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**ON THE SPECTRUM OF PSEUDORELATIVISTIC  
ELECTRONS HAMILTONIANS IN THE SPACES OF  
FUNCTIONS, HAVING FIXED PERMUTATIONAL AND  
POINT SYMMETRY**

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We consider the energy operator of  $n$  pseudorelativistic electrons in the field of  $k$  fixed nuclei in the space of functions, having arbitrary permutational and point symmetry. For this operator we found the location of essential spectrum and — when the total system charge is nonnegative — the leading term of the discrete spectrum counting function asymptotics.

## INTRODUCTION

In this paper we study the spectral properties of pseudorelativistic (PR) hamiltonians  $H_n$  of the systems  $Z_n$ , consisting of  $n$  electrons in the potential field of  $k$  fixed centers (nuclei). For PR operators their potential parts are nonrelativistic (NR), but the kinetic parts are relativistic operators. PR operators are nonlocal and namely this fact generates additional difficulties at the study their spectra as compared with NR operators for the same quantum systems. In spite on this fact many results, which were obtained early for NR systems  $Z_n$  and their operators, are proved later for PR operators. In particular the essential spectrum for PR operators  $H_n$  was found without symmetry account and with account of permutational [2] and rotational — respect to the groups  $O^+(3)$  and  $O(3)$  — symmetry for  $k = 1$  [3]. The discrete spectrum structure of  $H_n$  (including the spectral asymptotics) was discovered for the same cases for neutral and positive charged systems [6, 5, 3]. But for the important case  $k \geq 2$  (the case of molecules with infinitely heavy nuclei) the results on the spectrum with the rotational symmetry account were obtained only for NR case [4]. For  $k \geq 2$  the rotational symmetry of the system  $Z_n$  and hamiltonian  $H_n$  is not connected with the groups  $O^+(3)$  or  $O(3)$  (as for  $k = 1$ ), but with some (mainly finite) subgroup  $F_k$  from  $O(3)$ . This subgroup is determined by the positions of identical nuclei; the symmetry with respect to group  $F_k$  is named by POINT symmetry.

Here we consider PR operators  $H_n$  at any  $k$  in the spaces of functions, having arbitrary fixed types of permutational and POINT symmetry. In the paper for these operators

- a) location of the essential spectrum is discovered (Theorem 1);
- b) two-sided estimates of the discrete spectrum counting function are obtained in the terms of counting functions some NR two-particle operators (Theorem 3);
- c) the leading term of the spectral asymptotics is found (Theorem 4).

We only formulate our results and consider them, but do not adduce the proofs. It is connected with the inconvenience of the existing proofs (similar proofs occupy 30 pages even without symmetry account [6]) and with our hope to simplify them.

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## 1. OPERATORS

1.1. We consider the system  $Z_n = \{1, \dots, n\}$  of  $n$  pseudorelativistic electrons in the potential field of  $k$  nuclei, having infinitely heavy masses. Let  $e < 0$  and  $m$  be the charge and the mass of electron,  $r_j = (x_j, y_j, z_j)$  be the radius-vector of  $j$ -th electron,  $e_s > 0$  and  $A_s = (A_{s1}, A_{s2}, A_{s3})$  be the charge and the radius-vector of  $s$ -th nucleus,  $s = 1, \dots, k$ ;  $r = (r_1, r_2, \dots, r_n)$ ,  $R^{3n} = \{r\}$ . The PR energy operator of the system  $Z_n$  can be written in the form

$$\mathcal{H}_n = K_n + V_n(r),$$

where

$$K_n = \sum_{i=1}^n K(i), \quad K(i) = \sqrt{-\Delta_i + m^2}, \quad \Delta_i = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2},$$

$$V_n(r) = e^2 \sum_{i < j; i, j}^{1, n} |r_i - r_j|^{-1} + \sum_{i=1}^n \sum_{s=1}^k e e_s |r_i - A_s|^{-1}. \quad (1)$$

Here we took the Plank constant and the light velocity as units.

