BOUND ON RESONANCE EIGENVALUES OF SCHRÖDINGER OPERATORS

Heinz K.H. SIEDENTOP [1]
Institut für Mathematische Physik, Carolo-Wilhelmina, Mendelssohnstrasse 3, 3300 Braunschweig, Fed. Rep. Germany

Received 18 August 1983

A variational bound on both the real and the imaginary part of resonance eigenvalues is given for multiparticle Schrödinger operators with dilation analytic potentials.

1. Introduction. For selfadjoint operators there is a variety of methods for obtaining both upper and lower bounds on their eigenvalues, e.g. the minimax principle [1], the lower bound of Temple [2], and the "variance minimization" methods of Weinstein [3] (see also ref. [4], p. 321). All these are confined to selfadjoint operators; therefore, they cannot be used to localize eigenvalues of nonselfadjoint operators. In particular thus far bounds on resonance eigenvalues (real and imaginary part) which may be defined for a certain class of potentials as the poles of the resolvent of the complex dilated Schrödinger operator [5,6] seem to be unknown (see the review articles of Reinhardt [7], Junkers [8], p. 228 and Simon [9], open problem in §4.B).

Our starting point for the localization of resonances is the following bound on the multiplicity of eigenvalues [10,11]: Let A be an operator in $\mathcal{T}_{2p}(\mathcal{H})$, the ideal of all bounded operators on the complex Hilbert space $\mathcal{H}$ with $\mathrm{tr}(|A|^{2p}) < \infty$, $(p = 1, 2, 3, ...)$. Then for every $B \in \mathcal{T}_{2p}(\mathcal{H})$

$$\mathrm{tr}(|[(A-1)B + A]^p|^2) \geqslant \dim(\mathrm{Ker}(A-1)). \tag{1}$$

Choosing

$$B = A[(1-A)|_{[\mathrm{Ker}(1-A)]^\perp}]^{-1} P_{(1-A)(\mathcal{H})}, \tag{2}$$

$P_{(1-A)(\mathcal{H})}$ being the orthogonal projection on the image of $1-A$, minimizes the left-hand side of (1) such that there holds equality. Let H be a (multiparticle) Schrödinger operator defined by the corresponding quadratic form with dilation analytic pair potentials V_{ij} of class $\mathcal{F}_\alpha$ reduced on center of mass coordinates. (Here, and in the following we shall use the notations of refs. [12,13].) Choosing atomic coordinates H is given by

$$H = H_0 + V = -\sum_{i=1}^{N-1} (2\mu_i)^{-1}\Delta_i + \sum_{i,j=1;\, i<j}^{N-1} m_N^{-1}\nabla_i\nabla_j + \sum_{i=1}^{N-1} V_{iN}(\boldsymbol{\eta}_i) + \sum_{i,j=1;\, i<j}^{N-1} V_{ij}(\boldsymbol{\eta}_i - \boldsymbol{\eta}_j), \tag{3}$$

where $\mu_i^{-1} = m_i^{-1} + m_N^{-1}$, $\boldsymbol{\eta}_i = r_i - r_N$, and the derivatives are with respect to the coordinates $\boldsymbol{\eta}_1, ..., \boldsymbol{\eta}_{N-1}$. Let $\mathrm{U}(\vartheta)$ be the one-parameter group of dilatations.

$$[\mathrm{U}(\vartheta)\varphi](r) = \mathrm{e}^{d\vartheta/2}\varphi(\mathrm{e}^{\vartheta}r). \tag{4}$$

$V_{ij}(\vartheta) = U(\vartheta)V_{ij}U(\vartheta)^{-1}$ the dilated pair interactions, $G_0(\vartheta) = [E - H_0(\vartheta)]^{-1} = (E - \mathrm{e}^{-2\vartheta}H_0)^{-1}$ the Green function of the dilated kinetic energy, $V_{\mathrm{D}_i\mathrm{D}_j}(\vartheta) = I_{\mathrm{D}_i}(\vartheta) - I_{\mathrm{D}_j}(\vartheta)$ the difference of the dilated intercluster inter-

[1] Address after 1 August 1983: Department of Mathematics, California Institute of Technology, Pasadena, CA 91125, USA.

