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Abstract

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ON THE MIXED SPECTRUM OF CERTAIN MULTIDIMENSIONAL DIFFERENTIAL OPERATORS OF QUANTUM MECHANICS

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Consider the operator

$$H_n = T_n + V_n + W_n,$$

$$T_n = -a\sum_{i=1}^{n}\Delta_i, \qquad V_n = -b\sum_{i=1}^{n}|r_i|^{-1}, \qquad W_n = c\sum_{i\neq j}|r_{ij}|^{-1},$$

where $r_i = (x_i, y_i, z_i)$, $r_{ij} = r_i - r_j$, acting in the Hilbert space $\mathfrak{H}_n$ of complex-valued functions of $3n$ independent variables $r_1, \dots, r_n$, $n \geq 1$. For $a = \hbar^2/2m$, $b = ze^2$, $c = e^2$, H_n is the energy operator for an atom or ion with a fixed nucleus. If the interaction term W_n is omitted in H_n, then as n increases an ever greater number of eigenvalues lie on the continuous spectrum. However, the methods used up to now have yielded only isolated eigenvalues of the full operator H_n [1,2]. In this note it is shown that the symmetry properties of the operator H_n make it possible to distinguish eigenvalues belonging to one symmetry class on the limiting spectrum of another symmetry class. In this way it is established that, for $n \geq 4$, all eigenvalues of the operator H_n corresponding to physically realizable symmetry lie on its limiting spectrum, except, possibly, for some exceptional values.

1. Let $D_n^{(k)}$ be the irreducible representations of the permutation group of n symbols S_n; $\chi_n^{(k)}(R)$, $R \in S_n$, their characters; $\overline{D}_n^{(k)}$, $\overline{\chi}_n^{(k)}$ the associated irreducible representations and their characters; $k = 0, 1, \dots, [n/2]$*. For $n = 2$, in general expressions containing the indices n, k, one should put $D_2^{(1)} = \overline{D}_2^{(1)} = D_2^{(0)}$; $D_1^{(0)} = \overline{D}_1^{(0)}$ is the identity representation. In accordance with the Pauli principle, the representations $\overline{D}_n^{(k)}$, as well as the representation $D_2^{(0)}$, have physical meaning for the operator H_n (see [3], Chap. 22). If

$$R = \begin{pmatrix} i_1, \ldots, i_n \\ 1, \ldots, n \end{pmatrix} \in S_n,$$

then $T_R \psi(r_1, \ldots, r_n) = \psi(r_{i_1}, \ldots, r_{i_n})$ is a unitary operator in $\mathfrak{H}_n$. Put

$$P_n^{(k)} = \frac{l_n^{(k)}}{h_n} \sum_{R \in S_n} \chi_n^{(k)}(R) T_R, \qquad \mathfrak{H}_n^{(k)} = P_n^{(k)} \mathfrak{H};$$

$$\overline{P}_n^{(k)} = \frac{l_n^{(k)}}{h_n} \sum_{R \in S_n} \overline{\chi}_n^{(k)} T_R, \qquad \overline{\mathfrak{H}}_n^{(k)} = \overline{P}_n^{(k)} \mathfrak{H},$$

where $l_n^{(k)}$ is the common dimension of the representations $D_n^{(k)}$, $\overline{D}_n^{(k)}$; h_n is the order of the group S_n; $P_n^{(k)}$, $\overline{P}_n^{(l)}$ $(k, l = 1, \ldots, [n/2])$ are pairwise orthogonal projection operators, with the exception of certain pairs for which both operators are equal.

* We use the notation of Wigner' s book ([3]), adding to it the lower index n.

2. Let C_f^2 be the set of all finite twice continuously differentiable functions from $\mathfrak{H}$. The operator H_n is bounded below on C_f^2 (2). We extend it to a self-adjoint operator, retaining the previous notation. For $\psi \in C_f^2$,

$$H_n \bar{P}_n^{(k)} \psi = \bar{P}_n^{(k)} H_n \psi.$$

Put

$$C_f^2(\bar{D}_n^{(k)}) = C_f^2 \cap \overline{\mathfrak{H}}_n^{(k)} = \bar{P}_n^{(k)} C_f^2.$$

By $\bar{H}_n^{(k)}$ we denote the extension of the operator H_n, considered only on $C_f^2(\bar{D}_n^{(k)})$, to a self-adjoint operator acting in $\overline{\mathfrak{H}}_n^{(k)}$.