1.2. The operators  $K(i)$  are not local in the coordinate space, so it is more convenient to consider them in the momentum representation, where  $K(i)$  turn into multiplication operators  $\bar{K}(i)$ :

$$K(i) f(r_i) = \bar{K}(i) \bar{f}(p_i),$$

where  $\bar{K}(i) = \sqrt{p_i^2 + m^2}$ ,  $\bar{f}(p_i)$  is Fourier-transform of the function  $f(r_i)$ ,  $p_i$  is the momentum of  $i$ -th electron. By the technical reasons we take the operator  $\hat{K}(i) = \bar{K}(i) - m$  instead of the operator  $\bar{K}(i)$  and  $\hat{K}_n = \sum_{i=1}^n \hat{K}(i)$  instead of  $K_n$ ; for the potential  $V_n(r)$  we keep the form (1). Thus instead of the operator  $\mathcal{H}_n$  we shall study the operator

$$H_n = \hat{K}_n + V_n, \quad (2)$$

where the relativistic kinetic operator  $\hat{K}_n$  is the multiplication operator in the momentum space, the potential  $V_n(r)$  is the multiplication operator in the coordinate space. It is known [1], that the operator  $H_n$  is semi-bounded from below in  $\mathcal{L}_2(R^{3n})$ , if

$$e_s < -2/\pi e, \quad s = 1, 2, \dots, k, \quad (3)$$

where under the chosen units system  $e^2 = 137^{-1}$  is the value of fine-structure constant,  $e_s = -N_s e$ ,  $N_s$  is the number in Mendeleev periodic table of the element, whose atomic nucleus is considered. So the inequalities (3) mean that

$$N_s \leq 87, \quad s = 1, 2, \dots, k \quad (4)$$

and further we assume everywhere, that (4) hold. Using Friedrichs extension we extend the operator  $H_n$  from  $C_0^\infty$  to self-adjoint operator, again noted by  $H_n$ .

Along with  $H_n$  we shall consider the operator  $H_{n-1}$  of the system  $Z_{n-1} = \{1, 2, \dots, n-1\}$  of  $n-1$  electrons in the potential field of the same nuclei, which are contained in  $Z_n$ . This operator is defined by analogy with  $H_n$ , but in the space  $\mathcal{L}_2(R^{3n-3})$  instead of  $\mathcal{L}_2(R^{3n})$ ; here

$$R^{3n-3} = \{r'\}, \quad r' = (r_1, \dots, r_{n-1}).$$

## 2. SYMMETRY

2.1. Let  $O^+(3)$  and  $W$  be the rotations and inversions groups in  $R^3$ ,  $O(3) = O^+(3) \times W$  and  $F_k$  be such subgroup from  $O(3)$ , that the transformations  $g$  from  $F_k$  move identical nuclei one to the place of the other one. In other words for any  $s$ ,  $1 \leq s \leq k$  and  $g \in F_k$

$$g A_s = A_t, \quad g \in G_k \quad (5)$$

where the nucleus with number  $t$  is identical to the nucleus with number  $s$  ( $e_t = e_s$ ) and  $t$  depends on  $s$  and  $g$ . The group  $F_k$  is named by the group of the system  $Z_n$  POINT symmetry. Let  $S_n$  be the group of the permutations of  $n$  electrons,  $G_k = S_n \times F_k$  and  $G$  is one of the groups  $F_k$ ,  $S_n$ ,  $G_k$ . For  $g \in G$  we define the unitary operators  $T_g$ :

$$T_g \psi(r) = \psi(g^{-1}r), \quad \psi(r) \in \mathcal{L}_2(R^{3n}), \quad g \in G.$$

Using (5) it is easy to show, that

$$T_g V_n(r) = V_n(r) T_g, \quad g \in F_k$$

where the operators  $T_g$  act on the electrons coordinates. Consequently

$$T_g H_n = H_n T_g, \quad g \in G_k = S_n \times F_k. \quad (6)$$

Let  $\alpha$ ,  $\tau$  and  $\sigma = (\alpha, \tau)$  be the types of the irreducible representations of the groups  $S_n$ ,  $F_k$  and  $G_k$  respectively. We denote by  $\gamma$  the types of the irreducible representations of group  $G$  (that is  $\gamma = \alpha$  if  $G = S_n$ ,  $\gamma = \tau$  if  $G = F_k$  and  $\gamma = (\alpha, \tau)$  if  $G = G_k = S_n \times F_k$ ) and by  $P_n^{(\gamma)}$  — the projectors in  $\mathcal{L}_2(R^{3n})$  on the subspaces  $B_n^{(\gamma)} = P_n^{(\gamma)} \mathcal{L}_2(R^{3n})$  of the functions, which are transformed by the operators  $T_g$ ,  $g \in G$  according to the representations of the types  $\gamma$  of the group  $G$  (the expressions for  $P_n^{(\gamma)}$  are known, see for example [9]). By (6) the subspaces  $B_n^{(\gamma)}$  are invariant for the operator  $H_n$ .

