. To do this we first prove a theorem giving necessary and sufficient condition for the existence of solutions of an equation of the type

$$(A - \lambda)\phi = \psi \tag{14}$$

where  $A$  is a self-adjoint operator on a Hilbert space  $\mathcal{H}$  with domain  $\mathcal{D}_A$ ,  $\phi \in \mathcal{D}_A$ ,  $\psi \in \mathcal{H}$  and  $\lambda \in \Lambda(A)$  (= the spectrum of  $A$ ). To do this we first form the Sobolev triplet (Gelfand and Shilov 1967):

$$\Phi = \mathcal{D}_A \subset \mathcal{H} \subset \Phi' \tag{15}$$

where  $\Phi'$  is the dual of  $\Phi$ . For our result we need the following theorem (see, Gelfand and Shilov 1967).

*Theorem 3.2.* A symmetric linear operator  $A$ , defined on the space  $\Phi$  which admits a self-adjoint extension to the Hilbert space  $\mathcal{H}$ , has a complete set of eigendistributions belonging to the dual space  $\Phi'$ .

We can now assert our main theorems as follows.

*Theorem 3.3.* Let  $\lambda \in \Lambda_p(A)$  (= the point spectrum of  $A$ ) be an isolated point in the spectrum of  $A$ . Then a necessary and sufficient condition that equation (14) has a solution in  $\mathcal{H}$  is that  $P_A(\{\lambda\})\psi = 0$ , where  $P_A$  is the spectral measure induced by  $A$ . If a solution  $\phi$  exists, then  $(I - P_A(\{\lambda\}))\phi$  is unique.

*Theorem 3.4.* Let  $\lambda \in \Lambda_c(A)$  (= the continuous spectrum of  $A$ ). Then a necessary condition that equation (14) has a solution in  $\mathcal{H}$  is that  $\chi_\lambda(\psi) = 0$  where  $\chi_\lambda$  is the

eigendistribution belonging to the generalised eigenvalue  $\lambda$ . A sufficient condition that equation (14) has a solution in  $\mathcal{H}$  is that for some real  $\epsilon > 0$   $P_A([\lambda - \epsilon, \lambda + \epsilon])\psi = 0$ . Furthermore, if a solution exists, it is unique.

*Proof of theorem 3.3. Necessity:* Suppose a solution  $\phi$  exists in  $\mathcal{H}$ . Let  $\eta \in (P_A(\{\lambda\}))(\mathcal{H})$ , that is

$$(A - \lambda)\eta = 0. \tag{16}$$

We form the inner-product of equation (14) with  $\eta$ :

$$\langle \eta, (A - \lambda)\phi \rangle = \langle \eta, \psi \rangle \tag{17}$$

but since  $A$  is self-adjoint

$$\langle \eta, (A - \lambda)\phi \rangle = \langle (A - \lambda)\eta, \phi \rangle = 0. \tag{18}$$

Thus  $\psi$  is orthogonal to every vector in the range of  $P_A(\{\lambda\})$ , hence

$$P_A(\{\lambda\})\psi = 0. \tag{19}$$

*Sufficiency:* Since  $\lambda$  is isolated, it is possible to find an  $\epsilon > 0$  such that

$$([\lambda - \epsilon, \lambda + \epsilon] \cap \Lambda(A)) = \{\lambda\} \tag{20a}$$

so that

$$P_A([\lambda - \epsilon, \lambda + \epsilon]) = P_A(\{\lambda\}) = P \quad (\text{say}). \tag{20b}$$

Let

$$I - P = Q. \tag{21}$$

The restriction of  $A$  to  $Q(\mathcal{H})$  is the same as  $AQ$  restricted to the same subspace. By projecting equation (14) to  $Q(\mathcal{H})$  we have, since  $A$  and  $Q$  commute

$$(A - \lambda)Q\phi = Q\psi = (I - P)\psi = \psi \tag{22}$$

or

$$(AQ - \lambda)Q\phi = \psi. \tag{23}$$

The restriction of  $AQ$  to  $Q(\mathcal{H})$  is a self-adjoint operator on  $Q(\mathcal{H})$  and its spectrum is

$$\Lambda(AQ) = \Lambda(A) \setminus [\lambda - \epsilon, \lambda + \epsilon],$$

hence  $\lambda \notin \Lambda(AQ)$  and then  $(AQ - \lambda)^{-1}$ , by the resolvent theorem (see Reisz and Nagy 1965), is a bounded operator on  $Q(\mathcal{H})$  yielding

$$Q\phi = (AQ - \lambda)^{-1}\psi. \tag{24}$$

By setting  $\phi = Q\phi$ , we see that  $\phi$  is a solution of equation (14).