0.031-9163/83/0000–0000/$ 03.00 © 1983 North-Holland

actions of the cluster decompositions D_i and D_j,

$R_{D_i}(\vartheta) = [1 - G_0^{1/2}(\vartheta) V_{D_i}(\vartheta) G_0^{1/2}(\vartheta)]^{-1}$

dilated reduced Green function, and

$$H(\vartheta) = H_0(\vartheta) + \sum_{i,j=1;\, i<j}^{N} V_{ij}(\vartheta).$$

Now, the points of the discrete spectrum of $H(\vartheta)$ which are not in the discrete spectrum of H are called resonance eigenvalues of H [14].

In order to apply the inequality (1) to localize resonance eigenvalues of H we need an integral equation for the resonance states whose kernel lies in some trace ideal $\mathcal{T}_{2p}$ ($p = 1, 2, 3, ...$). An obvious candidate is the modified symmetrized Weinberg–van Winter equation

$$I_s(\vartheta, E)\varphi = \varphi\,, \tag{5}$$

where

$$I_s(\vartheta, E) = \sum_{S=\{D_N,\ldots,D_2\}} [G_0^{1/2}(\vartheta) V_{D_N D_{N-1}}(\vartheta) G_0^{1/2}(\vartheta)]\, R_{D_{N-1}}(\vartheta) \ldots R_{D_2}(\vartheta)$$
$$\times\, [G_0^{1/2}(\vartheta) V_{D_2 D_1}(\vartheta) G_0^{1/2}(\vartheta)]\,, \tag{6}$$

the sum running over all connected strings $S = \{D_N, D_{N-1}, \ldots, D_2\}$; i.e. for $E \notin \Sigma_\vartheta + e^{-2\vartheta} R_+$, where $\Sigma_\vartheta = \cup_D \{E_1 + \ldots + E_k \mid E_i$ is an element of the discrete spectrum of the dilated cluster hamiltonian $H_{C_i}(\vartheta)$, C_i being an element of the cluster decomposition $D\}$, $I_s(\vartheta, E)$ has the eigenvalue one of multiplicity $d_I(E)$, if $H(\vartheta)$ has the eigenvalue E of multiplicity $d(E)$ with $0 \leqslant d(E) \leqslant d_I(E)$.

Therefore, intending to use inequality (1) for the localization of the resonances by setting $A = I_s(\vartheta, E)$ we have to show $I_s(\vartheta, E)$ to be in some trace ideal $\mathcal{T}_{2p}(L^2(R^{3(N-1)}))$ for $p = 1, 2, 3, \ldots$ Then, for any choice of B, the resonance eigenvalues of H are, according to (1), necessarily confined to those regions of the complex plane which are included by the contour line

$$1 = g(E) = \mathrm{tr}(|[(I_s(\vartheta, E) - 1)B(E) + I_s(\vartheta, E)]^p|^2)\,,$$

i.e. the contour line where $g(E)$ drops below one.

2. Trace ideal properties of Weinberg–van Winter kernels and dilation analyticity of Schrödinger operators. We have the following trace ideal properties of $I_s(\vartheta, E)$:

Theorem 1: Let V_{ij}: $\{e^\vartheta r \mid r \in R^3, |\mathrm{Im}\, \vartheta| < \alpha\} \to C$, V_{ij} its restriction to the real line, $(V_{ij}(\vartheta))(r) = V_{ij}(e^\vartheta r)$ with $V_{ij}(\vartheta) \in R + L^{2p}(R^3)$ for every ϑ with $|\mathrm{Im}\, \vartheta| < \alpha$, $E \notin \Sigma_\vartheta + e^{-2\vartheta} R_+$, $\mathrm{Re}(e^{2\vartheta}E) < 0$. Then $I_s(\vartheta, E) \in \mathcal{T}_{2p}(L^2(R^{3(N-1)}))$.

