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A quantum KAM-like theorem II: fundamentals of localisation in quantum theory for resonance states

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Abstract. The quantum KAM-like theorem is extended to resonance states. The formulation uses dilatation analysis and existence condition of a unique transformation between eigenstates of integrable and non-integrable Hamiltonians. This condition determines the ability to assign local quantum numbers to eigenstates of non-integrable Hamiltonians and explains localisation phenomena.

1. Introduction

In a recent paper (Hose and Taylor 1983), hitherto referred to as I, an existence condition and a method of construction were presented for a solution of the Schrödinger equation of a non-integrable Hamiltonian in N degrees of freedom, that could be uniquely assigned N quantum numbers.

To state the condition let us first define an integrable Hamiltonian H_s as one which commutes with a set of N commuting dynamical operators (observables) J_K. The eigenstates of H_s are also eigenstates of the N observables J_K. Each one is thus uniquely labelled by a set of N quantum numbers corresponding to the eigenvalues of the dynamical operators J_K. For brevity, we shall designate the eigenstates of H_s simply as ϕ_J. If the integrable system exhibits dynamical symmetry such that the spectrum of H_s is degenerate, it is possible to find alternative sets of commuting observables which will also commute with H_s. In this case, several different eigenstates of H_s exist that are related by unitary transformations that transform states only within the single-energy degenerate subspaces of H_s. Note that the quantum numbers that label the vectors in different eigenstates correspond to different sets of commuting observables. In what follows we shall consider for simplicity, and without loss of generality, only one such eigenbasis of a set of commuting N observables J_K.

For methodological purposes of making connection with classical mechanics, let us say that the classical analogue of the set J_K is a set of N global actions that commute in the Poisson bracket sense with classical H_s. The eigenstates ϕ_J are therefore the quantum analogues of classical tori in the phase space (Percival 1977) of the

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integrable Hamiltonian H_s, and the quantum numbers labelling ϕ_J are simply the analogues of the values of the classical action variables on the torus.

Now given a non-integrable Hamiltonian H it was shown in I that the condition that a particular bound normalised and L^2 integrable eigenfunction ψ of H could be uniquely assigned a set of N quantum numbers J is

$$\langle |\langle \phi_J | \psi \rangle|^2 \rangle_{\frac{1}{2}} \tag{1.1}$$

where ϕ_J is simultaneously an eigenfunction of some H_s and the set of N commuting observables J_K. That this assignment is unique, if condition (1.1) is satisfied, is seen from the fact that both ψ and ϕ_J are basis vectors in two different complete orthonormal basis sets (the perturbed and the unperturbed) for the same Hilbert space. Note that if the pair ψ and ϕ_J satisfy condition (1.1) then neither one of them will satisfy the same condition with another basis vector belonging to the other orthonormal set. Hence, condition (1.1) is a one-to-one correspondence relation, and as such, it is a test for the ability to uniquely assign quantum numbers that label the integrable function ϕ_J, to the non-integrable ψ as well.

It was also previously shown (Hose and Taylor 1982, 1983) that condition (1.1) is the convergence criterion for an iterative method to construct the solution ψ from ϕ_J. Thus the ability to assign quantum numbers is at the same time the ability to construct the solution ψ from ϕ_J. In this respect, the theorem which was presented in I is a quantum Kolmogorov, Arnol'd and Moser (KAM) like theorem (Arnol'd 1978). The latter theorem proves the existence of localised motion in classical non-integrable Hamiltonian systems. It does so by showing that if an integrable Hamiltonian H_s is perturbed so as to make the new Hamiltonian non-integrable, and if the perturbation is sufficiently small, it is possible to construct from the unperturbed (and non-resonant) tori of H_s, via a series of successive canonical transformations, new slightly deformed tori of the non-integrable Hamiltonian. The same series of successive canonical transformations generates at each step a truncated integrable Hamiltonian that becomes closer and closer to the full non-integrable Hamiltonian. Now in I, it was shown that the iterative construction of ψ from ϕ_J generates at the same time a sequence of integrable effective Hamiltonians which are 'close' to the true non-integrable Hamiltonian (if condition (1.1) is satisfied) in the sense that the final effective Hamiltonian gives the same energy while operating on ϕ_J as does the full H by operating on ψ.

Unlike the KAM, the theorem of I does not prove *a priori* 'existence' in terms of analytic properties of H_s, albeit by placing almost unacceptable restrictions on the perturbation. The new theorem, in fact, places no unusual limitations on H_s and in this sense is more general. Here condition (1.1) is a test for existence *given* the exact solutions ψ which needs to be constructed as below or by other methods. Existence, in general, is then demonstrated by simply recalling that the eigenstates of a Hamiltonian which is known to be non-integrable, namely the Hénon–Heiles (Percival 1977) have been shown (Hose and Taylor 1982) to satisfy condition (1.1). Numerous other examples are available from, say, the success of the normal mode model to describe the low-lying vibrational states of molecules.

