Localization of Discrete Spectrum of Multiparticle Schrödinger Operators

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An upper bound on the dimension of eigenspaces of multiparticle Schrödinger operators is given. Its relation to upper and lower bounds on the eigenvalues is discussed.

1. Introduction

In the case of one- and two-particle Schrödinger operators $H$, upper bounds on the multiplicity of eigenvalues have been given in [1–4]. They generalize results of Birman [5], Schwinger [6], and others (for a review see Simon [7]), who gave global bounds on the number of eigenvalues, i.e. bounds on the total number of eigenvalues of $H$ below some $-x^2$, $x$ positive.

Multiparticle systems admit a wealth of processes, e.g. capture processes, breakup processes, rearrangements and excitations, which cannot occur or occur only rudimentarily in one- and two-particle systems. This dynamical complication is also reflected in the resolvent equation: E.g. the kernel of the homogeneous Lippman-Schwinger equation and the kernel of the Rollnik equation is not compact for particle number $N$ bigger than 2. Therefore a direct transcription to the $N$ particle case is feasible neither for the global bounds [5–7] nor for the local bounds [1–4].

Thus, the results on global bounds on the number of eigenvalues of multiparticle systems appeared relatively late: Yafaev [8] gave bounds on the total number of bound states of some threeparticle systems, whose interaction potentials are short range and negative, using the Faddeev equations. Simon [9] and Klaus and Simon [10] obtained bounds on the total number of eigenvalues for such potentials for the general $N$-body case, if the essential spectrum of the Schrödinger operator is given by two cluster breakups. Hill [11–13] has shown, that the $H^-$-ion has exactly one bound state and that the $H^{--}$-ion has no bound states at all. The complete absence of bound state for highly negative charged ions in general, i.e. their nonexistence, has been demonstrated by Ruskai [14, 15] and Sigal [16, 17]. In a further step Sigal [16, 18] gave a certain generalization of the Birman-Schwinger principle to the multiparticle case and showed a bound on the number of the eigenvalues of a Schrödinger operator being less than $E$:

$$\text{tr} \left| K_1(E) \right|^2 \leq \text{dim} \left\{ \varphi \in D(H) \mid \text{ex. } \lambda < E \text{ s.t. } H \varphi = \lambda \varphi \right\},$$

where

$$K_1(E) = J K(E) J^{-1}, \quad (J^2 u)(x) = (1 + |x|^2)^{-\delta/2} u(x)$$

and

$$K(E) = \sum_a J_a R_a(E) W_a.$$  

$J_a$ is a Ruelle-Simon partition of unity, $R_a$ is the resolvent of the intercluster Hamiltonian with respect to the cluster decomposition $a$ and

$$W_a = [J_a, -A] + J_a I_a.$$  

$I_a$ is the interaction between the clusters of $a$.

Local bounds on the number of eigenvalues, i.e. bounds on the dimension of $\text{Ker}(H - E)$

$$d(E) = \text{dim} \text{Ker}(H - E),$$

where $H$ is the Schrödinger operator

$$H = \sum_{i=1}^N \frac{1}{2m_i} A_i + \sum_{i,j=1}^N V_{ij}(x_i-x_j)$$

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reduced on the center of mass system and where $E$ is a negative real number below the bottom of the essential spectrum of $H$, are unknown. The purpose of the present paper is to give such a bound for a certain class of singular and long-range potentials.

In chapter two we collect some results, which we shall need in the following, and define our notation: The first section of this chapter contains the inequality on the dimension of eigenspaces of operators lying in some trace ideal $\mathfrak{I}_p (p = 1, 2, 3, \ldots)$; in the second section we give some notations which are useful for describing the breakup of multiparticle systems into clusters, and, furthermore, we show that the trace ideal properties of the symmetrized Weinberg-van Winter kernel depend on the decay properties of the interaction potentials. In chapter three we prove the bound on the dimension of eigenspaces of the Schrödinger operator $H$ using the Weinberg-van Winter equation. In addition we comment on using other integral equations for bound states, e.g. the geometric resolvent equation of Sigal [16, 18]. In chapter four we make explicit bound on chapter three for the simplest non-trivial system, the helium atom. The concluding chapter five discusses the relation of the bound states, e.g. the geometric resolvent equation. This is no longer possible for multiparticle systems, since that kernel is no longer compact. There is, however, a substitute for the Rollnik kernel in the case of multiparticle systems which is in some trace ideal $\mathfrak{I}_p$ of finite index $p$: In the following we shall recapitulate the machinery of the Weinberg-van Winter equation and show trace ideal properties of its kernel.