Let  $H_n^{(\gamma)}$  be the restriction of the operator  $H_n$  to the subspace  $B_n^{(\gamma)}$ . Our purpose is the study of the operator  $H_n^{(\gamma)}$  spectrum structure for  $\gamma = \sigma = (\alpha, \tau)$ ,  $G = G_k = S_n \times F_k$ .

2.2. Further we need in the description of permutational symmetry of the system  $Z_{n-1} = \{1, 2, \dots, n-1\}$  states. Let  $\alpha'$  be the types of irreducible representations of the group  $S_{n-1}$  permutations of  $n-1$  electrons,  $P_{n-1}^{(\alpha')}$  be the projector in  $\mathcal{L}_2(R^{3n-3})$  on the subspace  $B_{n-1}^{(\alpha')} = P_{n-1}^{(\alpha')} \mathcal{L}_2(R^{3n-3})$  of functions  $\varphi(r')$ ,  $r' = \{r_1, \dots, r_{n-1}\}$ , which are transformed by the operator  $T_g$ :  $T_g \varphi(r') = \varphi(g^{-1}r')$ ,  $g \in S_{n-1}$  according to the representation of the type  $\alpha'$  of the group  $S_{n-1}$ . It is clear, that the subspace  $B_{n-1}^{(\alpha')}$  is invariant for the operator  $H_{n-1}$ ; let  $H_{n-1}^{(\alpha')}$  be the restriction of the operator  $H_{n-1}$  to  $B_{n-1}^{(\alpha')}$ . We denote by  $E(\alpha)$  the set of such  $\alpha'$ , for which the representation of the type  $\alpha'$  of the group  $S_{n-1}$  is contained in the representation  $D_g^{(\alpha)}$ ,  $g \in S_n$  of the type  $\alpha$  of the group  $S_n$  after restriction  $D_g^{(\alpha)}$  from  $S_n$  to  $S_{n-1}$ . From physical point of view  $E(\alpha)$  is the set of all permutational symmetry types, which are possible for the states of the system  $Z_{n-1}$ , when the states of the system  $Z_n$  have the symmetry  $\alpha$ . We can describe the set  $E(\alpha)$  in explicit form. Let us do it for example for the types  $\alpha$ , permitted by Pauli principle for fermions systems. Such  $\alpha = \alpha_p$  correspond to all decompositions of number  $n$  into numbers 2 and 1:

$$\alpha_p \sim (\underbrace{2, \dots, 2}_p, \underbrace{1, \dots, 1}_{n-2p}), \quad p = 0, 1, \dots, \left[ \frac{n}{2} \right].$$

Then

$$E(\alpha_p) = \left\{ \alpha' \mid \alpha' \sim (\underbrace{1, 1, \dots, 1}_{n-1}) \right\} \text{ if } p = 0,$$

$$E(\alpha_p) = \left\{ \alpha' \mid \alpha' \sim (\underbrace{2, 2, \dots, 2}_{p-1}, 1) \right\} \text{ if } p = \frac{n}{2} \quad (n - \text{even}),$$

$$E(\alpha_p) = \left\{ \alpha'_1, \alpha'_2 \mid \alpha'_1 \sim (\underbrace{2, \dots, 2}_{p-1}, \underbrace{1, \dots, 1}_{n-2p+1}), \alpha'_2 \sim (\underbrace{2, \dots, 2}_p, \underbrace{1, \dots, 1}_{n-2p-1}) \right\}$$

$$\text{if } 0 < p < \frac{n}{2}.$$

Further we set

$$B_{n-1}(\alpha) = \sum_{\alpha' \in E(\alpha)} \oplus B_{n-1}^{(\alpha')}, \quad H_{n-1}(\alpha) = \sum_{\alpha' \in E(\alpha)} H_{n-1}^{(\alpha')}.$$