*Uniqueness:* Suppose that contrary to the assertion, there are two solutions  $\phi$  and  $\phi'$  such that  $Q\phi \neq Q\phi'$ . Since  $Q\psi = \psi$ , it follows that  $Q\phi$  and  $Q\phi'$  are also solutions of equation (14). This implies that  $Q(\phi - \phi')$  is a solution of

$$(A - \lambda)\eta = 0. \tag{25}$$

But every solution of equation (25) belonging to  $\mathcal{H}$  is an eigenvector of  $A$  belonging to

the eigenvalue  $\lambda$  and hence belongs to the range of  $P_A(\{\lambda\})$ . For every such vector  $\eta$

$$Q\eta = (I - P)\eta = \eta - \eta = 0 \tag{26}$$

contradicting  $Q\phi \neq Q\phi'$ . This completes the proof of theorem 3.3.

*Proof of Theorem 3.4. Necessity:* Note first that a solution in  $\mathcal{H}$ , if it exists, must necessarily belong to  $\Phi$ .

Suppose a solution exists. Let  $\chi_\lambda$  be the eigendistribution belonging to the generalised eigenvalue  $\lambda$ . Then evaluating  $\chi_\lambda$  at both sides of equation (14) gives us

$$\chi_\lambda(\psi) = \chi_\lambda((A - \lambda)\phi) = \chi_\lambda((\lambda - \lambda)\phi) = \chi_\lambda(0) = 0.$$

*Sufficiency:* The proof is the same as in the case of theorem 3.3.

*Uniqueness:* Suppose two solutions  $\phi$  and  $\phi'$  exist, then  $\phi - \phi'$  satisfies

$$(A - \lambda)(\phi - \phi') = 0$$

which implies that either  $\phi = \phi'$  or  $\lambda$  belongs to the point spectrum of  $A$ . The latter possibility is ruled out by our hypothesis. This completes our proof.

In view of the work done in proving the above theorem, we can assert the following theorem.

*Theorem 3.5.* Let  $\lambda \notin \Lambda(A)$ . Then equation (14) always has a unique solution in  $\mathcal{H}$ .

We would like to point out that a number of earlier results of Rejto (1968) and Sharma and Bowtell (1975) follow as immediate corollaries to these remarkably simple theorems.

#### 4. Autoionisation in helium

Let  $\mathcal{H}_H$  be the Hilbert space corresponding to the motion of the electron in the hydrogen atom relative to the centre of mass. The pure states describing the motion of the two electrons in helium relative to the centre of mass correspond to those elements of  $\mathcal{H}_H \otimes \mathcal{H}_H$  which satisfy certain symmetry requirements: such state vectors are either symmetric or antisymmetric with respect to the interchange of the order in pairs in  $\mathcal{H}_H \otimes \mathcal{H}_H$  whose linear combinations they are; the symmetric states are called singlets and the antisymmetric ones the triplets.

Let  $H$  be the quantum Hamiltonian for the motion of the electrons in helium. It can be written as

$$H = h \otimes I + I \otimes h + H_{12} = H_0 + H_{12} \tag{27}$$

where  $h$  is the hydrogen Hamiltonian,  $I$  the identity operator on  $\mathcal{H}_H$  and  $H_{12}$  represents the interelectronic interactions. The spectrum  $\Lambda(h)$  of  $h$  is completely known: it has point eigenvalues at (in natural atomic units)

$$-1/2n^2 \quad n \in \mathbb{Z}^+$$

and the whole of the positive real axis constitutes its continuous spectrum. Thus

$$\Lambda(h) = \{-1/2n^2 : n \in \mathbb{Z}^+\} \cup \{\mathbb{R}^+\} \cup \{0\} \tag{28}$$