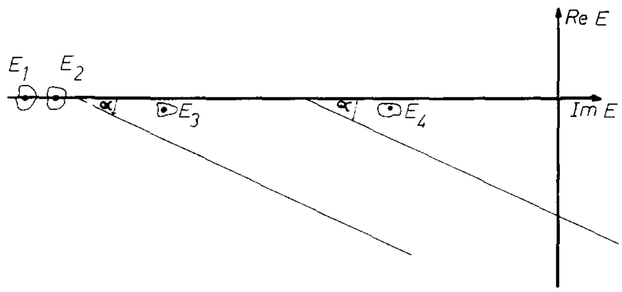

Fig. 1. Localization of eigenvalues of $H(\vartheta)$; $\alpha = \mathrm{Im}(2\vartheta)$. E_1 and E_2: eigenvalues belonging to bound states of H. E_3 and E_4: resonance eigenvalues. The eigenvalues are enclosed by the contour line $g(E) = 1$.

Proof: The proof proceeds analogously to the undilated case [15] where $I_s(E)$, the unmodified symmetrized Weinberg–van Winter kernel, was shown to lie in $\mathcal{I}_{2p}$ for E below the bottom of the essential spectrum. We only have to use a modified estimate for the free Green function reduced on the center of mass system in momentum space:

$$\sum_{i,j=2}^{N} a_{ij}P_i'P_j' \geqslant \sum_{i=2}^{N} c_i P_i'^2 \geqslant cP_\vartheta'^2 , \qquad c>0.$$

(We use Simon's notation [12], p. 189.) Therefore

$$|G_0^{1/2}(\vartheta)(P_2', \dots, P_N')| = |(E - H_0(\vartheta)]^{-1}(P_2', \dots, P_N')| = |e^{-2\vartheta} \sum a_{ij}P_i'P_j' - E|^{-1/2}$$

$$= e^{-2\mathrm{Re}\,\vartheta} \left| e^{2\vartheta}E - \sum a_{ij}P_i'P_j' \right|^{-1/2} \leqslant e^{-2\mathrm{Re}\,\vartheta} |e^{2\vartheta}E - cP_\vartheta'^2|^{-1/2} ,$$

where the inequality holds, if $\mathrm{Re}(e^{2\vartheta}E) < 0$. Using this estimate, and observing that the spectrum of the cluster decomposed hamiltonian H_D (hamiltonian minus the intercluster interactions of D) is contained in $\Sigma_\vartheta + e^{-2\vartheta}\mathrm{R}_+$ we may repeat the iteration of the above-mentioned proof.

In the following we restrict ourselves to spherical symmetric interaction potentials V_{ij}. Then, for real ϑ $V_{ij}(\vartheta)$ is multiplication by the function $V_{ij}(e^\vartheta r)$. Now, suppose $V(r)$ has an analytic continuation $V(z)$ to a sector $\{z \mid |\arg(z)| < \alpha\}$. Then, under the hypothesis of theorem one, V_{ij} is in the class $\mathcal{F}_\alpha$ which is a modification of a result of ref. [13].

3. Bounds on the dimension of eigenspaces of $H(\vartheta)$. The desired bound on the dimension of eigenspaces is now a simple corollary of inequality (1) and the result of section 2.

