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Abstract

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MATHEMATICS

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ON THE SPECTRUM OF THE ENERGY OPERATOR OF SYSTEMS OF MOLECULE TYPE ON SPACES OF FUNCTIONS OF A GIVEN SYMMETRY

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1. In this note the limiting spectrum of any permutation and rotational symmetry is found for the energy operator (5) of a system of molecule type (Theorem 1). For the energy operator of an atom with a moving nucleus (9), a discrete spectrum of any type of symmetry is detected. In this case the eigenvalues of some types of symmetry turn out to lie on the limiting spectrum of other types of symmetry (Theorem 2).

The spectrum of an operator of the form (5) for molecules without taking symmetries into account was studied in ⁽¹⁾. The case of atoms with fixed nuclei for physically realizable types of symmetry was considered in ^(2,3). The spectrum of systems of atom type without taking symmetries into account in an external electromagnetic field was investigated in ⁽⁴⁾.

2. Consider a quantum system of $(n+1)$ moving particles of $\bar{k}+1$ different types. \mathfrak{M}_k is the set of numbers of particles of the k -th type; $S(T)$ is the group of all permutations of indices of particles identical to one another, whose numbers are contained in the set $T = (t_1 \dots t_m) \subseteq N = (0, 1, \dots, n)$;

$$S_k = S(\mathfrak{M}_k), \quad S = S(N) = \prod_{k=0}^{\bar{k}} S_k; \quad D_{n_k}^{(\alpha_k)} \text{ is an irreducible representation}$$

of the group $S(\mathfrak{M}_k)$, determined by an arbitrary partition α_k of the number n_k of elements of \mathfrak{M}_k into positive integral summands:

$$\alpha_k = (\alpha_k^{(1)}, \dots, \alpha_k^{(m)}); \quad \sum_{i=1}^m \alpha_k^{(i)} = n_k \text{ (5)}; \quad D^{(\bar{\alpha})} = \prod_{k=0}^{\bar{k}} D_{n_k}^{(\alpha_k)}$$

is a representation of the group S ;

$$P_{n_k}^{(\alpha_k)} = \frac{l_{n_k}^{(\alpha_k)}}{n_k!} \sum_{R \in S} \chi^{(\alpha_k)}(R) T_R,$$

where $l_{n_k}^{(\alpha_k)}$ is the dimension of the representation $D_{n_k}^{(\alpha_k)}$; $\chi^{(\alpha_k)}(R)$ is the character of the element R in the representation $D_{n_k}^{(\alpha_k)}$; T_R is a unitary operator in the space of functions of $r_{q_1} \dots r_{q_{n_k}}$; $(q_1 \dots q_{n_k}) \equiv \mathfrak{M}_k$ (see (2));

$$P^{(\bar{\alpha})} = \prod_{k=0}^{\bar{k}} P_{n_k}^{(\alpha_k)}$$

is a projection operator in $\mathcal{L}^2(r_0 \dots r_n)$.

3. The Hamiltonian \mathcal{H} of the system under consideration has the form

$$\mathcal{H} = - \sum_{i=0}^n a_i \Delta_i + \sum_{\substack{i < j \\ i, j}}^{0, n} V_{ij}(r_i). \quad (1)$$

Here

$$\Delta_i = \partial^2 / \partial x_i^2 + \partial^2 / \partial y_i^2 + \partial^2 / \partial z_i^2; \quad r_i = (x_i, y_i, z_i); \quad r_{ij} = r_j - r_i;$$

$V_{ij}(r_{ij})$ are measurable functions satisfying the following conditions: for some δ , $0 < \delta < 1$,

$$\sup_{r_1, r_2} \int_{|r'_1 - r_1| + |r'_2 - r_2| \leq 1} |V_{ij}(r'_{12})|^2 (|r_1 - r'_1|^2 + |r_2 - r'_2|^2)^{-1-\delta/2} dr'_1 dr'_2 < +\infty,$$

$$i, j = 0, 1, \dots, \quad (2)$$

$$\lim_{|r_{12}| \rightarrow \infty} \int_{|r'_1 - r_1| + |r'_2 - r_2| \leq 1} |V_{ij}(r'_{12})|^2 dr'_1 dr'_2 = 0, \quad i, j = 0, 1, \dots \quad (3)$$