and the spectrum  $\Lambda(H_0)$  of  $H_0$  can now be easily seen to be

$$\Lambda(H_0) = \{\lambda = \nu + \mu : n, \mu \in \Lambda(h)\}. \tag{29}$$

When both  $\nu$  and  $\mu$  are point eigenvalues, then so is  $\lambda$ ; but if either  $\nu$  or  $\mu$  or both belong to the continuous spectrum of  $h$ , then  $\lambda$  also belongs to the continuous spectrum of  $H_0$ . Consequently  $H_0$  has a purely point spectrum in the interval  $[-1, -\frac{1}{2}[$  with eigenvalues  $\lambda_n$  given by

$$\lambda_n = -\frac{1}{2} - \frac{1}{2n^2} \quad n \in \mathbb{Z}^+. \tag{30}$$

The positive real axis constitutes the purely continuous spectrum of  $H_0$  whereas there is a superimposition of point and continuous spectra of  $H_0$  in the interval  $[-\frac{1}{2}, 0[$  or, in other words, there are a certain (in fact, denumerably infinite) number of point eigenvalues of  $H_0$  embedded in this interval which is part of the continuous spectrum of  $H_0$ . The values of these embedded eigenvalues are given by

$$\lambda_{n,m} = -\frac{1}{2n^2} - \frac{1}{2m^2} \quad n, m \in \mathbb{Z}^+ \setminus \{1\}. \tag{31}$$

In the non-relativistic approximation the total angular momentum of the electrons is conserved, consequently it is possible to decompose the subspaces of  $\mathcal{H}_H \otimes \mathcal{H}_H$  (which constitutes our model for helium) into a direct sum of subspaces of different angular momenta. Let

$$\mathcal{H}_H = \bigotimes_{l=0}^{\infty} \mathcal{H}_l \tag{32}$$

be the decomposition of  $\mathcal{H}_H$  according to angular momenta, then in the corresponding decomposition of  $\mathcal{H}_H$  according to total angular momenta, the term corresponding to total angular momentum  $n(n+1)$  has components in

$$\mathcal{H}_l \otimes \mathcal{H}_m \quad |l-m| \leq n \leq |l+m|.$$

Considering the case of total angular momentum 2, which gives rise to the so called P states, the appropriate subspace for these states is

$$\mathcal{H}_{He(P)} \subset (\mathcal{H}_0 \otimes \mathcal{H}_1) \oplus (\mathcal{H}_1 \otimes \mathcal{H}_0) \left( \bigoplus_{l,m} (\mathcal{H}_l \otimes \mathcal{H}_m) \oplus (\mathcal{H}_m \otimes \mathcal{H}_l) \right) \tag{33}$$

with  $l > 0$  and  $|l-m| \leq 1$ , where the direct sums over  $l$  and  $m$  are taken over only those values which produce P states of odd parity. (We consider here P states in preference to S states which are simpler in that the total angular momentum is zero. However, the lowest eigenvalue of the S-family which is embedded in the continuum is degenerate whereas the lowest eigenvalue of the P-family which is embedded in the continuum is non-degenerate thus making the P state simpler for the study of perturbations of eigenvalues embedded in the continuum.) Each of the subspaces in the direct sum (33) reduces  $H_0$ . Each subspace of a particular angular momentum not only reduces  $H_0$  but also  $H$ . The restriction  $H_0^P$  of  $H_0$  to  $\mathcal{H}_{He(P)}$  has spectrum

$$\Lambda(H_0^P) = \left\{ -\frac{1}{2} - \frac{1}{2n^2} : n \in \mathbb{Z}^+ \setminus \{1\} \right\} \cup [-\frac{1}{2}, 0] \cup \{\mathbb{R}^+\}. \tag{34}$$

The first of the sets in this union is purely discrete, in the interval of the second set are embedded infinitely many eigenvalues of  $H_0^p$  at points

$$-\frac{1}{2}\left(\frac{1}{n^2} + \frac{1}{m^2}\right) \quad n, m \in \mathbb{Z}^+ \setminus \{1\}. \tag{35}$$

It is generally believed, though it has not been proved rigorously, that when  $H_0$  is perturbed by  $H_{12}$ , the discrete eigenvalues remain discrete but the eigenvalues embedded in the continuum are absorbed by the continuum and the ‘ghosts’ they leave behind cause resonances. We shall consider the point eigenvalue embedded in the continuum at  $-\frac{1}{4}$  ( $n = m = 2$ ) and prove that the formal perturbation expansion corresponding to this simple eigenvalue has a Hilbert space solution only in the zero order.

*Theorem 4.1.* The formal first-order equations for the  $2s2p \ ^1_3P$  states of helium do not admit solutions in  $\mathcal{D}_{H_0}$ .