3. For functions $\psi \in \mathfrak{H}$ having, in each bounded domain, generalized derivatives in the sense of S. L. Sobolev, put, for $n \geq 1$,

$$W_2^1(\bar{D}_n^{(k)}) = \{\psi \in \overline{\mathfrak{H}}_n^{(k)},\ \|\operatorname{grad}\psi\| < \infty\},$$

where

$$\|\operatorname{grad}\psi\|^2 = \sum_i \|\operatorname{grad}_i \psi\|^2 = \int \left\{ \sum_i \left(\left|\frac{\partial\psi}{\partial x_i}\right|^2 + \left|\frac{\partial\psi}{\partial y_i}\right|^2 + \left|\frac{\partial\psi}{\partial z_i}\right|^2 \right) \right\} d\Omega;$$

$$L_n[\psi] = a\|\operatorname{grad}\psi\|^2 + (V_n\psi, \psi) + (W_n\psi, \psi);$$

$$\lambda_0(\bar{D}_n^{(k)}) = \inf L_n[\psi], \qquad \psi \in W_2^1(\bar{D}_n^{(k)}), \qquad \|\psi\| = 1;$$

$$\bar{\mu}_{n-1}^{(k)} = \min\{\lambda_0(\bar{D}_{n-1}^{(k)}), \lambda_0(\bar{D}_{n-1}^{(k-1)})\}, \qquad 0 < k \leq \left[\frac{n}{2}\right],$$

excluding $k = n/2$ for even n,

$$\bar{\mu}_{n-1}^{(0)} = \lambda_0(\bar{D}_{n-1}^{(0)}), \qquad \bar{\mu}_{n-2}^{(n/2)} = \lambda_0(\bar{D}_{n-1}^{(n/2-1)}).$$

The corresponding quantities relating to the representation $D_n^{(k)}$ will be denoted by $\lambda_0(D_n^{(k)})$, $\mu_{n-1}^{(k)}$.

Theorem 1. For all $n \geq 2$, the inequality

$$\lambda_0(\bar{D}_n^{(k)}) \leq \bar{\mu}_{n-1}^{(k)}$$

holds. In order that $\lambda_0(\bar{D}_n^{(k)})$ be an isolated eigenvalue of finite multiplicity of the operator $\bar{H}_n^{(k)}$, it is necessary and sufficient that the condition

$$\text{(E)} \quad \lambda_0(\bar{D}_n^{(k)}) < \bar{\mu}_{n-1}^{(k)}.$$

be satisfied.

The points $\lambda > \bar{\mu}_{n-1}^{(k)}$ form the entire limiting spectrum of the operator $\bar{H}_n^{(k)}$. The condition (E) expresses the energetic disadvantage of such a departure of one particle, under which the system passes from the state of symmetry $\bar{D}_n^{(k)}$ to a state of symmetry $\bar{D}_{n-1}^{(k)}$ or $\bar{D}_{n-1}^{(k-1)}$.

4. Let

$$\lambda_0^{(k)} \leq \lambda_1^{(k)} \leq \dots \leq \lambda_{p-1}^{(k)} \quad (p \geq 1)$$

be eigenvalues, and let $u_0, u_1, \dots, u_{p-1}$ be the corresponding orthonormal eigenfunctions of the operator $\bar{H}_n^{(k)}$;

$$Q_p = \{\psi \in W_2^1(\bar{D}_n^{(k)});\ (\psi, u_l) = 0;\ l = 0, 1, \dots, p-1\},$$

$$\lambda_p(\bar{D}_n^{(k)}) = \inf L[\psi], \qquad \psi \in Q_p, \qquad \|\psi\| = 1.$$

Theorem 2. For $n \geq 2$, the inequality

$$\lambda_p(\bar{D}_n^{(k)}) \leq \bar{\mu}_{n-1}^{(k)} \quad (p \geq 1)$$

holds. In order that $\lambda_p(\bar{D}_n^{(k)})$ be an isolated eigenvalue of finite multiplicity of the operator $\bar{H}_n^{(k)}$, it is necessary and sufficient that the condition

$$(\text{E}_1) \quad \lambda_p(\bar{D}_n^{(k)}) < \bar{\mu}_{n-1}^{(k)}.$$

be satisfied.