(see (4)) and

$$\begin{aligned}
 V_{ij}(x, y, z) &= V_{i'j'}(x, y, z), \quad (i, i') \in \mathfrak{M}_k, \quad (j, j') \in \mathfrak{M}_{k'}, \quad k, k' = 0, 1, \dots, \bar{k}, \\
 V_{ij}(-x, -y, -z) &= V_{ij}(x, y, z), \quad (i, j) \in \mathfrak{M}_k, \quad k = 0, 1, \dots, \bar{k}, \\
 a_i &= a_j, \quad (i, j) \in \mathfrak{M}_k, \quad k = 0, 1, \dots, \bar{k}.
 \end{aligned} \tag{4}$$

The conditions (2), (3) are satisfied, in particular, by the potentials $V_{ij}(r_{ij}) = |r_{ij}|^{-\gamma}$, $0 < \gamma < 1.5$ ⁽⁶⁾. The relations (4) reflect the identity of particles in each of the sets \mathfrak{M}_k .

The operator \mathcal{H} , in the space invariant for it (by virtue of (4))

$$\mathfrak{H}' = \{\psi(r_0 \dots r_n), \psi \in \mathcal{L}^2, P^{(\alpha)}\psi = \psi\}$$

has purely continuous spectrum. Separating the motion of the center of mass and introducing relative coordinates $r'_i = r_i - r_0$, $i = 1, 2, \dots, n$, we arrive at the problem of investigating the spectrum of the operator

$$H = H_{0,1,\dots,n} = -\sum_{i=1}^n (a_i + a_0)\Delta_i - a_0 \sum_{\substack{i \neq j \\ i,j}}^{1,n} (\nabla_i, \nabla_j) + \sum_{\substack{i < j \\ i,j}}^{0,n} V_{ij}(r_{ij}) \tag{5}$$

in the space invariant for it

$$\mathfrak{H}^{(\bar{\alpha})} = \{\varphi(r_1 \dots r_n), \varphi \in \mathcal{L}^2, P^{(\bar{\alpha})}\varphi(\mathbf{r} - \mathbf{r}_0) = \varphi(\mathbf{r} - \mathbf{r}_0)\},$$

where $\mathbf{r} - \mathbf{r}_0 = (r_1 - r_0, \dots, r_n - r_0)$. If

$$V_{ij}(r_{ij}) = V_{ij}(|r_{ij}|), \tag{6}$$

then the original system possesses, along with permutational, also rotational and reflection symmetry. In this case it is important to know the spectrum of H in the space

$$\mathfrak{H}^{\bar{\sigma}} = \mathfrak{H}^{\bar{\alpha}, l, \omega} = \{\varphi(r_1 \dots r_n), \varphi \in \mathcal{L}^2, P^{\bar{\sigma}}\varphi(\mathbf{r} - \mathbf{r}_0) = \varphi(\mathbf{r} - \mathbf{r}_0)\},$$

where $P^{\bar{\sigma}} = P^{(\bar{\alpha})} \times P^{l, \omega}$ is the projection operator, l is the weight of a representation of the rotation group, and ω is the parity ⁽³⁾.

Let $H^{\bar{\sigma}}$ be the self-adjoint extension of H in the set of functions

$$\{\varphi(r_1 \dots r_n), \varphi \in C_0, \varphi \in \mathfrak{H}^{\bar{\sigma}}\},$$

where the sign $\in C_0$ indicates finiteness and infinite differentiability of the function in all arguments.