*Proof.* The first-order equation is

$$(H_0 + \frac{1}{4})\psi_1 = (E_1 - H_{12})\psi_0 \tag{36}$$

with

$$E_1 = \langle \psi_0, H_{12}\psi_0 \rangle \tag{37}$$

and

$$H_0\psi_0 = -\frac{1}{4}\psi_0. \tag{38}$$

$-\frac{1}{4}$  is an eigenvalue of  $H_0$  embedded in the continuum and therefore in order that a solution exists the necessary conditions in both theorems 3.3 and 3.4 must be satisfied. It is easy to verify that the necessary condition in theorem 3.3 is satisfied. The necessary condition in theorem 3.4 is

$$\chi_{1/4}((E_1 - H_{12})\psi_0) = 0. \tag{39}$$

The left-hand side of equation (39) has been evaluated analytically by Horak and Lewis (1976) and the value is non-zero. Hence the formal first-order equation does not have a solution in  $\mathcal{D}_{H_0}$ . We are finished.

We shall now show how equation (36) can be suitably projected onto a subspace to yield, in the coordinate representation, an ordinary differential equation which contains that part of equation (36) which causes all the difficulty. We consider the subspace

$$(\mathcal{H}_0 \otimes \mathcal{H}_1) \oplus (\mathcal{H}_1 \otimes \mathcal{H}_0).$$

In the coordinate representation  $\mathcal{H}_0$  can be represented by  $L_2^2([0, \infty[)$  which is the Hilbert space of those real-valued functions on  $[0, \infty[$  which are normed by the inner-product defined by

$$\langle f, g \rangle = \int_0^\infty f(r)g(r)r^2 dr. \tag{40}$$

Elements of  $\mathcal{H}_1$  have representations of the form  $fY_1^1$  where  $f \in L_2^2([0, \infty[)$  and  $Y_1^1$  is



a spherical harmonic. In this representation the restriction  $h|_{\mathcal{H}_l}$  of  $h$  to  $\mathcal{H}_l$  has the realisation

$$h|_{\mathcal{H}_l} = L_l = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} - \frac{1}{r} + \frac{l(l+1)}{r^2} \quad l = 0, 1. \tag{41}$$

If we take  $\mathcal{H}_{00}$  to be the subspace spanned by the eigenvector belonging to the lowest eigenvalue  $-\frac{1}{2}$  of  $L_0$  and consider the direct sum

$$(\mathcal{H}_{00} \otimes \mathcal{H}_1) \oplus (\mathcal{H}_1 \otimes \mathcal{H}_{00})$$

then this is that subspace of  $\mathcal{H}_{\text{He}(P)}$  which in the language of physicists is spanned by the so called  $1snp$  and  $1skp$  ( $n$  is a discrete parameter and  $k$  is a continuous parameter) states of helium. Let  $P$  be the projection on this subspace, then  $P$  commutes with  $H_0$  and in our particular representation, straightforward calculation reduces

$$P(H_0 + \frac{1}{4})\psi_1 = P(E_1 - H_{12})\psi_0 \tag{42}$$

to

$$\begin{aligned} & \left( -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} - \frac{1}{r} + \frac{1}{r^2} - \frac{1}{4} \right) \psi_1 \\ &= (L_1 - \frac{1}{4})\psi_1 \\ &= \frac{1}{27\sqrt{3}} e^{-2r} r(3r+2) \\ & \pm \left( \frac{e^{-2r}}{(243\sqrt{3})r^2} (27r^4 + 18r^3 + 48r^2 - 128r - 128) + \frac{64 e^{-r/2}}{243\sqrt{3}} (2-r) \right) \end{aligned} \tag{43}$$

where the + sign is to be taken for singlets and the - sign for the triplets. Since  $\frac{1}{4}$  belongs to the continuous spectrum of  $L_1$ , theorem 3.4 in the preceding section tells us that equation (43) has a Hilbert space solution only if  $\chi_{1/4}(\phi) = 0$ , where  $\phi$  represents the right-hand side of equation (43). The work of Sharma and Bowtell (1973) and Horak and Lewis (1976) shows that this is non-zero showing that a Hilbert space solution does not exist. However, it is possible that a solution in the space  $\Phi'$  (the dual of  $\mathcal{D}_{L_1}$ ) exists and both Sharma and Bowtell (1973) and Horak and Lewis (1976) claim to have found such a solution. The work above explains in a nutshell the mathematics which lies behind the work of these authors who seem to do all their work formally without caring much about rigorous justification of their works. The work of Sharma and Bowtell (unpublished) provides rather accurate estimates of the so called widths calculated according to the formula given by Fermi's golden rule with  $H_1$  as in equation (27): the values are in poor agreement with experiment. The calculation uses the same pair  $(H, H_0)$  as used by Simon (1973) whose work being purely qualitative does not provide any numerical values.