5. **Theorem 3.** If b, c in the expression H_n satisfy the condition

$$b > (n-1)c,$$

then for $k = 0, 1, \ldots, [\frac{n}{2}]$:

1) for $\bar{H}_n^{(k)}$ there exists an infinite sequence of points of the discrete spectrum

$$\lambda_p(\bar{D}_n^{(k)}) \to \bar{\mu}_{n-1}^{(k)} \qquad (p \to \infty);$$

2) for $n \geq 3$ one has

$$\bar{\mu}_{n-1}^{(0)} = \bar{\mu}_{n-1}^{(1)} < \bar{\mu}_{n-1}^{(k)},$$

except for $(n, k) = (3, 1)$.

6. Theorems 1, 2, and 3, 1) are valid without changes for the representations $D_n^{(k)}$. Assertion 3, 2), as applied to $D_n^{(k)}$, is replaced by the following: for $n \geqslant 3$, $k \geqslant 2$, the inequality $\mu_{n-1}^{(1)} < \mu_{n-1}^{(k)}$ holds.

7. Since for neutral atoms and positive ions $Z \geqslant n$, the condition $b > (n-1)c$ is always satisfied for them. We give some consequences of Theorems 1-2. Since $\lambda_p(\bar{D}_n^{(k)}) \to \bar{\mu}_{n-1}^{(k)}$ $(p \to \infty)$, it follows, by 3, 2), that $\lambda_p(\bar{D}_n^{(k)}) > \mu_{n-1}^{(0)} = \mu_{n-1}^{(1)}$ for all p, except, possibly, for a finite number. By Theorem 1, all these $\lambda_p(\bar{D}_n^{(k)})$ belong to the limiting spectrum of the operator $H_n^{(l)}$, $l = 0, 1$. For $n = 3$ (the lithium atom) $D_3^{(1)} = \bar{D}_3^{(1)}$, $\mu_2^{(0)} = \mu_2^{(1)} = \bar{\mu}_2^{(1)} < \bar{\mu}_2^{(0)}$. Therefore the realized eigenvalues $\lambda_p(\bar{D}_3^{(0)})$ all, except perhaps for a finite number, lie in the limiting spectrum of the realized symmetry $\bar{D}_3^{(1)}$. Apparently, an analogous situation holds for $n > 3$. It follows from Theorems 1-3 that, for all n, there exists an infinite sequence of eigenvalues of the realized symmetry that do not lie in the realized limiting spectrum. Among them is the least of all, $\lambda_0(\bar{D}_n^{(k)})$, corresponding to the ground state.

8. The proofs of Theorems 1 and 2 are based on the following proposition.

Theorem 4. Let $\psi_m \in C_2^f(\bar{D}_n^{(k)})$,

$$\|\psi_m\|_{L^2} + \|\operatorname{grad} \psi_m\|_{L^2} \leqslant M \quad (m = 1, 2, \ldots),$$

$$\int_\Omega |\psi_m|^2 \, d\Omega \to 0 \quad (m \to \infty)$$

for any bounded domain Ω. Then

$$\lim_{m \to \infty} L_n[\psi_m] \geqslant \bar{\mu}_{n-1}^{(k)}.$$

This proposition means that an arbitrary decay of a system from a state of symmetry $\bar{D}_n^{(k)}$ cannot be energetically more advantageous than the departure of one particle, under which the system passes into a state of symmetry $\bar{D}_{n-1}^{(k)}$ or $\bar{D}_{n-1}^{(k-1)}$.

For the proof of Theorem 3 it is established that the inequality $b > (n-1)c$ implies the energy inequalities (E), (E_1). The proof of Theorem 4 is based on the decomposition of configuration space used earlier in ([2]).

These results carry over, without essential difficulties, to other irreducible representations of the group S_n, and also to potentials of a more general form than Coulomb potentials. The relations between the quantities $\lambda_0(D_n^{(k)})$, $\lambda_0(\bar{D}_n^{(k)})$ remain unclear, except for the cases indicated in Theorem 3, 2).

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References

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3. E. Wigner, *Group Theory and Its Application to the Quantum-Mechanical Theory of Atomic Spectra*, IL, 1961.

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