2.2.: In the following we shall use as far as possible the nomenclature of Simon [19]: A cluster decomposition $D$ of $\{1, \ldots, N\}$ is a family of disjoint subsets of $\{1, \ldots, N\}$ whose union is $\{1, \ldots, N\}$. The elements of $D$ are called clusters.

Given a cluster decomposition we write $i D j$, iff $i$ and $j$ are in the same cluster of $D$, and $i D j$, iff $i$ and $j$ lie in different clusters of $D$.

Let $H = H_0 + \sum_{i < j, i, j = 1}^N V_{ij}$ be an $N$-body Schrödinger operator. Then

$$V_D := \sum_{i, j = 1, i < j, i D j} V_{ij}$$

is called the cluster potential,

$$H_D := H_0 + V_D$$

the cluster Hamiltonian, and

$$I_D := \sum_{i, j = 1, i < j, \sim i D j} V_{ij}$$

the intercluster interaction.

Let $D_1$ and $D_2$ be two cluster decompositions. $D_2$ is called a refinement of $D_1$, $D_1 \subset D_2$, iff $D_2$ is obtained from $D_1$ by further partitioning. A string $S$ is an ordered family of cluster decompositions $(D_N, D_{N-1}, \ldots, D_1)$ with $D_N \supset D_{N-1} \supset \ldots \supset D_2$ such that $D_i (i = k, \ldots, N)$ contains $l$ elements. We call the string connected, iff $k = 1$. $i(S):= k$ is called the index of the string.
Finally set 
\[ V_{D_r D_{r-1}} := I_{D_r} - I_{D_{r-1}} = V_{D_{r-1}} - V_{D_r} \]  
(11) 
and 
\[ R_{D_r} := (1 - G_0^{1/2} V_{D_r} G_0^{1/2})^{-1}, \]  
(12) 
where \( G_0 = (z - H_0)^{-1} \) is the free resolvent. \( R_{D_r} \) is called the reduced Green's function.

Using these notations, we define the Weinberg-van Winter kernel \( I(E) \) to be 
\[ I(E) = \sum_{S = [D_0, \ldots, D_{r-1}]} (E - H_{D_0})^{-1} V_{D_0 D_{r-1}} (E - H_{D_{r-1}})^{-1} \]  
\[ \cdot \cdot \cdot \cdot (E - H_{D_{r-2}}) V_{D_{r-2} D_{r-1}} \cdot (E - H_{D_{r-1}})^{-1} V_{D_{r-1} D_r} \]  
(13) 
(see [19–22]) and the symmetrized Weinberg-van Winter kernel \( I_s(E) \) to be 
\[ I_s(E) = \sum_{S = [D_0, \ldots, D_{r-1}]} (G_0^{1/2} V_{D_0 D_{r-1}} G_0^{1/2}) \]  
\[ \cdot R_{D_{r-1}} \cdots R_{D_r} (G_0^{1/2} V_{D_r D_{r-1}} G_0^{1/2}), \]  
(14) 
In the following for all occurring operators we suppose the center of mass being removed, i.e. we separate out the center of mass motion and choose the configuration space of the \( N \)-body system with \( m_1, \ldots, m_N \) to be the hyperplane 
\[ X = \left\{ x \in \mathbb{R}^{3N} \mid \sum_{i=1}^{N} m_i x_i = 0 \right\} \] 
and define the scalar product in \( X \) to be 
\[ \langle x, y \rangle = 2 \sum_{i=1}^{N} m_i x_i y_i. \]