Experimental results are in better agreement with semi-empirical values obtained from Fermi's rule with a different pair  $(H, H_0)$ , but semi-empirical calculations, to say the least, are semi-empirical.

We now show that whenever a self-adjoint operator is perturbed by another self-adjoint operator satisfying condition (3), the family of perturbed operators corresponding to the different values of the perturbation parameter always has a spectral concentration at each point eigenvalue of the unperturbed operator.

*Theorem 4.2.* Let  $H_0$  be a self-adjoint operator with domain  $\mathcal{D}_{H_0}$  in a Hilbert space  $\mathcal{H}$ . Let  $H^\epsilon$  be the family of operators  $H_0 + \epsilon H_1$  where  $H_1$  is a self-adjoint operator with domain  $\mathcal{D}_{H_1} \supset \mathcal{D}_{H_0}$ . Then the family  $H_\epsilon$  has a spectral concentration at each eigenvalue  $\lambda$  of  $H_0$ .

*Proof.* Let  $\phi$  be an eigenvector belonging to the eigenvalue  $\lambda$ , that is

$$H_0\phi = \lambda\phi \quad \text{or} \quad (H_0 + \epsilon H_1 - \lambda)\phi = \epsilon H_1\phi.$$

This implies that

$$\|(H_0 + \epsilon H_1 - \lambda)\phi\| = \epsilon \|H_1\phi\|$$

and provided  $\epsilon$  is small enough  $\phi$  is indeed an approximate eigenvector of  $H_\epsilon = H_0 + \epsilon H_1$  belonging to the value  $\lambda$ . Moreover if  $P$  is the projection on the eigenspace of  $H_0$  belonging to  $\lambda$ , then

$$(I - P)\phi = 0.$$

Thus  $\phi$  satisfies the condition of being an asymptotic eigenvector and according to the theorem of Conley and Rejto (1966) there is at least a first-order concentration of spectrum at  $\lambda$ . This completes the proof of our theorem.

*Remark.* Theorem 4.2 tells us that under a suitable perturbation a point eigenvalue always yields a spectral concentration. It is known from the experimental study of doubly excited states of helium that the autoionising states are associated with the vanishing of point eigenvalues embedded in the continuum under perturbation. Hence there is a heuristic link between spectral concentration and autoionisation.

## 5. Pure state or mixed state

From time to time it has been suggested by a variety of authors that a proper theory for decaying states is more likely to be found in statistical quantum mechanics rather than in the quantum theory of isolated systems. This seems to be the most probable area where a good solution of the problem is likely to be found. Slow decay, experimental or otherwise, of an isolated system does not seem very meaningful and the phenomenon is more easily understandable in terms of ensembles. The foundations of quantum theory provided by Birkhoff and von Neumann (1936) and others (see, for example, Mackey 1963, Varadarajan 1968) incorporates into the theory the collective behaviour of an ensemble through the so called mixed states. A mixed state in the theory is represented by a positive self-adjoint operator of unit trace and does not have a representation by a vector in the underlying Hilbert space. The expected value of an observable represented by the operator  $A$  in a state represented by the operator  $S$  is simply  $\text{Tr}(AS) = \text{Tr}(SA)$ . If  $S$  and  $A$  do not commute  $AS$  will not be self-adjoint but  $\text{Tr}(AS)$  is always real. It is possible that  $S$  corresponding to a decaying state is not very different from  $P$  the projection on the eigenspace of  $H_0$  belonging to the eigenvalue which dissolves into the continuum. It is also possible that  $S$  corresponding to a decaying state is not uniquely defined and as Sharma and SriRanganathan (1977) have pointed out, the lack of precise definition whether in the experimental profile or in the theoretical model is in some way the very essence of resonances. Exponential decays and Lorentzian lineshapes may very well arise from

the overwhelming desire of experimentalists to identify their results somehow with something which is acceptable even though such identifications might lack proper foundations. The situation as we see it is far from satisfactory and we hope that answering some of the objections we have raised will, in due course, shed some light on this very difficult problem.

