

Absence of Positive Eigenvalues in a Class of Multiparticle Quantum Systems

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I. Introduction

One of the hardest questions in the spectral analysis of Schrödinger Hamiltonians is that of controlling the presence of eigenvalues embedded in the continuous spectrum. While the problem is of limited physical interest, it is of technical importance in scattering theory. Its difficulty is illustrated by three classes of examples:

1) Two-body systems (with center of mass removed) with a potential behaving like $r^{-1} \sin r$ as $r \rightarrow \infty$ are known which possess positive eigenvalues [24, 25, 16].

2) Multiparticle systems which are the special type consisting of one particle of infinite mass together with two clusters which do not interact with one another can have negative energy embedded eigenvalues, e.g.

$$-\Delta_1 - \Delta_2 - 2/r_1 - 2/r_2 \quad \text{on } L^2(\mathbb{R}^6).$$

3) There are multiparticle systems with a symmetry so that eigenvalue with one set of quantum numbers are embedded in a continuum with a different set of quantum numbers [15, 6, 17, 18].

Previous study of this question has responded to examples of type (2) and (3) by concentrating on proving the absence of positive energy eigenvalues and we will restrict ourselves to this question. For two-body systems with center of mass removed (equivalently one-body systems), the question has been more or less answered in that there are theorems which guarantee the absence of positive energy eigenvalues in a large number of cases and which only break down at the point where counterexamples of type (1) exist. The earliest results of this genre are due to Kato [11]; the strongest results, due to Weidmann [25], are for central potentials although there are almost as strong results for general potentials due to Agmon [1, 2] and Simon [16]. Much less is known in the multiparticle case. The earliest result which is for the special case of atomic Hamiltonians is due to Weidmann [26]. Later Weidmann [27] introduced a virial theorem technique; the main applications he made of this technique was to prove:

a) repulsive potential have no positive eigenvalues (see also Lavine [12]);

b) if all the two-body potentials are homogeneous with a common degree $-\alpha$ ($0 < \alpha < 2$), there are no positive eigenvalues;

c) if each two-body potential is a Yukawa potential, there are no eigenvalues in (a, ∞) where $a > 0$ depends on the coupling constants and rate of fall off of the potentials (see also Alberverio [5]). Among other things, we will extend results (b) and (c) in this paper to (b'). If each two-body potential, V_{ij} , is homogeneous with some degree $-\beta_{ij}$ ($0 < \beta_{ij} < 2$) there are no positive eigenvalues. (c') If each V_{ij} is a Yukawa potential, there are no positive eigenvalues.

Our result depends on employing two sets of ideas which have appeared recently in the study of N -body Schrödinger operators. The first is the powerful technique of dilatation analyticity introduced by Combes [9], developed by Balslev and Combes [7] and further extended and exploited by Simon [20, 17, 19]. The applicability of dilatation analytic ideas to the study of positive eigenvalues already appears in [17, 19, 22] where it is proved that local, central, dilatation analytic potentials in the two-body case cannot have positive eigenvalues (by appealing to the Agmon-Simon theorem) and where it is shown how to recover Weidmann's result (b) when $\alpha = 1$. E. Balslev (private communication) has remarked that this later argument can be easily extended to the case $0 < \alpha \leq 1$.

The second set of ideas is that eigenfunctions can often be proved to fall off exponentially. This was proved by O'Connor for discrete eigenvalues in great generality [13]. (Earlier results exist due to Ahlrichs [4] and Schnol [14]). For dilatation analytic systems, this result has been extended to embedded eigenvalues at non-threshold points by Combes [10] and Thomas [22]. All these results prove fall off in the weak sense that $\Psi \in D(\exp a|x|)$ for some $a > 0$ but in many cases, one can prove pointwise exponential bounds [21].