Using condition (1.1) to assign quantum numbers requires a test ϕ_J; that is a preselected H_s and a set of N commuting observables J_K. Condition (1.1) guarantees unique assignment only within the choice of H_s and the set J_K. It does not discard the possibility that other H_s's and sets J_K exist that could satisfy (1.1). The question now comes up as to how do we know we have tested all possible H_s that determine whether

a state could be assigned by N quantum numbers or not. The answer is we do not know for sure. This is exactly similar to the classical KAM theorem where given an arbitrary H one could not be sure how many H_s exist that would make the perturbation 'sufficiently small'. If one set of J_K are found that satisfies equation (1.1), then the quantum numbers of ϕ_J can be assigned to ψ. If, in practice, an H_s and set J_K can not be found to satisfy (1.1), it can not be said with certainty that quantum numbers can not be assigned. If several H_s's and J_K sets satisfy (1.1), then several different quantum number sets can be assigned to ψ. Physically, the one with the largest value of the left-hand side of (1.1) is the best description: this being in accordance with the probability amplitude interpretation of quantum theory.

In I, the relation of assigning quantum numbers to the question of mode, orbital, or compact space, localisation was discussed. Clearly ϕ_J is local in analogy to classical tori. If condition (1.1) holds, since, in the probability amplitude sense, ψ is dominated by ϕ_J; ψ is localised on ϕ_J and the quantum numbers J are local, as opposed to global, quantum numbers of ψ. In a recent paper (Hose *et al* 1984) it is shown that the eigenfunctions of the Hénon–Heiles Hamiltonian that satisfy conditions (1.1) have Wigner transforms which are slightly distorted ϕ_J 'tori'. Moreover, it has been shown for this case (Hose and Taylor 1982) that those and only those ψ's that satisfy condition (1.1) have eigenvalues that could be computed by semi-classical Einstein–Brillouin–Keller (EBK) quantisation (Noid and Marcus 1977). This of course, is due to the fact that the EBK method only works for states associatable with classical tori; i.e. states that satisfy condition (1.1). From projections onto different ϕ_J, the wavefunctions satifying condition (1.1) could be further divided into classes which could then be uniquely associated in the $\bar{h} \to 0$ limit with the tori corresponding to librating and precessing quasi-periodic trajectories (Hose and Taylor 1982, Hose *et al* 1984). It is in the nature of the localisation that physical applications are found. This paper only discusses how to rigorously recognise localisation i.e. by the ability to assign N local quantum numbers.

As noted in I, condition (1.1) is inappropriate for resonances. A resonance is localised and is often quantised by EBK (Noid and Koszykowski 1980, Wolf and Hase 1980, Hedges and Reinhardt 1982) semi-classical methods, but it does not correspond to an eigenfunction of H; i.e. it is a wavepacket. The continuum functions at the centre of the resonance are not of L^2 type and condition (1.1) becomes meaningless. An extension of I is clearly required. Fortunately, the extension is not difficult using the dilatation analytic method (Reinhardt 1982). In § 2 the theory is reformulated using this method. A dilatation analogue of equation (1.1) is used and derived in § 3. The reader would be advised to be familiar with I before venturing forth, as the new proof is basically similar but notationally more complicated.

Section 4 and the appendix give examples stressing the ideas given previously. Section 4 also points to differences in the present criterion for convergence of perturbation theory and that given by the Kato–Rellich theorem (Kato 1966, Rellich 1969). The latter defines a parameter λ in

$$H = H_s + \lambda V$$

and looks for analyticity in λ of the eigenvalues and associated eigenprojectors. Note that such a smallness parameter, which is the only way to assure that $|\lambda V| \ll |H_s|$ in classical mechanics, is not useful in quantum theory. In the latter, smallness can be achieved even when λ is large if ψ in $|\langle\psi|\lambda V|\psi\rangle|$ is small where V is large. As such, a different approach is needed and supplied here and in I.

2. Theoretical background

For a system with N degrees of freedom consider a bound unit normalised eigenstate ϕ_J satisfying

$$H_s\phi_J = \varepsilon_J\phi_J \tag{2.1}$$

where H_s is an integrable Hamiltonian. That is, there exist N operators J_K, one of which could be H_s, such that

$$[J_K, H_s] = [J_K, J_{K'}] = 0 \tag{2.2}$$

i.e. that we have a complete set of commuting observables at our disposal that satisfy

$$J_K\phi_J = j_K\phi_J$$

where J denotes the vector $\{j_K\}$ of N quantum numbers. ϕ_J is uniquely indexed by J.