Lemma 4. Let $T_1 = (i_0 \dots i_t)$, $T_2 = (j_1 \dots j_{n-t})$, $i_0 \equiv 0$, $j_s < j_p$, $i_s < i_p$, $s < p$, $T_1 \cup T_2 = N$; $\check{S} = \check{S}(T_1) \times \check{S}(T_2)$, $\check{D}(R) = D^{(\check{\alpha})}(R)$, $R \in \check{S}$. Each irreducible component $\check{D}^{(\check{\gamma})}(R)$ of the representation $\check{D}(R)$ of the group \check{S} is a direct product of certain irreducible representations $D^{(\check{\alpha}')}$ and $D^{(\check{\alpha}'')}$ of the groups $S(T_1)$ and $S(T_2)$ (7)

$$\check{D}^{(\check{\gamma})} = D^{(\check{\alpha}')} \times D^{(\check{\alpha}'')} \quad (7)$$

Let $\pi(\check{\alpha}; T_1, T_2)$ be the set of all such pairs $(\check{\alpha}', \check{\alpha}'')$ of types of irreducible representations of the groups $S(T_1)$ and $S(T_2)$, for each of which (7) holds for some irreducible component of the representation $\check{D}(R)$; $\tau(\check{\alpha}; T_1)$ is the set of all types of irreducible components of the representation $D'(R) = D^{(\check{\alpha})}(R)$, $R \in S(T_1)$, of the group $S(T_1)$.

Let, further, l', ω' and l'', ω'' be arbitrary irreducible types of the full rotational symmetry (f.r.s.) for functions, respectively, of $r_{i_1} \dots r_{i_t}$, $r_{j_1} \dots r_{j_{n-t}}$, and $r_1 \dots r_n$; $\pi(l, \omega; T_1, T_2)$ is the set of all tetrads $(l', \omega'; l'', \omega'')$

* That is, l', ω' are indices of irreducible representations of the rotation and reflection groups for which $P^{l', \omega'} \mathcal{L}^2(r_{i_1} \dots r_{i_t}) \neq 0$; analogous relations hold for l'', ω'' and l, ω .

l'', ω'' , for which the tensor product of the representations $D^{l', \omega'}$ and $D^{l'', \omega''}$ contains the representation $D^{l, \omega}$, i.e. (8)

$$|l' - l''| \leq l \leq l' + l'', \quad \omega = \omega' \cdot \omega'' \quad (8)$$

$\tau(l, \omega; T_1)$ is the set of all types l', ω' of p.v.s. functions of $r_{i_1} \dots r_{i_t}$, for each of which there exists such a type l'', ω'' of p.v.s. functions of $r_{j_1} \dots r_{j_{n-t}}$ that $(l', \omega'; l'', \omega'') \in \pi(l, \omega; T_1, T_2)$.

Let

$$\pi(\check{\sigma}; T_1, T_2) = \{(\check{\sigma}', \check{\sigma}''), \quad (\check{\alpha}' = (\check{\alpha}', l', \omega'), \quad \check{\sigma}'' = (\check{\alpha}'', l'', \omega''))\},$$

$$(\check{\alpha}', \check{\alpha}'') \in \pi(\check{\alpha}; T_1, T_2), \quad (l', \omega'; l'', \omega'') \in \pi(l, \omega; T_1, T_2)\},$$

$$\tau(\check{\sigma}; T_1) = \{\check{\sigma}' = (\check{\alpha}', l', \omega'), \quad \check{\alpha}' \in \tau(\check{\alpha}, T_1), \quad (l', \omega') \in \tau(l, \omega; T_1)\}.$$

We shall call the pair $(\check{\sigma}', \check{\sigma}'')$ compatible with $\check{\sigma}$ if $(\check{\sigma}', \check{\sigma}'') \in \pi(\check{\sigma}; T_1, T_2)$.

p. 5. Put

$$\mathcal{H}_{j_1 \dots j_{n-t}} = - \sum_{k=1}^t a_{i_k} \Delta_k + \sum_{\substack{l < m \\ l, m}}^{1, t} V_{j_k j_m} (r_{j_k i_m}),$$

$$H_{i_0 \dots i_t} = - \sum_{s=1}^t (a_{i_s} + a_0) \Delta_{i_s} - \sum_{\substack{s \neq l \\ s, l}}^{1, t} a_0 (\nabla_{i_s}, \nabla_{i_l}) + \sum_{\substack{s < l \\ s, l}}^{0, t} V_{i_s i_l} (r_{i_s i_l}),$$