The operator  $H_{n-1}(\alpha)$  is the restriction of the operator  $H_{n-1}$  to the subspace  $B_{n-1}(\alpha)$ ; let

$$\mu_n^{(\alpha)} = \inf H_{n-1}(\alpha). \quad (7)$$

### 3. RESULTS ON THE ESSENTIAL SPECTRUM

3.1. Let the group  $F_k$  be finite.

**Theorem 1.** *For  $\forall \sigma = (\alpha, \tau)$  the essential spectrum  $s_{\text{ess}}(H_n^{(\sigma)})$  of the operator  $H_n^{(\sigma)}$  consists of all points of half-line  $[\mu^{(\alpha)}, +\infty)$ .*

Let us consider this result. According to [2] the half-line  $[\mu^{(\alpha)}, +\infty)$  is the set of all points of the essential spectrum  $s_{\text{ess}}(H_n^{(\alpha)})$  of the operator  $H_n^{(\alpha)}$ . So Theorem 1 says that for finite groups  $F_k$  the equality  $s_{\text{ess}}(H_n^{(\alpha, \tau)}) = s_{\text{ess}}(H_n^{(\alpha)})$  holds for  $\forall \tau$ .

Let us compare the case of finite groups  $F_k$  with the situation, when  $F_k$  is infinite. We consider only  $F_k = O^+(3)$  and  $F_k = O(3) = O^+(3) \times W$  (see 2.1). These groups  $F_k$  are rotational symmetry groups for all PR atoms and their ions with infinitely heavy nuclei (that is for the case  $k = 1, A_1 = (0, 0, 0)$ ). We denote by  $l$  and  $\omega$  the types of irreducible representations of groups  $O^+(3)$  and  $W$ ; so  $\tau = l$  if  $F_k = O^+(3)$ ,  $\tau = (l, \omega)$  if  $F_k = O(3) = O^+(3) \times W$ .



When  $F_k = O^+(3)$  then  $\inf s_{\text{ess}}(H_n^{(\alpha, l)}) = \mu^{(\alpha)}$  [3] similarly to the case finite  $F_k$ . But when  $F_k = O(3)$ , the value  $\inf s_{\text{ess}}(H_n^{(\alpha, l, \omega)})$  depends not only on  $\alpha$ , but on  $\tau = (l, \omega)$  as well [3]. So for two infinite groups —  $O^+(3)$  and  $O(3)$  — the situations are different and it means, that dependence or independence  $\inf s_{\text{ess}}(H_n^{(\alpha, \tau)})$  on  $\tau$  is not connected with group  $F_k$  infiniteness or finiteness.

3.2. To understand the reasons of dependence (or independence) of value  $\inf s_{\text{ess}}(H_n^{(\alpha, \tau)})$  on  $\tau$  for different  $F_k$ , let us note, that when we find the lower bound of the operator  $H_n$  essential spectrum in the space  $B_n^{(\sigma)}$ ,  $\sigma = (\alpha, \tau)$ , we have to estimate from below the operator  $H_{n-1}$  in the space  $B_{n-1}(\sigma)$  of such functions  $\varphi(\tau') \in \mathcal{L}_2(R^{3n-3})$ , that have the types of the permutational symmetry  $\alpha'$  and the rotational (point) symmetry  $\tau'$ , which are possible for the states of subsystem  $Z_{n-1}$ , when the states of the whole system have the symmetry of the type  $\sigma$ . For any  $F_k \subseteq O(3)$  and  $\sigma = (\alpha, \tau)$  such possible types  $\sigma' = (\alpha', \tau')$  are described by the following conditions:

$\alpha'$  is permitted, iff  $\alpha' \in E(\alpha)$ ;

$\tau'$  is permitted iff  $\exists \tau''$ , for which

$$D_g^{(\tau')} \otimes D_g^{(\tau'')} \supseteq D_g^{(\tau)}, \quad g \in F_k \quad (8)$$

and

$$\text{a) } P^{(\tau')} \mathcal{L}_2(R^{3n-3}) \neq 0, \quad \text{b) } P^{(\tau'')} \mathcal{L}_2(R^3) \neq 0. \quad (9)$$

Here  $D_g^{(\gamma)}$  is irreducible representation of the type  $\gamma$  of the group  $F_k$ . It follows from the representations theory, that for  $\forall \tau, \tau'$  we can find  $\tau''$  for (8). The conditions (9) hold for any  $\tau', \tau''$ , when  $F_k = O^+(3)$  and for any finite  $F_k$  [4]. So for these cases all  $\tau'$  are permitted and it means, that  $B_{n-1}(\alpha, \tau) = B_{n-1}(\alpha)$ . This fact results in the independence of the value  $\inf s_{\text{ess}}(H_n^{(\alpha, \tau)})$  on  $\tau$  for the mentioned cases.