Further consider that ψ and a generally complex eigenvalue E is associated with an isolated non-degenerate pole of the resolvent of the Hamiltonian H. As such, the pole may be physically observable as a bound state or a resonance. ψ and E are given by a wave equation obtained by complex dilatation (Aguilar and Combes 1971, Balslev and Combes 1971, Simon 1973, Reinhardt 1982) of the real axis Schrödinger equation

$$H(\zeta)\psi(\zeta) = E\psi(\zeta) \tag{2.3}$$

with

$$\langle\psi(\bar{\zeta})|\psi(\zeta)\rangle = 1 \tag{2.4}$$

but $\|\psi(\zeta)\|$ is generally not equal to one. ζ is the complex scaling that uncovers the pole at E. In what follows the results of I for bound states are recovered by setting $\operatorname{Im}\zeta = 0$ in which case all scalar products retain their usual sense. Since dilatation is essentially only a change of coordinate scale for bound states equation (2.1), all quantities therein can be considered dilatated

$$H_s(\zeta)\phi_J(\zeta) = \varepsilon_J\phi_J(\zeta). \tag{2.1'}$$

The object now is to show the conditions under which there exists a method of construction of a $\psi(\zeta)$ uniquely related to ϕ_J. The existence is demonstrated by giving a convergent perturbation iteration method that constructs $\psi(\zeta)$ out of ϕ_J. The condition of convergence and the uniqueness is guaranteed by

$$|\langle\psi_E(\bar{\zeta})|\phi_J(\zeta)\rangle|^2 > \tfrac{1}{2}. \tag{1.1'}$$

Convergence will be proven in § 3 and uniqueness follows.

We can always extend the $\phi_J(\zeta)$'s and $\psi_E(\zeta)$ to a complete set such that

$$1 = \sum_K |\phi_K(\zeta)\rangle\langle\phi_K(\bar{\zeta})|, \qquad \langle\phi_K(\bar{\zeta})|\phi_L(\zeta)\rangle = \delta_{KL}$$

$$1 = \sum_{E'} |\psi_{E'}(\zeta)\rangle\langle\psi_{E'}(\bar{\zeta})|, \qquad \langle\psi_E(\bar{\zeta})|\psi_{E'}(\zeta)\rangle = \delta_{EE'}.$$

Insertion of the former into (1.1') immediately shows that if the weight of $\phi_J(\zeta)$ in $\psi_E(\zeta)$ is greater than one half, no other ϕ_K can do this. Likewise, if ψ_E is more than one half weight on ϕ_K no other $\psi_{E'}$ can do this. The uniqueness is demonstrated. To construct $\psi(\zeta)$ out of $\phi_J(\zeta)$, a projector

$$P^{\zeta} \equiv P(\zeta) = |\phi_J(\zeta)\rangle\langle\phi_J(\bar{\zeta})| \tag{2.5a}$$

is defined along with its complement

$$Q^\zeta \equiv Q(\zeta) = 1 - P^\zeta \tag{2.5b}$$

$$[Q^\zeta]^2 = Q^\zeta, \qquad [P^\zeta]^2 = P^\zeta, \qquad P^\zeta Q^\zeta = 0. \tag{2.5c}$$

Equation (2.1′) can then be rearranged using the Feshbach–Löwdin partitioning to give

$$H^\zeta_{\text{eff}}(E) P^\zeta \psi(\zeta) = E P^\zeta \psi(\zeta) \tag{2.6a}$$

or equivalently

$$H^\zeta_{\text{eff}}(E) \phi_J(\zeta) = \varepsilon_J \phi_J(\zeta) \tag{2.6b}$$

with

$$H^\zeta_{\text{eff}}(E) \equiv H^\zeta_{PP} + H^\zeta_{PQ}[1/(E - H^\zeta_{QQ})] H^\zeta_{QP} \equiv P^\zeta H^\zeta A^\zeta(E) \tag{2.7}$$

where

$$P^\zeta H(\zeta) P^\zeta \equiv H^\zeta_{PP}, \qquad Q^\zeta H(\zeta) P^\zeta = H^\zeta_{QP} \text{ etc.}$$

Also

$$\psi(\zeta) = (P^\zeta + Q^\zeta)\psi(\zeta) = \{1 + [1/(E - H^\zeta_{QQ})] H^\zeta_{QP}\} \phi_J(\zeta) = A^\zeta(E) \phi_J(\zeta). \tag{2.8}$$

$A^\zeta(E)$ is a dilatated wave operator and if it exists it constructs $\psi(\zeta)$ out of $\phi_J(\zeta)$. Multiplying (2.6*a*) by $\phi_J(\bar{\zeta})$ and integrating, gives after eliminating $\langle \phi_J(\bar{\zeta}) | \psi(\zeta) \rangle$ from both sides of equation

$$E = \langle \phi_J(\bar{\zeta}) | H^\zeta_{\text{eff}}(E) | \phi_J(\zeta) \rangle. \tag{2.9}$$