## 6. Concluding remarks

To sum up, we have looked at some of the mathematical models of resonances and found that the subject is full of unresolved difficulties of the most fundamental kind. The results in the theories are often proved by methods which lack elegance and produce non-unique definitions and solutions. It remains a difficult task to establish contact between the rigorous quantum theory built on sound mathematical foundations (see, Varadarajan 1968 where further references will be found) and the models usually used to describe resonances. We have proved theorems which give the necessary and sufficient conditions for the existence of Hilbert space solutions of formal perturbation and kindred equations and which establish certain uniqueness properties of the solutions which exist. We have proved that whenever a state vector belonging to a point eigenvalue is perturbed, we have, with certain mild restrictions on the perturbation, the phenomenon of spectral concentration and it is possible that in cases where the spectral concentration does not constitute a point eigenvalue of the perturbed operator, we have the phenomenon which probably corresponds to a resonance. We have shown that the autoionising  $2s2p^{1,3}P$  states of helium do not admit Hilbert space solutions of the formal perturbation equations except in the zero order, though a formal solution which does not belong to the underlying Hilbert space probably exists and belongs to the dual of the domain of the unperturbed Hamiltonian. We have shown that in cases where a complex eigenvalue is obtained by interfering with a self-adjoint operator, the phenomenon is not related to deficiency indices. We have looked into the mathematical backgrounds of the work of Sharma and Bowtell (1973) on the autoionising states of helium and have made some progress towards finding the rigorous mathematical framework in which the theory can have a proper mathematical formulation.

## References

- Balslev E and Combes J 1971 *Commun. Math. Phys.* **22** 280–94  
 Birkhoff G and von Neumann J 1936 *Ann. Math., Princeton, N.J.* **37** 823–43  
 Breit G and Wigner E P 1936 *Phys. Rev.* **49** 519–31  
 Conley C C and Rejto P A 1966 *Perturbation Theory and its Applications in Quantum Mechanics* ed C H Wilcox (New York: Wiley) pp 129–43  
 Gamow G 1928 *Z. Phys.* **51** 204–12  
 Gelfand I M and Shilov G E 1967 *Generalized Functions* vol. 3 (New York: Academic) pp 190–1  
 Gleason A M 1957 *J. Math. Mech.* **6** 885–93  
 Horak Z J and Lewis M N 1976 *Czech. J. Phys. B* **26** 1088–93  
 Howland J S 1972 *University of Virginia Preprint*  
 Landau L D and Lifshitz E M 1958 *Quantum Mechanics* (Oxford: Pergamon)  
 Mackey G 1963 *The Mathematical Foundations of Quantum Mechanics* (New York: Benjamin)  
 Naimark M A 1968 *Linear Differential Operators* part 2 (London: Harrap)  
 Nakayama T and DeWitt H 1964 *J. Quant. Spectr. Rad. Transfer* **4** 623–38

- Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill)
- Rejto P A 1968 *Israel J. Math.* **6** 311–37
- Rellich F 1936 *Math. Annln.* **113** 677–85
- Riesz F and Nagy B Sz 1965 *Functional Analysis* (New York: Ungar)
- Segal I E 1947 *Ann. Math., Princeton, N.J.* **48** 930–48
- Sharma C S 1972 *Mathematical Foundations of Non-relativistic Quantum Theory* (duplicated lecture notes on an intercollegiate course given at the University of London)
- Sharma C S and Bowtell G 1973 *Can. J. Phys.* **51** 1637–45
- 1975 *Quantum Chemistry: the State of the Art* eds. V R Saunders and J Brown (Didcot: Science Research Council)
- Sharma C S and SriRanganathans 1977 *Nuovo Cim. B* **42** 65–70
- Simon B 1973 *Ann. Math., NY* **97** 247–74
- Titchmarsh E C 1958 *Eigenfunction Expansions Associated with Second-Order Differential Equations* (London: Oxford University Press)
- Weisskopf V and Wigner E 1930 *Z. Phys.* **63** 54–73
- Wong J 1967 *J. Math. Phys.* **8** 2039–42
- Varadarajan V S 1968 *Geometry of Quantum Theory* vol. 1 (New York: Van Nostrand)