Theorem 2: Let V_{ij}: $\mathrm{R}_+ \to \mathrm{R}$ be a function with analytic continuation into the sector $\{z \mid |\arg(z)| < \alpha\}$. Let $(V_{ij}(\vartheta))(r(\ )) \in \mathrm{R} + \mathrm{L}^2(\mathrm{R}^{3(N-1)})$, $|\mathrm{Im}(\vartheta)| < \alpha$, which is in this case multiplication by $V_{ij}(e^\vartheta r)$, let E be away from $\Sigma_\vartheta + e^{-2\vartheta}\mathrm{R}_+$, and from the negative real axis, $\mathrm{Re}(e^{2\vartheta}E) < 0$, and $d(E)$ as defined in section 2 i.e. those resonance eigenvalues which are in the discrete spectrum of $H(\vartheta)$. Then

$$g(E) = \mathrm{tr}(\,|[(I_s(\vartheta, E) - 1)B + I_s(\vartheta, E)]^p|^2) \geqslant d(E) \tag{7}$$

for any $B \in \mathcal{I}_{2p}(\mathrm{L}^2(\mathrm{R}^{3(N-1)}))$. Furthermore, for

$$B = -1 + ((1 - I_s(\vartheta, E))|_{[\mathrm{Ker}(1 - I_s(\vartheta, E))]^\perp})^{-1} P_{[1 - I_s(\vartheta, E)]}(\mathrm{L}^2(\mathrm{R}^{3(N-1)})) , \tag{8}$$

equality holds in (7) except for those E which correspond to spurious solutions, i.e. to points E where $I_s(\vartheta, E)$ has the eigenvalue one of multiplicity $d_\mathrm{I}(E)$ but $H(\vartheta)$ does not have the eigenvalue E, or, if $H(\vartheta)$ has E as an eigenvalue, its multiplicity is less than $d_\mathrm{I}(E)$.

4. Conclusions. The operator I_s depends analytically on E. Thus for suitable choices of B_E (sufficient smoothness properties concerning the E dependence) the function $g(E)$ will be smooth, too, and we may speak of contour lines of $g(E)$, especially of the contour line $g(E) = 1$. As mentioned in the introduction the resonance eigenvalues lying in the discrete spectrum of $H(\vartheta)$ are, if this line is closed, necessarily enclosed by it. Thus, we may localize resonance eigenvalues. Furhtermore, if the operator B is in a certain sense near to the minimal operator B_min as defined by (8), the bounds on the resonance will become very sharp.

There exist definite procedures for obtaining such approximated operators B_min, e.g. the modified Fredholm series [16,17] yields a convergent series for B_min, though it might be numerical more efficient to use some other approximation method for B_min; but, no matter which approximation method is actually used, we obtain rigorous bounds on resonances.

References

[1] E. Fischer, Monatsh. Math. Phys. 16 (1905) 234.
[2] G. Temple, Proc. R. Soc. A119 (1928) 276.
[3] D.H. Weinstein, Proc. Acad. Sci. (USA) 20 (1934) 529.
[4] K. Yoshida, Functional analysis, 5th ed. (Springer, Berlin, 1978).
[5] J. Aguilar and J.M. Combes, Commun. Math. Phys. 22 (1971) 269.
[6] E. Balslev and J.M. Combes, Commun. Math. Phys. 22 (1971) 280.
[7] W.P. Reinhardt, Ann. Rev. Chem. 33 (1982) 223.
[8] B.R. Junkers, Adv. At. Mol. Phys. 18 (1982) 207.
[9] B. Simon, Int. J. Quant. Chem. 14 (1978) 529.
[10] H.K.H. Siedentop, Phys. Lett 93A (1983) 286.
[11] H.K.H. Siedentop, Dimension of eigenspaces of Schrödinger operators – Local Birman–Schwinger bound, Rep. Math. Phys., to be published.
[12] B. Simon, Quantum mechanics for hamiltonians defined as quadratic forms (Princeton Univ. Press, Princeton, 1971).
[13] B. Simon, Commun. Math. Phys. 27 (1972) 1.
[14] M. Reed and B. Simon, Methods of modern mathematical physics IV: Analysis of operators (Academic Press, New York, 1978).
[15] H.K.H. Siedentop, Localization of discrete spectrum of multiparticle Schrödinger operators, to be published.
[16] E. Seiler and B. Simon, Commun. Math. Phys. 45 (1975) 99.
[17] B. Simon, Trace ideals and their applications (Cambridge Univ. Press, London, 1979).