Assuming, without loss of generality that the spectrum of H^ζ_{QQ} is known, the perturbed energy which we need to know to define $A^\zeta(E)$ and $H^\zeta_{\text{eff}}(E)$, can be solved for by an iteration procedure starting from an initial guess, for example some number ε^0, by putting (2.7) into (2.9) and then iterating the result. The result is expressible as having $H^\zeta_{\text{eff}}(E)$ given now in a continued fraction form

$$\begin{aligned} H^\zeta_{\text{eff}}(\mathrm{E}) = H^\zeta_{PP} + H^\zeta_{PQ} & \frac{1}{-H^\zeta_{QQ} + \langle \phi_J(\bar{\zeta}) | H^\zeta_{PP} + H^\zeta_{PQ}} H^\zeta_{QP} \\ & H^\zeta_{qp} \frac{1}{-H^\zeta_{QQ} + \langle \phi_J(\bar{\zeta}) | H^\zeta_{PP} + H^\zeta_{pq}} H^\zeta_{QP} | \phi_J(\zeta) \rangle \\ & \qquad \frac{1}{\vdots} H^\zeta_{QP} | \phi_J(\zeta) \rangle. \\ & \qquad -H^\zeta_{QQ} + \varepsilon^0 \end{aligned} \tag{2.10}$$

Comparing equations (2.7) and (2.10) it is seen that the continued fraction form (2.10) yields at the same time a continued fraction for A^ζ. This gives by (2.8) an approximation to $\psi(\zeta)$. Note how each iterate E_i defines a sequence of $H^\zeta_{\text{eff}}(E_i)$ and $\psi_i(\zeta) = A^\zeta(E_i)\phi_J(\zeta)$. The infinite continued fraction expression (2.10) is strictly equivalent to $H^\zeta_{\text{eff}}(E)$ defined in equation (2.7). If the iteration procedure diverges, it means that $H^\zeta_{\text{eff}}(E)$ is defined only at the perturbed energy (or by infinite continued fraction) and is therefore energy dependent. Intermediate iterates have no physical meaning. However, if the iteration converges, then to any desired accuracy there exists a finite continued fraction approximation to $H^\zeta_{\text{eff}}(E)$, $A^\zeta(E)$, $\psi(\zeta)$ and E. At each iteration

equations (2.7), (2.8), (2.9) still hold; i.e. dynamics is preserved and the limiting procedure of $\phi_J(\zeta)$ going to $\psi_E(\zeta)$ is definitive. At each step $H^{\zeta}_{\text{eff}}(E)$ becomes the 'close' Hamiltonian, which as will be shown, is integrable, and which approaches the non-integrable $H(\zeta)$ in the sense that it defines as above, convergent, unique and consistent (*via* (2.7), (2.8) and (2.9)) approximations to $A^{\zeta}(E)$ (i.e. $\psi_E(\zeta)$—the 'deformed torus'). As such, the $\psi(\zeta)$ can be labelled by the J of the ϕ_J. The J are the good local quantum numbers of $\psi(\zeta)$. The convergence criterion is equation (1.1').

That each iterate of $H^{\zeta=0}_{\text{eff}}$ is integrable is due to the fact that equation (2.10) is always in $P^{\zeta=0}$ space. Since the $P^{\zeta=0}$ space is just $\phi_J(\zeta=0)$ which is an eigenfunction of N commuting observables J_K, the latter commutes with $H^{\zeta=0}_{\text{eff}}(E)$. By $H^{\zeta=0}_{\text{eff}}$ we mean that only bras and kets, not integrals, are back rotated. Note that if this convergence had not been guaranteed, the successive $H^{\zeta=0}_{\text{eff}}$ would have depended on energy and commutation would not have guaranteed that the J_K are constants of motion. The reason is that for an energy dependent Hamiltonian $H(E)$,

$$[J_K, H(E)] \neq \dot{J}_K.$$

Clearly other iteration schemes, e.g. Newton–Raphson, give methods that can solve for E iteratively and convergently if the initial iterate is chosen sufficiently close to the exact E. The Schrödinger equation is solvable by many means. What these methods do not do is to give a uniqueness criterion and they do not relate the energy and wavefunction iterations and convergence (see equation (2.7)–(2.9)). Hence other iteration methods do not assign quantum numbers. Substituting equation (2.8) into the left-hand side of equation (1.1'), and demanding that the limit of the result evaluated at $E^{(0)}, E^{(1)}, \ldots$ be greater than 0.5 is a necessary and sufficient condition for a solution with N local quantum numbers to exist.

Having accomplished our aims stated at the beginning of this section, we turn to the proof that equation (1.1') is the convergence criterion.