In the following we need an integral equation for the bound states whose kernel lies in some trace ideal. Theorem one shows that the symmetrized Weinberg-van Winter kernel yields such an integral equation:

**Theorem 1:** Let \( V_{ij} \in R + L^2(\mathbb{R}^3) \), for some \( p = 1, 2, 3, \ldots \), and \( E < \Sigma \), being the bottom of the essential spectrum of the Schrödinger operator reduced on center of mass coordinates. Then it holds:

a) \( I_s(E) \in \mathcal{S}_{2p}(L^2(X)) \).

b) If \( H \) has \( E \) as an eigenvalue, then \( I_s(E) \) has the eigenvalue one. If \( \psi \) is an eigenfunction of \( H \), then 
\[ (E - H_0)^{1/2} \psi \]  
is the corresponding eigenfunction of \( I_s(E) \).

Proof: a) The proof is by induction and follows an idea of Hunziker [23] (see also Simon [19], pp. 187). We only have to modify the step from \( n \) to \( n + 1 \). We use the notations of Simon [19].

In order to show \( I_s(E) \) to be in \( \mathcal{S}_{2p}(L^2(X)) \) we consider each individual term of \( I_s(E) \) separately, i.e., a general term 
\[ T = (G_0^{1/2} V_{x_{n+1} G_0^{1/2}} R_{D_{n+1}} (G_0^{1/2} V_{x_{n+1} G_0^{1/2}}) \cdots \]  
\[ \cdot R_{D_{r-1}} (G_0^{1/2} V_{D_r} G_0^{1/2}), \]  
(16) 
where \( i_r \) and \( j_r \) are indices in different clusters of \( D_r \) but the same cluster of \( D_{r-1} \). Furthermore we introduce the coordinates \( x_{k}^r := x_{a_is} \) \( (k = 2, \ldots, N) \), which are a complete independent set of coordinates in \( X \).

We deal with the kernel \( \mathcal{T} \) of \( T \) in momentum space and prove that 
\[ \tau(P_2, \ldots, P_N, \tilde{P}_2, \ldots, \tilde{P}_N) \]  
\[ = |\mathcal{T}(P_2, \ldots, P_N, \tilde{P}_2, \ldots, \tilde{P}_N)| \] 
defines an operator \( \tau \) such that 
\[ \tau \in \mathcal{S}_{2p}(L^2(X)). \]  
(17) 
This implies \( T \in \mathcal{S}_{2p} \).

First we note that 
\[ T_r := [(G_0^{1/2} V_{N} G_0^{1/2}) R_{D_{n+1}}] \cdots [(G_0^{1/2} V_{r+1} G_0^{1/2}) R_{D_{1}}], \]  
(18) 
has no forces between clusters of \( D_r \), so it has a kernel with \( \delta(P_2 - P_3) \cdots \delta(P_r - P_r) \), that is 
\[ (T_r f)(P_2, \ldots, P_N) = \int d\tilde{P}_{r+1} \ldots \]  
\[ \cdots d\tilde{P}_N \mathcal{T}(P_2, \ldots, P_r, \tilde{P}_{r+1}, \ldots, \tilde{P}_N) \cdot f(P_2, \ldots, P_r, \tilde{P}_{r+1}, \ldots, \tilde{P}_N). \]  
(19) 
Let \( t^{(P_2, \ldots, P_0)} \) be the operator which has the absolute value of \( \mathcal{T}(P_2, \ldots, P_0) \) as kernel. We shall show inductively that the \( \mathcal{S}_{2p}(L^2(P_{r+1}, \ldots, P_N)) \)-norm is uniformly bounded in \( P_2, \ldots, P_r \); i.e. there exists a \( d_r \) such that for all \( P_2, \ldots, P_r \) 
\[ |t^{(P_2, \ldots, P_0)}|_{\mathcal{S}_{2p}(L^2(P_{r+1}, \ldots, P_N))} < d_r < \infty. \]  
(20) 
Start the induction with \( r = N \) so \( \mathcal{T}(P_2, \ldots, P_0) = 1 \). Clearly \( t^{(P_2, \ldots, P_0)} \) fulfills (20).