where $r_{i_0 i_t} = r_{i_t}$. Let $(\vec{\sigma}', \vec{\sigma}'') \in \pi(\vec{\sigma}; T_1, T_2)$,

$$Q' = \{g(r_{i_1} \dots r_{i_t}) \in C_0, P^{\vec{\sigma}'} g(r_{i_1} - r_0, \dots, r_{i_t} - r_0) = g(r_{i_1} - r_0, \dots, r_{i_t} - r_0), \|g\| = 1\},$$

$$Q'' = \{\varphi(r_{j_1} \dots r_{j_{n-t}}) \in C_0, P^{\vec{\sigma}''} \varphi(r_{j_1} \dots r_{j_{n-t}}) = \varphi(r_{j_1} \dots r_{j_{n-t}}), \|\varphi\| = 1\},$$

$$Q_0 = \{\psi(r_1 \dots r_n) \in C_0, P^{\vec{\sigma}} \psi(r - r_0) = \psi(r - r_0)\}$$

$$\lambda^{\vec{\sigma}'}(i_1 \dots i_t | i_0) = \inf_{g \in Q'} (H_{i_0 \dots i_t} g, g); \quad \lambda^{\vec{\sigma}''}(j_1 \dots j_{n-t}) = \inf_{\varphi \in Q''} (\mathcal{H}_{j_1 \dots j_{n-t}} \varphi, \varphi),$$

$$\lambda_0^{\vec{\sigma}} = \inf(H_{0,1 \dots n} \psi, \psi), \quad \psi \in Q_0,$$

$$\mu^{\vec{\sigma}} = \min\{\inf[\lambda^{\vec{\sigma}'}(i_1 \dots i_t | i_0) + \lambda^{\vec{\sigma}''}(j_1 \dots j_{n-t})]\},$$

$$T_1 \cup T_2 = N, \quad (\vec{\sigma}', \vec{\sigma}'') \in \pi(\vec{\sigma}; T_1, T_2),$$

where first, for fixed $T_1 = (i_0 \dots i_t)$ and $T_2 = (j_1 \dots j_{n-t})$, the lower bound is taken over all pairs of symmetry types $(\vec{\sigma}', \vec{\sigma}'')$ compatible with $\vec{\sigma}$, and then the minimum over all possible decompositions $T_1 \cup T_2 = N$.

(A) Suppose that for some k the number of elements of \mathfrak{M}_k is odd.*

Theorem 1. *The entire limiting spectrum of the operator $H^{\vec{\sigma}}$ coincides with all points of the ray $[\mu, +\infty)$.*

For the existence of a discrete spectrum it is necessary and sufficient that

$$\lambda_0^{\vec{\sigma}} < \mu^{\vec{\sigma}}.$$

The theorem applies to the operators H^σ of any quantum systems for which the particle interaction potentials satisfy conditions (2)–(4), (6). In particular, it is valid for the energy operator of an arbitrary molecule for which (A) holds. Theorem 1 expresses the following

* That is, the system does not admit a separation into two physically indistinguishable subsystems.

energy principle. For a quantum system to have bound states of symmetry $\bar{\sigma}$, whose energy levels do not lie in the continuous spectrum of the same type of symmetry, it is necessary and sufficient that the decomposition of the system into any mutually noninteracting subsystems T_1 and T_2 of symmetry types $(\bar{\sigma}', \bar{\sigma}'')$ compatible with $\bar{\sigma}$ be energetically unfavorable.

If in the expression H , $V_{ij} \geq 0$, $i, j \neq 0$, then

$$\mu^{\bar{\sigma}} = \min_{T_1 \subset N} \left\{ \inf_{\bar{\sigma}' \in \tau(\bar{\sigma}; T_1)} \lambda^{\bar{\sigma}'}(i_1 \dots i_{n-1} | i_0) \right\}, \quad \text{where } T_1 = (i_0, \dots, i_{n-1}).$$

p. 6. Consider a system of atomic type: $\mathfrak{M}_0 = (0)$, $\mathfrak{M}_1 = (1, 2, \dots, n)$,

$$H = - \sum_{i=1}^n (a_1 + a_0) \Delta_i - a_0 \sum_{\substack{i \neq j \\ i, j}}^{1, n} (\nabla_i, \nabla_j) - b \sum_{j=1}^n |r_j|^{-1} + c \sum_{\substack{i < j \\ i, j}}^{1, n} |r_i|^{-1}. \quad (9)$$