3. The convergence condition in the complex dilatated case

Let H be the Hamiltonian of § 2 which we suppose to be dilatation analytic. Thus $H(\zeta), \zeta \in \mathbb{C}$ is well defined. Suppose that E is a real or complex eigenvalue of $H(\zeta)$ with correspnding eigenprojector $P_E(\zeta)$. In case E is not degenerate we have

$$P_E(\zeta) = |\psi(\zeta)\rangle\langle\psi(\bar{\zeta})| \tag{3.1}$$

where $|\psi(\zeta)\rangle$ is normalised according to

$$\langle\psi(\bar{\zeta})|\psi(\zeta)\rangle = 1. \tag{3.2}$$

Thus $P_E(\zeta) = P_E^2(\zeta)$ but is not necessarily Hermitian. Note that $\|\psi(\zeta)\| \neq 1$ in general. Let $|(\phi(\zeta)\rangle$ be a dilatation analytic vector with $\langle\phi(\bar{\zeta})|\phi(\zeta)\rangle = 1$ so that

$$P^{\zeta} = |\phi(\zeta)\rangle\langle\phi(\bar{\zeta})| \tag{3.3}$$

is the associated projector. Eventually $|\phi(\zeta)\rangle$ will be an eigenvector of $H_s(\zeta)$ as discussed in § 2. Let now $Q^{\zeta} = 1 - P^{\zeta}$. Then, according to the Feshbach decomposition we have

$$[z - H(\zeta)]^{-1} = [z - H^{\zeta}_{QQ}]^{-1} + \{P^{\zeta} + [z - H^{\zeta}_{QQ}]H^{\zeta}_{QP}\}G_P(\zeta, z)\{P^{\zeta} + H^{\zeta}_{PQ}[z - H^{\zeta}_{QQ}]^{-1}\} \tag{3.4}$$

where

$$G_P(\zeta, z) = \{z - H^\zeta_{PP} - H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-1} H^\zeta_{QP}\}. \tag{3.5}$$

Equation (3.4) makes sense for z not contained in the spectra of $H(\zeta)$ and H^ζ_{QQ}. We assume now that E is an isolated eigenvalue of $H(\zeta)$ which is not contained in the spectrum of $H_{QQ}(\zeta)$. This may not be true for every possible choice of P^ζ and every ζ but it is likely that for Hamiltonians associated with atomic and molecular systems no problems arise. Now the pole of $[z - H(\zeta)]^{-1}$ at $z = E$ corresponds to the pole at $z = E$ of $G_P(\zeta, z)$. Since P^ζ is one-dimensional this means that E must be the unique solution of

$$EP^\zeta - H^\zeta_{PP} - H^\zeta_{PQ}[E - H^\zeta_{QQ}]^{-1} H^\zeta_{QP} = 0 \tag{3.6}$$

or

$$E - \langle \phi(\bar{\zeta}) | H(\zeta) | \phi(\zeta) \rangle - \langle \phi(\bar{\zeta}) | H^\zeta_{PQ}[E - H^\zeta_{QQ}]^{-1} H^\zeta_{QP} | \phi(\zeta) \rangle = 0. \tag{3.7}$$

In case ϕ remains square integrable for $\zeta = 0$ (this happens if ϕ is an eigenvector of the undilatated H_s) we can dilatate back the second terms with the result

$$E - \langle \phi | H | \phi \rangle - \langle \phi(\bar{\zeta}) | H^\zeta_{PQ}[E - H^\zeta_{QQ}]^{-1} H^\zeta_{QP} | \phi(\zeta) \rangle = 0. \tag{3.8}$$

This equation (and also (3.7)) has a unique iterative solution, provided for z in neighbourhood of E

$$|\partial_z \langle \phi(\bar{\zeta}) | H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-1} H^\zeta_{QP} | \phi(\zeta) \rangle| < 1 \tag{3.9}$$

or alternatively,

$$|\langle \phi(\bar{\zeta}) | H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-2} H^\zeta_{QP} | \phi(\zeta) \rangle| < 1. \tag{3.10}$$

Equations (3.9) and (3.10) are based upon the assumption made earlier that $[z - H^\zeta_{QQ}]^{-1}$ is analytic in a neighbourhood of E so that

$$\langle \phi(\bar{\zeta}) | H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-1} H^\zeta_{QP} | \phi(\zeta) \rangle$$

also had this property.

Let now Γ be a small circle in $\mathbb{C}$ with E in its interior and avoiding other points of the spectrum of $H(\zeta)$. Then

$$\begin{aligned} P^\zeta_E &= (2\pi \mathrm{i})^{-1} \oint_\Gamma \mathrm{d}z [z - H(\zeta)]^{-1} \\ &= (2\pi \mathrm{i})^{-1} \oint_\Gamma \mathrm{d}z \{P^\zeta + [z - H^\zeta_{QQ}]^{-1} H^\zeta_{QP}\} G_P(\zeta, z) \{P^\zeta + H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-1}\} \\ &= (2\pi \mathrm{i})^{-1} \oint_\Gamma \mathrm{d}z (z - E)^{-1} \{P^\zeta + [z - H^\zeta_{QQ}]^{-1} H^\zeta_{QP}\} (z - E) G_P(\zeta, z) \\ &\quad \times \{P^\zeta - H^\zeta_{PQ}[z - H^\zeta_{QQ}]^{-1}\} \\ &= \{P^\zeta + [E - H^\zeta_{QQ}]^{-1} H^\zeta_{QP}\} \lim_{z \to E} (z - E) G_P(\zeta, z) \{P^\zeta + H^\zeta_{PQ}[E - H^\zeta_{QQ}]^{-1}\}. \end{aligned} \tag{3.11}$$