Now, suppose we know \( t^{(P_2, \ldots, P_0)} \) obeys the claim. Let \( S^{(P_2, \ldots, P_r)} \) be the operator which has the
absolute value of the kernel of $T_{r}(G_{0}^{1/2}V_{r}G_{0}^{1/2})$ as kernel:

$$
\begin{align*}
S_{r}^{(P_{r},\ldots,P_{r-1})}(P_{r},\ldots,P_{N},\tilde{P}_{r},\ldots,\tilde{P}_{N}) &= |S_{r}^{(P_{r},\ldots,P_{r-1})}(P_{r+1},\ldots,P_{N},\tilde{P}_{r+1},\ldots,\tilde{P}_{N})| \\
&\cdot |G_{0}^{1/2}(P_{r},\ldots,P_{r-1},\tilde{P}_{r},\ldots,\tilde{P}_{N})| V_{r}(P_{r}-\tilde{P}_{r}) \\
&\cdot |G_{0}^{1/2}(P_{r},\ldots,P_{r-1},\tilde{P}_{r},\ldots,\tilde{P}_{N})|,
\end{align*}
$$
(21)

where $\tilde{V}_{r}$ is the suitably normalized Fourier transform of $V_{r}$, and

$$
|G_{0}^{1/2}(P_{r}^{2},\ldots,P_{r}^{N})| = -i (\Sigma a_{ij} P_{r}^{i} P_{r}^{j} - E)^{-1/2},
$$
(22)

where $a_{ij}$ is a positive definite matrix. Since $a_{ij}$ is positive definite we can find $C > 0$ such that

$$
\Sigma a_{ij} P_{r}^{i} P_{r}^{j} \geq C \Sigma P_{r}^{2}.
$$
(23)

Thus

$$
|G_{0}^{1/2}(P_{r}^{2},\ldots,P_{r}^{N})| \leq C P_{r}^{2} - E^{-1/2}.
$$
(24)

As a result,

$$
\begin{align*}
S_{r}^{(P_{r},\ldots,P_{r-1})}(P_{r},\ldots,P_{N},\tilde{P}_{r},\ldots,\tilde{P}_{N}) &= |S_{r}^{(P_{r},\ldots,P_{r-1})}(P_{r+1},\ldots,P_{N},\tilde{P}_{r+1},\ldots,\tilde{P}_{N})| \\
&\cdot |C P_{r}^{2} - E^{-1/2} \tilde{V}_{r}(P_{r}-\tilde{P}_{r})| C P_{r}^{2} - E^{-1/2}.
\end{align*}
$$
(25)

We now decompose the potential $V_{r} = V_{r}^{'} + V_{r}^{''}$ in a part $V_{r}^{'} \in R$ and a part $V_{r}^{''} \in L^{2p}(R^{3})$. Let

$$
W_{r}(P_{r},\tilde{P}_{r}) = |C P_{r}^{2} - E^{-1/2}.
$$

$W_{r}$ is Hilbert-Schmidt (Simon [19], p. 22). Using Russo’s inequality (Simon [24], p. 57)

$$
|K|_{q} \leq (|K|_{q,\hat{q}}) K^{*}_{q,\hat{q}}_{1/2},
$$
(26)

where $K$ is an integral operator with kernel $K(x,y)$ and $K(x,y) = \hat{K}(y,x)$, we get

$$
|W_{r}^{(2p)}|_{2p} \equiv \left\{ \int dy \int dx \left| C x^{2} - E^{-p} \left( \int dy \hat{V}_{r}^{(2p)} \right) \right|^{2p} \right\}^{1/2p}.
$$
(27)