But for  $F_k = O(3)$  the relations (9) are wrong for some  $\tau', \tau''$ , since  $P^{(\gamma)} \mathcal{L}_2(R^6) = 0$  for  $\gamma = (0, -1)$ ,  $P^{(\gamma)} \mathcal{L}_2(R^3) = 0$  for

$\gamma = (l, (-1)^{l+1})$ ,  $l = 0, 1, \dots$ . The reason of it consists in the property, of spherical harmonics  $Y_{lm}$  in  $R^3$ : they have parity  $(-1)^l$ . This implies, that not all  $\tau'$  are permitted for given  $\tau$ . For example, if  $n \geq 4$ ,  $G_k = O(3)$  and  $\tau = (0, \omega)$ ,  $\omega = \pm 1$ , then the types  $\tau'_l = (l, (-1)^{l+1}\omega)$ ,  $l = 0, 1, 2, \dots$  are not permitted, since for  $\tau = \tau'_l$  there is the single type  $\tau''$ , for which (8) holds:  $\tau'' = \tau''_l = (l, (-1)^{l+1})$ , but for  $\tau'' = \tau''_l$  (9.b) is wrong. These considerations show, that depending on  $\tau$  some types  $\tau'$  of rotational symmetry are impossible for functions  $\varphi(r') \in B_{n-1}(\sigma)$ ,  $\sigma = (\alpha, \tau)$  and consequently  $B(\alpha) \neq B(\alpha, \tau)$ . It means  $\inf s_{\text{ess}}(H_n^{(\sigma)}) \equiv \inf H_{n-1}(\sigma)$  may depend on  $\tau$ , when  $F_k = O(3)$ .

3.3. The considerations of 3.2 show, WHY the lower bound of essential spectrum of the operator  $H^{(\sigma)}$ ,  $\sigma = (\alpha, \tau)$  has not to do depend on  $\tau$ . After these considerations we may do not prove the "hard part" of the Theorem 1, which consists in the finding of  $\inf s_{\text{ess}}(H_n^{(\sigma)})$ . Actually  $s_{\text{ess}}(H_n^{(\sigma)}) \subseteq s_{\text{ess}}(H_n^{(\alpha)})$  for  $\sigma = (\alpha, \tau)$  at  $\forall \tau$  so it is sufficient to prove that  $[\mu^{(\alpha)}, +\infty) \equiv s_{\text{ess}}(H_n^{(\alpha)}) \subseteq \subseteq s_{\text{ess}}(H_n^{(\sigma)})$ . But such proof is the "easy part" of the proof HWZ-type theorems and it may be done in standard manner on the base of the relations (8), (9) and the results of [4].

#### 4. RESULTS ON THE DISCRETE SPECTRUM

4.1. Let the group  $F_k$  be finite. We denote by  $Q_n$  the total charge of the system  $Z_n$ :  $Q_n = ne + \sum_{s=1}^k e_1$ .

**Theorem 2.** *Let  $Q_n \geq 0$ . Then the number  $\mu_n^{(\alpha)} = \inf H_{n-1}(\alpha)$  is the point of the discrete spectrum of the operator  $H_{n-1}(\alpha)$ .*

So the lower bound of the essential spectrum  $s_{\text{ess}}(H_n^{(\sigma)})$  of considered operator  $H_n$  in the space of functions, having symmetry  $\sigma = (\alpha, \tau)$  is the discrete eigenvalue of the operator  $H_{n-1}$  in the space  $B_{n-1}(\alpha)$  of the functions, whose permutational symmetry is

possible for the states  $\varphi(r'_1, \dots, r'_{n-1})$  of the subsystem  $Z_{n-1}$ , when the states of the system  $Z_n$  have the symmetry  $\alpha$ .