Now, omitting ζ and $\bar{\zeta}$ for brevity

$$\begin{aligned} z-\langle\phi|H|\phi\rangle-\langle\phi|H_{PQ}[z-H_{QQ}]^{-1}H_{QP}|\phi\rangle \\ &= z-\langle\phi|H|\phi\rangle-\langle\phi|H_{PQ}[z-H_{QQ}]^{-1}H_{QP}|\phi\rangle-E+\langle\phi|H|\phi\rangle \\ &\quad +\langle\phi|H_{PQ}[E-H_{QQ}]^{-1}H_{QP}|\phi\rangle \\ &= z-E-\langle\phi|H_{PQ}\{[z-H_{QQ}]^{-1}-[E-H_{QQ}]^{-1}\}H_{QP}|\phi\rangle \\ &= (z-E)\{1+\langle\phi|H_{PQ}[z-H_{QQ}]^{-1}[E-H_{QQ}]^{-1}\}H_{QP}|\phi\rangle \end{aligned} \tag{3.12}$$

so that

$$\lim_{z\to E}(z-E)G_p(\zeta,z)=[1+\langle\phi(\bar{\zeta})|H^{\zeta}_{PQ}[E-H^{\zeta}_{QQ}]^{-2}H^{\zeta}_{QP}|\phi(\zeta))]^{-1}P^{\zeta} \tag{3.13}$$

and

$$\langle\phi(\bar{\zeta})|P^{\zeta}_{E}|\phi(\zeta)\rangle=[1+\langle\phi(\bar{\zeta})|H^{\zeta}_{PQ}[E-H^{\zeta}_{QQ}]^{-2}H^{\zeta}_{QP}|\phi(\zeta))]^{-1}. \tag{3.14}$$

From this result we conclude that the convergence condition (3.10) for the iteration procedure is equivalent to

$$|\langle\phi(\bar{\zeta})|P^{\zeta}_{E}|\phi(\zeta))|>\tfrac{1}{2} \tag{3.15}$$

i.e.

$$|\langle\phi(\bar{\zeta})|\psi(\zeta))\langle\psi(\bar{\zeta})|\phi(\zeta))|>\tfrac{1}{2}. \tag{3.16}$$

In case E is a real isolated eigenvalue of H, not contained in the spectrum of H_{QQ}, we can dilatate back with the result $|\langle\phi|\psi\rangle|^2>\frac{1}{2}$, the condition obtained earlier by Hose and Taylor. We thus have obtained the proposed extension of overlap condition $|\langle\phi|\psi\rangle|^2>\frac{1}{2}$ for the case of resonances. In fact, this extension is also needed in the case of continuum-embedded eigenvalues which cannot be removed from the continuous spectrum by symmetry arguments. In that case E would still be in the spectrum of the undilatated H_{QQ} so that $[z-H_{QQ}]^{-1}$ would not exist. Examples demonstrating the extension to resonances is given in the appendix.

We end this section with two further remarks. The first is that it often happens that ϕ, the eigenfunction of the undilatated H_s, has sufficient decay to compensate for the blowing up of $\psi(\zeta=0)$. Thus $\langle\phi|\psi\rangle$ has a meaning and equals $\langle\phi(\bar{\zeta})|\psi(\zeta)\rangle$ even if $\psi(\zeta=0)$ is not square integrable but the uniqueness property is lost. Our second remark concerns the dilatation formalism applied to molecular systems in the Born–Oppenheimer approximation. Now the Hamiltonian is no longer dilatation analytic but there exists a variant, the 'exterior scaling' version (Simon 1979), which can be used. The whole formalism presented so far remains in force in this case. We also note that the exterior scaling method has computational advantages for atoms with inner shell electrons, since it does not deform the wavefunctions in the interior of the atom.

4. Different schemes for following eigenvalues

The difference between the assignment of quantum numbers by means of continuously following the eigenvalues or by means of the 50%-overlap criterion can already be demonstrated on 2×2-matrices. Thus let $H(\lambda)$ be the matrix

$$H(\lambda)=\begin{pmatrix}1-\lambda & \zeta\lambda\\ \zeta\lambda & -1+\lambda\end{pmatrix}=\begin{pmatrix}\varepsilon_1(\lambda) & \zeta\lambda\\ \zeta\lambda & \varepsilon_2(\lambda)\end{pmatrix} \tag{4.1}$$