In any proof of the absence of positive eigenvalues, there must appear a distinction between positive (embedded) eigenvalues and negative embedded eigenvalues [because of examples (2) and (3)]. If (by induction) we know there are no positive thresholds, then a distinction appears naturally in the dilatation analytic framework if we can rotate the essential spectrum through an angle of π at which point all the negative eigenvalues become embedded (or reembedded) in continuous spectrum. Positive eigenvalues are also distinguished from resonances by this mechanism. In fact, one has the following situation. Consider a Hamiltonian $H(i\frac{\pi}{4})$. It can have positive eigenvalues, negative eigenvalues or resonance eigenvalues. The negative eigenvalues are "covered" by essential spectrum as θ passes through $i\pi/2$, the resonances are covered as θ varies through some critical value θ_0 but the positive eigenvalues persist when θ passes through 0 because of a mechanism associated with the self-adjointness of $H(0)$. Thus, of all the eigenvalues of $H(i\frac{\pi}{4})$, only

the positive eigenvalues persist for θ running through a (closed) strip of width π .

The ability to rotate the essential spectrum by an angle of π or greater is dependent on the potentials being from a special class:

Definition. A quadratic form V on $L^2(\mathbb{R}^3)$ is said to be in class $\mathcal{F}_{\pi/2}$ if F and only if:

1) V is symmetric and $Q(V) \supset Q(H_0)$ where $H_0 = -\Delta$ and Q is the quadratic form domain.

2) $(H_0 + 1)^{-1/2} V (H_0 + 1)^{-1/2}$ is compact.

3) Let $U(\theta)$ be the group of dilatations and define $F(\theta) = (H_0 + 1)^{-1/2} \cdot U(\theta) V U(\theta)^{-1} (H_0 + 1)^{-1/2}$ for $\theta \in \mathbb{R}$. $F(\theta)$ has an extension to the strip $\{\theta \mid |\operatorname{Im} \theta| \leq \pi/2\}$ which is regular (continuous and analytic on the interior). Throughout we use ideas from [7, 19] freely. We also define:

Definition. A quadratic form on $L^2(\mathbb{R}^3)$ is called local if it is the form of a multiplication operator.

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II. Statement of the Main Result

Our main theorem whose proof appears in § IV is:

Theorem 1. Let $\tilde{H} = -\sum_{i=1}^N (2\mu_i)^{-1} \Delta_i + \sum_{i < j=1}^N V_{ij}$ on $L^2(\mathbb{R}^{3N})$ with each V_{ij} a local potential in class $\mathcal{F}_{\pi/2}$. Let H be the operator on $L^2(\mathbb{R}^{3N-3})$ obtained by removing the center of mass motion from \tilde{H} (i.e. $\tilde{H} = T \otimes 1 + 1 \otimes H$ with $T = -(2\sum \mu_i)^{-1} \Delta_R$). Then H has no positive eigenvalues.

Remark. Locality is critical for the result to be true [17]. As immediate Corollaries, we have:

Theorem 2. If $V_{ij}(r)$ is homogeneous of order $-\beta_{ij}$ with $0 < \beta_{ij} < 2$, then H has no positive eigenvalues. In particular, purely Coulombic Hamiltonians have no positive energy eigenvalues.

Proof. If V_{ij} is homogeneous of order $-\beta_{ij}$ then

$$U(\theta) V_{ij} U(\theta)^{-1} = e^{-\beta_{ij}\theta} V_{ij}$$

so $V_{ij}(\theta)$ is entire. In particular $V_{ij} \in \mathcal{F}_{\pi/2}$.

Theorem 3. If each V_{ij} is of the form

$$V_{ij}(r) = r^{-1} \int_0^\infty e^{-ar} dv_{ij}(\alpha)$$

where each v_{ij} is a finite measure, then H has no positive eigenvalues.

Proof. Clearly

$$[U(\theta) V_{ij} U(\theta)^{-1}] (r) = e^{-\theta} r^{-1} \int_0^\infty \exp(-\alpha e^\theta r) dv_{ij}(\alpha)$$

is in $L^2 + (L^\infty)_\varepsilon$ if $|\arg e^\theta| = |\operatorname{Im} \theta| \leq \pi/2$.

Remark. We are in the rather strange situation of being able to prove non-existence of positive eigenvalues for Yukawa potentials but not for exponential potentials!

III. Exponential Fall Off of Eigenfunctions at Complex θ

As preparation for the proof of the main theorem, we now study the analytic continuation of eigenfunctions associated with positive eigenvalues. As an inductive hypothesis, we will suppose throughout that there are no positive thresholds. We also suppose that the hypotheses of Theorem 1 hold.