Let  $U$  be the eigenspace of the operator  $H_{n-1}(\alpha)$ , corresponding to the eigenvalue  $\mu_n^{(\alpha)}$ . Since  $T_{g'}H_{n-1} = H_{n-1}T_{g'}$ ,  $g' \in G'_k = S_{n-1} \times F_k$ , then  $U$  is invariant for the operators  $T_{g'}$ . It is evident, that operators  $T_{g'}$  form a representation of the group  $G'_k$  in the subspace  $U$ . To simplify our consideration we assume that this representation is irreducible (that is  $U$  is not degenerated with respect to the symmetry). We denote by  $\sigma'_0$  the type of the irreducible representation  $g' \rightarrow T_{g'}$ ,  $g' \in G'_k$  in  $U$ ; since  $G'_k = S_{n-1} \times F_k$ , then  $\sigma'_0 = (\alpha'_0, \tau'_0)$  for some types  $\alpha'_0$  and  $\tau'_0$  of irreducible representations of  $S_{n-1}$  and  $F_k$ . Further for any numbers  $\varepsilon > 0$ ,  $R > 0$  we introduce two-particle NR operators

$$h_{\pm\varepsilon}(R) = \left( \frac{-1 \pm \varepsilon}{2m} \right) \Delta_n + (1 \pm \varepsilon) Q_{n-1} e^{|r_n|^{-1}}, \quad (10)$$

which are considered on the smooth functions, supported in the region  $|r_n| \geq R$ . Let  $h_{\pm\varepsilon}^{(\gamma)}(R)$  be the restriction of the operator  $h_{\pm\varepsilon}(R)$  to the subspace of functions, having point symmetry of the type  $\gamma$ . At last for any real number  $\lambda$  and self-adjoint operator  $W$  we denote by  $N(\lambda, W)$  the counting function of the discrete spectrum  $s_d(W)$  of the operator  $W$  on half-line  $(-\infty, \lambda]$ .

4.2. Now we can formulate our main result.

**Theorem 3.** *Let  $Q_n \geq 0$ . Then the discrete spectrum of the operator  $H_n^{(\sigma)}$  is infinite at arbitrary  $\sigma = (\alpha, \tau)$  and for any  $\varepsilon > 0$ ,  $\lambda_0 > 0$  there are such numbers  $R > 0$  and  $C_i = C_i(\varepsilon, R)$ ,  $i = 1, 2$ , that for  $\forall \lambda$ ,  $0 < \lambda \leq \lambda_0$  the following estimates of the operator  $H_n^{(\sigma)}$  discrete spectrum counting function hold:*

$$\begin{aligned} |\sigma| \sum_{\gamma \in \Gamma} b(\tau; \tau'_0, \gamma) |\gamma|^{-1} N(-\lambda, h_{-\varepsilon}^{(\gamma)}(R)) - C_1 &\leq N(\mu_n^{(\alpha)} - \lambda; H_n^{(\sigma)}) \leq \\ &\leq |\sigma| \sum_{\gamma \in \Gamma} b(\tau; \tau'_0, \gamma) |\gamma|^{-1} N(-\lambda; h_{+\varepsilon}^{(\gamma)}(R)) + C_2, \end{aligned} \quad (11)$$

where  $\Gamma$  is the set of all types of group  $F_k$  irreducible representations, the coefficient  $b(\tau; \tau'_0, \gamma)$  shows, now many times the repre-

sentation of the group  $F_k$  of the type  $\tau$  is contained in the tensor product of the representations of the types  $\tau'_0$  and  $\gamma$ :

$$b(\tau; \tau'_0, \gamma) = |F_k|^{-1} \sum_{g \in F_k} \chi_g^{(\tau'_0)} \chi_g^{(\gamma)} \bar{\chi}_g^{(\tau)}, \quad (12)$$

$\chi_g^{(p)}$  is the character of the element  $g$  in the group  $F_k$  representation of the type  $p$ ,  $p = \tau'_0, \tau, \gamma$ ;  $|\gamma|, |\sigma|$  are the dimensions of the representations of the types  $\gamma$  and  $\sigma$ ,  $|F_k|$  is the number of the group  $F_k$  elements.

In the Theorem 3 we obtained two-sided estimates of the discrete spectrum  $n$ -particle PR operator  $H_n^{(\sigma)}$  counting function in the terms of counting functions of two-particle NR operators  $h_{\pm\epsilon}^{(\gamma)}(R)$ .