and let $H_s = H(0)$. The eigenvalues of $H(\lambda)$ are $E_{1,2}(\lambda) = \pm[(1-\lambda)^2 + \lambda^2\zeta^2]^{1/2}$ and the eigenvectors are $\psi_1(\lambda) = (\cos\frac{1}{2}\alpha, \sin\frac{1}{2}\alpha)$, $\psi_2(\lambda) = (-\sin\frac{1}{2}\alpha, \cos\frac{1}{2}\alpha)$ with $\tan\alpha = \zeta\lambda/(1-\lambda)$, so that $\cos\alpha = (1-\lambda)[(1-\lambda)^2 + \lambda^2\zeta^2]^{-1/2}$. Thus the eigenvectors of H_s are obtained by setting $\lambda = 0$, i.e. $\phi_1 = (1, 0)$, $\phi_2 = (0, 1)$ and the overlaps of interest are

$$\begin{aligned} \Theta_1(\lambda) &= |\langle\psi_1(\lambda)|\phi_1\rangle|^2 = \cos^2\tfrac{1}{2}\alpha = \tfrac{1}{2}(1+\cos\alpha) \\ \Theta_2(\lambda) &= |\langle\psi_1(\lambda)|\phi_2\rangle|^2 = \sin^2\tfrac{1}{2}\alpha = \tfrac{1}{2}(1-\cos\alpha). \end{aligned} \tag{4.2}$$

For $0 \leq \lambda < 1$, $\Theta_1(\lambda) > \frac{1}{2}$ so that the overlap criterion associates ϕ_1 with $\psi_1(\lambda)$. For $\lambda > 1$ we have to continue $\cos\alpha(\lambda)$ analytically so that it becomes negative and consequently $\Theta_1(\lambda) < \frac{1}{2}$ and $\Theta_2(\lambda) > \frac{1}{2}$ in this case. Now the overlap criterion associates ϕ_2 with $\psi_1(\lambda)$. On the other hand $E_1(\lambda)$ and $E_2(\lambda)$ change continuously with λ (see figure 1) so that $\psi_j(\lambda)$ is still associated with ϕ_j for $\lambda > 1$ if we apply the continuity criterion.

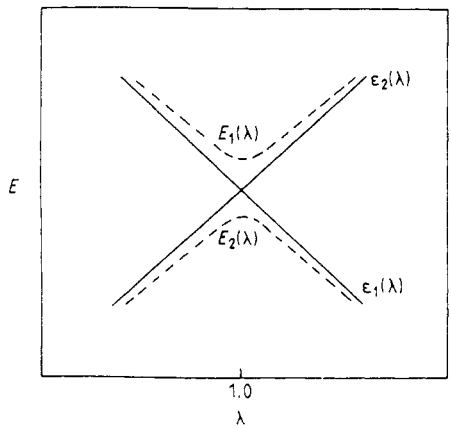

Figure 1. Perturbed and unperturbed eigenvalues as a function of the perturbation parameter λ.

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Appendix

In this appendix we consider a model example in order to show that the 50%-overlap condition can actually be met in the case of resonances. Thus let $\lambda \in \mathbb{R}$ and let

$$H_\lambda = P^2 + \lambda|\phi\rangle\langle\phi|, \qquad \phi(P) = \sqrt{\frac{a}{2\pi^2}}\,\frac{1}{P}\,\frac{1}{P^2+a^2}, \qquad a > 0 \tag{A1}$$

act in $L^2(\mathbb{R}^3, dP)$. The corresponding dilatated Hamiltonian is

$$H_\lambda(\zeta) = P^2 \exp[-2\zeta] + \lambda |\phi(\zeta)\rangle\langle\phi(\bar{\zeta})| = H_0(\zeta) + V_\lambda(\zeta). \tag{A2}$$

Here $\phi(P, \zeta) = \exp[-\frac{3}{2}\zeta]\phi(P\exp[-\zeta])$. For sake of definiteness, we take $\operatorname{Im}\zeta > 0$. The eigenvalue problem

$$H_\lambda(\zeta)|\psi_\lambda(\zeta)\rangle = E_\lambda|\psi_\lambda(\zeta)\rangle \tag{A3}$$

has the solution (non-normalised)

$$|\psi_\lambda(\zeta)\rangle = [E_\lambda - H_0(\zeta)]^{-1}|\phi(\zeta)\rangle \tag{A4}$$

where E_λ is the solution of the implicit equation

$$\langle\phi(\bar{\zeta})|[E_\lambda - H_0(\zeta)]^{-1}|\phi(\zeta)\rangle = \lambda^{-1}. \tag{A5}$$

The eigenprojector associated with E_λ is

$$P_\lambda(\zeta) = |\psi_\lambda(\zeta)\rangle\langle\hat{\psi}_\lambda(\bar{\zeta})| \tag{A6}$$

where $|\hat{\psi}_\lambda(\zeta)\rangle$ is $|\psi_\lambda(\zeta)\rangle$ normalised according to

$$\langle\hat{\psi}_\lambda(\bar{\zeta})|\psi_\lambda(\zeta)\rangle = 1. \tag{A7}$$