Combining the trace ideal properties of $W_{r}$ and $W_{r}^{''}$ yields $W_{r}^{''} \in \mathfrak{L}_{2p}$. Thus

$$
\begin{align*}
S_{r}^{(P_{r},\ldots,P_{r-1})}(I_{2p},\ldots,P_{N}) &= |S_{r}^{(P_{r},\ldots,P_{r-1})}(I_{2p},\ldots,P_{N})| \\
&\cdot |W_{r}(P_{r}^{2},\ldots,P_{N})| \\
&\cdot |W_{r}^{''}(P_{r}^{2},\ldots,P_{N})| \\
&\cdot |W_{r}^{''}(P_{r}^{2},\ldots,P_{N})|.
\end{align*}
$$
(28)

Thus, the existence and uniform boundedness in $P_{r}^{2},\ldots,P_{r-1}$ of the $\mathfrak{L}_{2p}$-norms of $S_{r}^{(P_{r},\ldots,P_{r-1})}$ follows. Now $t_{r}^{(P_{r},\ldots,P_{r-1})} = S_{r}^{(P_{r},\ldots,P_{r-1})}$ has a uniformly bounded operator norm (uniform in $P_{r}^{2},\ldots,P_{r-1}$). Thus $t_{r}^{(P_{r},\ldots,P_{r-1})}$ has uniformly bounded $\mathfrak{L}_{2p}$-norms. This completes the induction.

b) See Reed and Simon [25], p. 344.

We remark that the theorem has an obvious transcription to the unsymmetrized Weinberg-van Winter kernel. We have to require the potentials $V_{ij}$ to be in $L^{2}(R^{3}) + L^{2p}(R^{3}) (p = 1, 2, \ldots)$ in this case.

3. Upper Bound on the Dimension of Eigenspaces of Schrödinger Operators

Using the Weinberg-van Winter equation, its trace ideal properties and its relation to the bound states, we get the following result:

**Theorem 2:** Let $E < \Sigma$ and $V_{ij} \in R + L^{2p}(R^{3})$. Then

$$
g(E) = \text{tr} \left[ \left\{ (I_{E} - 1) B + I_{E} |E|^{2} \right\} \right] \leq \dim \text{Ker} (H - E).
$$
(30)
Furthermore for
\[
B = \begin{bmatrix}
-1 - ((I_s(E) - 1) (\text{Ker} (I_s(E) - 1)))^{-1}
\end{bmatrix}
\]
the left hand side of (30) is minimal.

Proof: Follows from (6) and (7) and the trace Winter equation and its relation to the bound states of \( H \).

Remarks:

a) It is not necessary that the operator \( B \) as defined in (31) yields equality in (30); but choosing this \( B \), the left hand side of (30) can only be greater than the right hand side for a particular \( E \), if \( I_s(E) \psi = \psi \) has a “spurious” solution, i.e. \( I_s(E) \) has the eigenvalue one, but \( H \) reduced on the center of mass frame does not have \( E \) as an eigenvalue. This situation can actually occur (see Federbush [26]). One could circumvent this difficulty by using instead of the symmetrized Weinberg-van Winter kernel some other kernel, e.g. the Faddeev-Yakubovski kernel [27, 28], which does not have spurious solutions.

b) Our bound has an obvious transcription to the case where one uses the unsymmetrized Weinberg-van Winter kernel instead of the symmetrized one. In this case one has to require \( V_{ij} \in L^2(\mathbb{R}^3) + L^2(\mathbb{R}^3) \).

c) We can also handle systems with external forces as long as the corresponding potentials \( V_i \) are in \( R + L^2(\mathbb{R}^3) \) (or \( L^2(\mathbb{R}^3) + L^2(\mathbb{R}^3) \)). The Hamiltonian of such an \( N \)-particle system has the same form as an \( N + 1 \)-particle Hamiltonian reduced on the center of mass frame except that the matrix \( a_{ij} \) (see (21)) is not diagonal in the latter case, which is unessential.

d) It is also possible to handle restrictions due to permutational symmetries of the systems. One can e.g. use the modification of the Weinberg-van Winter kernel by Balslev [29] instead of \( I(E) \) or \( I_s(E) \).