Theorem 2. Let $\alpha = (\alpha^{(1)}, \dots, \alpha^{(s)})$, $\alpha^{(1)} \geq \alpha^{(2)} \geq \dots \geq \alpha^{(s)} > 0$, $1 \leq s \leq n$, $\sum_{i=1}^s \alpha^{(i)} = n$, and let $\sigma = (\alpha, l, \omega)$ be any type of symmetry of functions of $r_1 \dots r_n$, $(l, \omega) \neq (0, -1)$ for $n = 2^*$. Then the entire limiting spectrum of the operator H^σ consists of all points of the ray $[\mu^\sigma, +\infty)$, where $\mu^\sigma = \inf \lambda^{\sigma'}(1, 2, \dots, n-1 | 0)$, $\sigma' \in \tau(\sigma; T_1)$, $T_1 = (0, 1, \dots, n-1)$.

If the numbers b and c in (9) are such that

$$b > (n-1)c \geq 0,$$

then there exists an infinite sequence of points of the discrete spectrum λ_p^σ , $p = 0, 1, \dots$, of the operator H^σ , accumulating at μ^σ , and for $\sigma \neq \sigma_0 \equiv (\alpha_0, 0, +1)$, where $\alpha_0 = (n, 0)$, one has $\lambda_0^{\sigma_0} < \lambda_0^\sigma$.

By definition, $\tau(\sigma; T_1) = \tau(\alpha; T_1) \times \tau(l, \omega; T_1)$. The set $\tau(\alpha; T_1)$ consists of those symmetry types $\alpha'_i = (\alpha^{(1)} \dots \alpha^{(i-1)}, \alpha^{(i)} - 1, \alpha^{(i+1)} \dots \alpha^{(s)})$, determined by the given $\alpha = (\alpha^{(1)} \dots \alpha^{(s)})$, for which $\alpha^{(i)} - 1 \geq \alpha^{(i+1)}$; moreover, if $\alpha^{(s)} = 1$, then $\alpha'_s = (\alpha^{(1)} \dots \alpha^{(1)} \dots \alpha^{(s-1)})$ (see (5), p. 191). The set $\tau(l, \omega; T_1)$ was found in (3).

Corollary of Theorem 2. Let $\sigma_{i,m} = (\alpha_i, m, (-1)^m)$, $i = 0, 1$; $m = 0, 1, \dots$; $\sigma_0 = \sigma_{0,0}$, where $\alpha_0 = (n, 0)$, $\alpha_1 = (n-1, 1)$. Then

$$\mu^{\sigma_0} = \mu^{\sigma_{i,m}} < \mu^\sigma, \quad \sigma \neq \sigma_{i,m}, \quad i = 0, 1; \quad m = 0, 1, \dots \quad (10)$$

It follows from (10) that for $\sigma \neq \sigma_{i,m}$ the limiting spectrum and the eigenvalues of the operator H^σ , with the exception of at most a finite number of them, lie in the limiting spectrum of the operators $H^{\sigma_{i,m}}$, $i = 0, 1$; $m = 0, 1, \dots$

p. 7. If $\vec{\sigma} = \vec{\alpha}$, i.e., we are interested only in the permutation symmetry of the wave functions, then restriction (A) of p. 5 is dropped. The formulations of Theorems 1 and 2 remain valid if there and in the definitions of $\mu^{\vec{\sigma}}$ and H^σ one replaces $\vec{\sigma}$ by $(\vec{\alpha})$, $(\vec{\sigma}', \vec{\sigma}'')$ by $(\vec{\alpha}', \vec{\alpha}'')$, σ by α , σ_0 by α_0 , and $\sigma_{i,m}$ by α_i .

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* The space $\mathfrak{H}^{\alpha,0,-1}$ is empty for any α when $n = 2$ ⁽³⁾.

Note: Figure translations are in progress. See original paper for figures.

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