Lemma 1. *Suppose that $H\Psi = E\Psi$ with $E > 0$. Then $U(\theta)\Psi$ has a continuation in the region $B \equiv \{\theta \mid |\operatorname{Im} \theta| \leq \pi/2\}$, continuous in B , analytic in its interior.*

Proof. By standard dilatation analytic theory, E is an eigenvalue of $H(\theta)$ for all $\theta \in B$ and the eigenprojections are finite rank and analytic in θ (see e.g. [3]). By a lemma of O'Connor [13], the corresponding eigenfunction have the same analyticity properties. \square

Lemma 2. *Under the same hypotheses as Lemma 1, $U(\theta)\psi$ falls off exponentially for any θ with $\operatorname{Im} \theta \neq 0$ in the sense that there exists a $b > 0$ so that:*

$$\int |\exp(br) (U(\theta)\psi)(r)|^2 d^{3N-3}r < \infty .$$

Remarks. 1) It is easy to extend this result to real θ by a Phragmon-Lindelöf argument, see Thomas [22].

2) One can obtain explicit lower bounds on b .

Proof. This is a result of Thomas [22]. The proof is so short, we sketch it for the reader's convenience. For $\theta \in B$ and for each $\alpha \in \mathbb{R}^{3N-3}$, let:

$$H(\theta, \alpha) = e^{i\alpha \cdot x} (H(\theta)) e^{-i\alpha \cdot x} = e^{-2\theta} t(-i\nabla - \alpha) + V(\theta)$$

where $t(p)$ is the free kinetic energy as a quadratic form in p . Clearly, $H(\theta, \alpha)$ is an analytic family or type (B) as a function of α . Thus the eigenvalue E extends to an analytic function and the corresponding eigenprojections, $P(\alpha)$ are analytic. By the usual dilatation analytic argument, $E(\alpha) = E$ for all real α and thus for all α and $P(\alpha) = e^{i\alpha \cdot x} P(0) e^{-i\alpha \cdot x}$ for α real. By O'Connor's Lemma [13], $U(\theta)\psi$ is an analytic vector for $e^{i\alpha \cdot x}$ which implies that $U(\theta)\psi \in D(\exp(br))$ for some b . \square

IV. Proof of Theorem 1

By induction, we can suppose that H has no strictly positive thresholds, since the only threshold when $N = 2$ is at 0. Suppose $E > 0$ and $H\psi = E\psi$. We will show that $\psi = 0$. Fix $g \in C_0^\infty(\mathbb{R}^{3N-3} \setminus \{0\})$, a function with compact support away from $r = 0$; say $\text{supp } g \subset \{r \mid |r| \geq R > 0\}$. For $z \in [0, \infty)$, let

$$\begin{aligned} F(z) &= z^{3N} \int \overline{g(r)} \psi(zr) dr \\ &= z^{3N/2} \langle g, U(\ln z) \psi \rangle. \end{aligned}$$

By Lemma 1, $F(z)$ has a continuation in the region

$$D = \{z \mid |\arg z| \leq \pi/2, |z| > 0\}$$

Moreover

$$\begin{aligned} |F(z)| &\leq z^{3N/2} \|g\| \sup_{z \in D} \|U(\ln z) \psi\| \\ &= z^{3N/2} \|g\| \|U(i\pi/2) \psi\| \end{aligned}$$

where the equality $\sup_{z \in D} \|U(\ln z) \psi\| = \|U(i\pi/2) \psi\|$ follows from the unitarity of $U(\theta)$ when $\theta \in \mathbb{R}$ and a Phragmon-Lindelöf theorem (see [3]). Moreover

$$\begin{aligned} |F(\pm i\beta)| &\leq |\beta|^{3N} \int_{|r| \geq R} |g(r)| |U(\pm i\frac{\pi}{2}) \psi(\beta r)| dr \\ &\leq |\beta|^{3N} \int_{|r| \geq R} |g(r)| e^{b(r-R)\beta} |U(\pm i\frac{\pi}{2}) \psi(\beta r)| dr \\ &= e^{-\beta b R} |\beta|^{3N/2} \int |g(r)| |U(\ln \beta) [e^{b \cdot} U(\pm i\frac{\pi}{2}) \psi](r)| dr \\ &\leq e^{-\beta b R} |\beta|^{3N/2} \|g\| \|e^{b \cdot} U(\pm i\frac{\pi}{2}) \psi\| \end{aligned}$$

The last norm is finite by Lemma 2.