4. Explicit Bounds for Coulomb Systems

The bounds of chapter three contain the reduced resolvents \( R_D \). In order to make them explicit we have to have some knowledge about the kernel of reduced resolvents. We shall given explicit expressions for these kernels in the case of the simplest multiparticle Coulomb system, the helium atom in Born-Oppenheimer approximation. The corresponding Schrödinger operator is
\[
H(z) = -\Delta_1 - \Delta_2 - r_1^{-1} - r_2^{-1} + x r_1^2 \quad (32)
\]
where \( x = 1/Z \) with \( Z \) the charge of the nucleus (Thirring [30], p. 191). We can use the unsymmetrized form of the Weinberg-van Winter kernel because the singular part of the Coulomb potential is square integrable. It reads (Thirring [30], p. 220)
\[
I(E) = (E - H_0)^{-1} (E - H_0 + rz_1^2) - (E - H_0)^{-1} (E - H_0 + rz_2^2)
\]
\[
\cdot (-r_1^{-1} + x r_1^2) + (E - H_0)^{-1} (E - H_0 + rz_1^2) - (E - H_0)^{-1} (E - H_0 + rz_2^2) - (E - H_0)^{-1} (E - H_0 + rz_2^2)
\]
\[
\cdot (-r_2^{-1} + x r_2^2) \quad (33)
\]
Because of the Born-Oppenheimer approximation \( H_0 \) is just the six dimensional Laplacian. Thus
\[
(E - H_0)^{-1} (p, p') = \delta(p - p') (E - p^2)^{-1} \quad (34)
\]
The potentials occurring in (33) are explicitly known. The only operators whose integral kernels are not at hand, are the reduced resolvents in (33). In order to give an explicit kernel for these terms we first note that \( (E - H_0 - a/r_i)^{-1} \) is the only occurring type of reduced resolvent. The two other terms, especially \( (E - H_0 + x/r_1)^{-1} \), can be brought into this form by change of variables.
In momentum space the operator \( E - H_0 - a/r_1 \) becomes

\[
(E - p^2) \delta(p - p') - \left( \frac{a}{r_1} \right) (p_1 - p'_1) \delta(p_2 - p'_2). \tag{35}
\]

Thus

\[
(E - H_0 - a/r_1)^{-1} (p_1, p_2, p'_1, p'_2) = \delta(p_2 - p'_2) \\
\cdot (Z + A - a/r_1)^{-1} (p', p'_1) |Z = E - p|^2. \tag{36}
\]

Now, using the integral representation for the one-particle Coulomb Green's function (Schwinger [31]), we get

\[
(E - H_0 - a/r_1)^{-1} (p, p') = \delta(p_2 - p'_2)
\]

\[
\int_0^1 dq \quad \left[ \frac{1}{q^{1/2} (E - p^2)} \right]^2
\]

\[
\left[ (p_1 - p'_1)^2 q - (1 - q)^2 (E - p^2)/(4 (E - p'_2)) \right]^2 \tag{37}
\]

which is the last step in making the Weinberg-van Winter kernel explicit in the case of the helium atom.

Fig. 1. Construction of upper and lower bounds to an eigenvalue \( E_{\text{ext}} \) of multiplicity one below the bottom of the essential spectrum \( \Sigma \).

5. Upper and Lower Bounds on the Eigenvalues

As in the one-particle case, the bound on the dimension of eigenspaces can be used to localize the eigenvalues of the Schrödinger operator below the bottom of the essential spectrum (see [3, 32]): Eigenvalues can only occur where the bound is bigger or equal to one, i.e. the eigenvalues are necessarily in between the points where \( g(E) \) drops below one. In order to get a localization of the eigenvalues it is necessary to choose the trial operator \( B \) sufficiently near to the minimal operator

\[
B = \sum_{n, m = 1}^M a_{n, m} |e_n\rangle \langle e_m|.
\tag{38}
\]

where \( e_n \) are suitably chosen orthonormal functions and where the coefficients \( a_{n, m} \) are chosen such that \( g(E) \) becomes minimal. The functions \( e_n \) and the coefficients \( a_{n, m} \) may depend on the parameter \( E \).

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