It follows from (A4) that

$$P_\lambda(\zeta) = \frac{|\psi_\lambda(\zeta)\rangle\langle\psi_\lambda(\bar{\zeta})|}{\langle\phi(\bar{\zeta})|[E_\lambda - H_0(\zeta)]^{-2}|\phi(\zeta)\rangle}. \tag{A8}$$

For large $|\lambda|$ we expect $|\psi_\lambda(\zeta)\rangle$ to approach $|\phi(\zeta)\rangle$. Let us therefore consider

$$\begin{aligned}\Theta(\lambda) = \langle\phi(\bar{\zeta})|P_\lambda(\zeta)|\phi(\zeta)\rangle &= \frac{\langle\phi(\bar{\zeta})|\psi_\lambda(\zeta)\rangle\langle\psi_\lambda(\bar{\zeta})|\phi(\zeta)\rangle}{\langle\phi(\bar{\zeta})|[E_\lambda - H_0(\zeta)]^{-2}|\phi(\zeta)\rangle} \\ &= [\lambda^2\langle\phi(\bar{\zeta})|E_\lambda - H_0(\zeta)]^{-2}|\phi(\zeta)\rangle]^{-1} \\ &= [-\lambda^2\partial_{E_\lambda}\langle\phi(\bar{\zeta})|[E_\lambda - H_0(\zeta)]^{-1}|\phi(\zeta)\rangle]^{-1} \\ &= [-\lambda^2\partial_{E_\lambda}\lambda^{-1}(E_\lambda)]^{-1} = [\partial_{E_\lambda}\lambda(E_\lambda)]^{-1}.\end{aligned} \tag{A9}$$

Here we used (A4) and (A5) and (A9) should be read in the sense that

$$\begin{aligned}\lambda^{-1}(E) &= \langle\phi(\bar{\zeta})|[E - H_0(\zeta)]^{-1}|\phi(\zeta)\rangle \\ \partial_{E_\lambda}\lambda(E_\lambda) &= \partial_E\lambda(E)|_{E=E_\lambda}.\end{aligned} \tag{A10}$$

If we put $E = k^2$ a straightforward calculation starting from (A5) results in

$$k^2 + \mathrm{i}ak = \lambda. \tag{A11}$$

We find for $\lambda < 0$ the physical solution

$$k = \tfrac{1}{2}\mathrm{i}a\{[1 - (4\lambda/a^2)]^{1/2} - 1\}$$

with the corresponding negative energy

$$k^2 = -\tfrac{1}{4}a^2\{2 - 4\lambda/a^2 - 2[1 - (4\lambda/a^2)]^{1/2}\}.$$

In the region $0 < \lambda < \frac{1}{4}a^2$ there are two virtual states but for $\lambda > \frac{1}{4}a^2$ there is a resonance with associated complex eigenvalue $E = k^2$,

$$k = \tfrac{1}{2}(4\lambda - a^2)^{1/2} - \tfrac{1}{2}\mathrm{i}a$$

so that

$$\text{Re } E_\lambda = \lambda - \tfrac{1}{2}a^2, \qquad \text{Im } E_\lambda = -ia(\lambda - \tfrac{1}{4}a^2)^{1/2}.$$

Since

$$\lambda = k^2 + iak = E + ia\sqrt{E} \tag{A12}$$

we have

$$\partial_E \lambda(E) = 1 + \tfrac{1}{2}iaE^{-1/2} = 1 + ia/2k \tag{A13}$$

so that for $\lambda \to 0$ we have

$$|\Theta(\lambda)| = \left|\frac{2k}{2k+ia}\right| = \left|\frac{[1-(4\lambda/a^2)^{1/2}-1]}{[1-(4\lambda/a^2)]^{1/2}}\right|. \tag{A14}$$

In this case, k is positive imaginary and $\Theta(\lambda)$ is real. The 50%-condition now gives

$$(1-4\lambda/a^2)^{1/2} - 1 > \tfrac{1}{2}(1-4\lambda/a^2)^{1/2} \qquad \text{or} \qquad |\lambda| > \tfrac{3}{4}a^2 \tag{A15}$$

For $\lambda > \frac{1}{4}a^2$ on the other hand, we have a resonance eigenstate of the dilatated Hamiltonian. Now the 50%-condition requires

$$\left|\frac{(4\lambda - a^2)^{1/2} - ia}{(4\lambda - a^2)^{1/2}}\right| = \left|1 - \frac{i}{(4\lambda/a^2 - 1)^{1/2}}\right| > \tfrac{1}{2} \tag{A16}$$

and this is always true for $\lambda > \frac{1}{4}a^2$.

In conclusion, we see that the 50%-condition holds for $\lambda < -\frac{3}{4}a^2$ (bound state with negative real eigenvalue) and for $\lambda > \frac{1}{4}a^2$ (resonance with complex eigenvalue). Thus in these cases we can take $H_s = \lambda|\phi\rangle\langle\phi|$. (Note that it only acts in the s-states subspace.)

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