Thus F is a polynomially bounded function in the right half plane, falling off exponentially along the imaginary axis. By a theorem of Carlson [8] (see also Titchmarsh [23]), $F \equiv 0$. Thus $F(1) = \langle g, \psi \rangle = 0$. Since the set of allowable g 's is dense, $\psi = 0$. \square

References

1. Agmon, S.: Lower bounds for Schrödinger type equations. Proc. Tokyo International Conf. on Functional Analysis 1969
2. Agmon, S.: Lower bounds for solutions of Schrödinger operators. J. Anal. Math. **23**, 1 (1970)
3. Aguilar, J., Combes, J. M.: A class of analytic perturbations for one-body Schrödinger hamiltonians. Commun. math. Phys. **22**, 269 (1971)
4. Ahlrichs, R.: Asymptotic behavior of atomic bound state wave functions. Univ. of Karlsruhe Preprint

5. Albeverio, S.: On bound states in the continuum for N-body systems and the virial theorem. *Ann. Phys.* **71**, 167 (1972)
6. Balslev, E.: Spectral theory of Schrödinger operators of many-body systems with permutation and rotation symmetries. *Ann. Phys.* **73**, 49 (1972)
7. Balslev, E., Combes, J.M.: Spectral properties of many body Schrödinger operators with dilatation-analytic interactions. *Commun. math. Phys.* **22**, 280 (1971)
8. Carlson, F.: University of Upsala Thesis (1914)
9. Combes, J.M.: An algebraic approach to quantum scattering. Unpublished report (1969)
10. Combes, J.M.: On the exponential fall off for bound state systems of many particle systems. *Commun. math. Phys.*, to appear
11. Kato, T.: Growth properties of solutions of the reduced wave equation with a variable coefficient. *Commun. Pure Appl. Math.* **12**, 403 (1959)
12. Lavine, R.: Commutators and scattering theory, I. Repulsive interactions. *Commun. Math. Phys.* **20**, 301—323 (1971)
13. O'Connor, A.: Exponential Decay of bound state wave functions. *Commun. math. Phys.* **32**, 319—340 (1973)
14. Schnol, I.: *Math. sb.* **42**, 273—286 (1953)
15. Sigolov, A., Zhislin, G.: On the spectrum of an energy operator for atoms. *Izv. Ak. Nauk. USSR Mat.* **29**, 853 (1965)
16. Simon, B.: On positive eigenvalues of one-body Schrödinger operators. *Commun. Pure Appl. Math.* **22**, 531—538 (1969)
17. Simon, B.: Resonances in n-body quantum systems with dilatation analytic potentials. *Ann. Math.* **97**, 247 (1973)
18. Simon, B.: Continuum embedded eigenvalues for spatially cut off $P(\varphi)^2$ hamiltonians. *Proc. A.M.S.* **35**, 223 (1972)
19. Simon, B.: Quadratic form techniques and the Balslev-Combes theorem. *Commun. math. Phys.* **27**, 1 (1972)
20. Simon, B.: Convergence of time-dependent perturbation theory for antiionizing states of atoms. *Phys. Lett.* **36A**, 23 (1971)
21. Simon, B.: Pointwise bounds on eigenfunctions and wave packets in N-body quantum systems. *Proc. A.M.S.*, to appear
22. Thomas, L.: Asymptotic behavior of eigenfunctions for multiparticle Schrödinger hamiltonians. *Commun. math. Phys.*, to appear
23. Titchmarsh, E. C.: *The theory of functions.* Oxford Press 1932
24. von Neumann, J., Wigner, E.: Über merkwürdige diskrete Eigenwerte. *Z. Phys.* **30**, 465 (1929)
25. Weidmann, J.: Zur Spektraltheorie von Sturm-Liouville Operatoren. *Math. Zeit.* **98**, 268 (1967)
26. Weidmann, J.: On the continuous spectrum of Schrödinger operators. *Commun. Pure Appl. Math.* **19**, 107—110 (1966)
27. Weidmann, J.: The virial theorem and its application to the spectral theory of Schrödinger operators. *Bull. A.M.S.* **73**, 452—456 (1967)

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