ON FINITENESS OF THE DISCRETE SPECTRUM OF THE ENERGY OPERATORS OF MULTIATOMIC MOLECULES

S.A. Vugal'ter and G.M. Zhislin

Conditions are obtained for the discrete spectrum of the Hamiltonians of multiatomic molecules to be finite in the case when the boundary of the continuum of a Hamiltonian is determined by decomposition of the corresponding molecule into any number of neutral complexes.

Introduction

Among the problems involving investigation into the discrete spectra of the energy operators of many-particle quantum systems, particular attention attaches to the problem of studying the discrete spectrum of the many-particle Schrödinger operator with Coulomb potentials. The studies [1-6] were devoted to qualitative investigation of the structure of the discrete spectra of such operators. It was shown that the discrete spectrum of the Hamiltonian for atoms is infinite, while for doubly negative ions it is finite. For singly charged negative ions, conditions were found for the discrete spectrum to be finite, but the fulfillment of these conditions could be proved only for all (-) ions only without allowance for symmetry (with allowance for symmetry, only for the negative hydrogen ion).

For the energy operators of molecules, the case mainly investigated corresponds to that when the boundary of the continuum is determined by decompositions of the molecule into only two subsystems. It was shown that in such a case the discrete spectrum is finite if these subsystems are electrically neutral, and the discrete spectrum is infinite if these subsystems have different charges.

When there are determining decompositions into more than two subsystems, it is known only that the discrete spectrum is infinite if among the determining decompositions there is at least one into two differently charged stable subsystems.

In the present paper, we investigate the discrete spectrum of the energy operator in the presence of determining decompositions into three and more subsystems. The main result of the paper is the identification of a class of multiatomic molecules with determining decompositions into an arbitrary number of neutral subsystems for which the discrete spectra of the energy operators of these molecules are finite. For triatomic molecules this is done with allowance for the permutational and rotational symmetry; in the general case, with allowance for only the permutational symmetry.

The condition for a spectrum to be finite obtained in the paper (Theorems 1.1-1.3) is analogous to the requirement of absence of virtual levels of the Hamiltonians of subsystems in the case of systems with short-range interaction, for which the start of the essential spectrum is the number zero [7, 8]. The qualitative meaning of this condition is that the lower bounds of the Hamiltonians of definite subsystems are conserved when some fairly small, rapidly decreasing perturbations are introduced.

+ Such decompositions are called determining decompositions; see Sec.1.
Let $Z_t = (1, \ldots, n)$ be a system of $n$ quantum numbers with Coulomb interaction,

$$H = -\frac{1}{2} \Delta_t + \sum_{i,j=1,i<j}^{n} e_i e_j |r_{ij}|^{-\frac{1}{2}}$$

be the energy operator of the system $Z_t$, written down after separation of the center-of-mass motion and introduction of the scalar product

$$(r, \bar{r})_t = \sum_{i=1}^{n} m_i (r_i, \bar{r}_i).$$

Here, $r = (r_1, \ldots, r_n)$, $r_i$ is the radius vector of particle $i$ of the system $Z_t$, $\Delta_t$ is the Laplacian on $R_t = \{r \in H^2, \sum_{i=1}^{n} m_i r_i = 0\}$, $m_i$, $e_i$ are the mass and charge of particle $i$, and $r_{ij} = r_i - r_j$.

We extend the operator $H$, which is defined on $C_0^2(R_t)$, to a self-adjoint operator on $L^2(R_t)$, retaining the previous notation.

Let $S$ be the group of permutations of the identical particles in $Z_t$, $\alpha$ be the arbitrary type of the irreducible representation $D^\alpha$ of $S$, $l$ be the weight of the irreducible representation $D^{(l)}$ of the group $O^+(3)$, $\omega = \pm 1$ be the type of the irreducible representation $D_\omega$ of the inversion group $W$, and $G = S \times O^+(3) \times W$. Suppose further $\sigma = (\alpha, l, \omega)$ and $P' = P_{\sigma}^\sigma P_{\sigma}'$, where $P_{\sigma}^\sigma$, $P_{\sigma}'$, $P_{\sigma}$ are projection operators in $L^2(R_t)$ onto the subspaces of functions that transform in accordance with representations that are multiples, respectively, of $D^\alpha$, $D^{(l)}$, $D_\omega$. Obviously, the representation of the group $G$ on the space $\Theta' = P_{\sigma}^\sigma L^2(R_t)$ by the operators

$$T_g: T_g \psi(r) = \psi(g^{-1}r), g \in G,$$

is a multiple of an irreducible representation of type $\sigma$.

We denote the restriction of the operator $H$ to $\Theta'$ by $H^\sigma$.

When we take into account only the permutational symmetry of the system $Z_t$, the operator $H$ will be studied on the space $\Theta'' = P_{\sigma}^\sigma L^2(R_t)$ (and not on the space $\Theta'' = P_{\sigma}^\sigma P_{\sigma}^\sigma L^2(R_t)$). In this case, we set $G = S, \sigma = \alpha, P'' = P_{\sigma}^\sigma, H'' = H^\sigma$, etc.

Let $Z = (C_1, \ldots, C_k)$ be an arbitrary decomposition of the system $Z_t$ into pairwise nonintersecting nonempty subsystems $C_i$; $|Z| = k, \omega(Z) = \{(i, j) | i < j, (i, j) \notin C_i, t = 1, \ldots, k\}$, $R_i(Z) = \{r \in R_t, r_j = 0, j \notin C_i\}$, $R_i(Z) = \bigcup_{C_i \in Z} R_i(C_i)$.

We denote by $\Delta_t(C_i)$, $\Delta_t(Z)$, $\Delta_t(C_i)$, $V_t(C_i)$, $V_t(C_i)$, $V_t(Z)$, respectively, the Laplacians and gradients in $R_i(Z)$, $R_t(Z)$, and $R_i(Z)$, and by $P_i(C_i)$, $P_i(Z)$, $P_i(Z)$ the projection operators in $R_t$ onto these subspaces. Let $q(Z) = P_i(Z) r_i, z(Z) = P_i(Z) r_i, q(C_i) = P_i(C_i) r_i$.

The energy operators of the relative motion of the subsystem $C_i$ and the composite (i.e., consisting of noninteracting subsystems) system $Z$ have, respectively, the form

$$H[i] = -\frac{1}{2} \Delta_t[C_i] + \sum_{i,j \in C_i, i < j} e_i e_j |r_{ij}|^{-\frac{1}{2}}$$

and

$$H(Z) = -\frac{1}{2} \Delta_t(Z) + \sum_{C_i \in Z} \sum_{i,j \in C_i, i < j} e_i e_j |r_{ij}|^{-\frac{1}{2}}.$$

It is obvious that $H = H(Z) - \frac{1}{2} \Delta_t(Z) + I(Z)$, where $I(Z) = \sum_{(i,j) \in Z} e_i e_j |r_{ij}|^{-\frac{1}{2}}$.

We extend the operators $H(Z)$ and $H(C_i)$, respectively, from $C_0^2(R_t(Z))$ and $C_0^2(R_t[C_i])$ to self-adjoint operators on $L^2(R_t(Z))$ and $L^2(R_t[C_i])$, retaining the previous notation.

Let $S[C_i]$ be the group of permutations of the identical particles in the subsystem $C_i$, $S(Z) = S[C_i] \times \ldots \times S[C_k]$, $S(Z)$ be the group generated by the group $S(Z)$ and permutations of the identical subsystems.

* Throughout this paper, orthogonality in the space $R_\sigma$ is understood in the sense of the scalar product $\langle \cdot, \cdot \rangle_t$. 358