4.3. It is easy to prove, that

$$\lim_{\lambda \rightarrow 0+0} \frac{N(-\lambda; h_{\pm\epsilon}^{(\gamma)}(R))}{N(-\lambda; h_{\pm\epsilon}^{(\gamma)}(0))} = 1 \quad (13)$$

and

$$\lim_{\lambda \rightarrow 0+0} \frac{N(-\lambda; h_{\pm\epsilon}^{(\gamma)}(0))}{N(-\lambda; h_0^{(\gamma)}(0))} = 1 + \delta(\pm\epsilon) \quad (14)$$

where the operator  $h_{\pm\epsilon}(0)$  is two-particle hydrogen like type operator with the known spectrum and eigenfunctions,  $\delta(\pm\epsilon) \rightarrow 0$  if  $\epsilon \rightarrow 0$ . The calculations show, that

$$\lim_{\lambda \rightarrow 0+0} \frac{N(-\lambda; h_0^{(\gamma)}(0))}{N(-\lambda; h_0(0))} = \frac{|\gamma|^2}{|F_k|} \quad (15)$$

where  $N(-\lambda; h_0(0))$  is the known counting function of the operator  $h_0(0)$  discrete spectrum:

$$N(-\lambda; h_0(0)) = f(\lambda) = 6^{-1} 2^{-1/2} m^{3/2} \lambda^{-3/2} |Q_{n-1}e|^3.$$

If we use the relations (13)–(15) then we obtain from the Theorem 3 the following result:

**Theorem 4.** *Let  $Q_n \geq 0$ . Then for  $\forall \sigma = (\alpha, \tau)$*

$$\lim_{\lambda \rightarrow 0+0} \frac{N(\mu_n - \lambda; H_n^{(\sigma)})}{|\sigma| d(\tau, \tau'_0) f(\lambda)} = 1 \quad (16)$$

where

$$d(\tau, \tau'_0) = |F_k|^{-1} \sum_{\gamma} b(\tau; \tau'_0, \gamma) |\gamma| = |F_k|^{-1} |\tau| |\tau'_0| \quad (17)$$

and coefficients  $b(\tau; \tau'_0, \gamma)$  are given by the relation (12).

#### 4.4. Remarks.

1. Theorem 4 discovers the principal term of the spectral asymptotics of the discrete spectrum  $s_d(H_n^{(\sigma)})$  of the operator  $H_n^{(\sigma)}$  and its dependence on the point symmetry type  $\tau$ . By Theorem 1  $s_{\text{ess}}(H_n^{(\alpha)}) = s_{\text{ess}}(H_n^{(\alpha, \tau)})$  and consequently

$$s_d(H_n^{(\alpha)}) = \bigcup_{\tau \in \Gamma} s_d(H_n^{(\alpha, \tau)}). \quad (18)$$

So Theorem 4 and relation (18) describe the inner structure of the operator  $H_n^{(\alpha)}$  discrete spectrum with respect to all types point symmetry of the eigenfunctions of this spectrum.

By the way from the relations (16)–(18) we can get the leading term of the discrete spectrum counting function asymptotics for the operator  $H_n^{(\alpha)}$ . Actually taking into account that  $|\sigma| = |\alpha| |\tau|$  and summing the functions  $|\sigma| d(\tau, \tau'_0) f(\lambda)$  over all  $\tau$  we obtain  $|\alpha| |\tau'_0| f(\lambda)$ , where the number  $|\tau'_0|$  may be considered as the multiplicity of the group  $S_n$  irreducible representation of the type  $\alpha'_0$  in  $U$  (see 4.1). This result is agreed with [6].

2. By (16), (17) the leading term of spectral asymptotics of  $s_d(H_n^{(\sigma)})$  depends on the type  $\tau'_0$  of the point symmetry PR system  $Z_{n-1}$  ground state, when the states of the system  $Z_n$  have the symmetry  $\sigma = \alpha$  ( $\tau'_0$  is the type of the point symmetry of functions

from eigenspace  $U$  of the operator  $H_{n-1}(\alpha)$ , corresponding to its minimal eigenvalue  $\mu_n^{(\alpha)}$ , see §4.1).

Unfortunately, we do not know  $\tau'_0$  and there are no any restrictions on the possible types  $\tau'_0$ . So to get all possible variants of asymptotics for fixed  $\sigma = (\alpha, \tau)$  we are obliged (according (17)) to consider all  $\tau'_0$ , having the different  $|\tau'_0|$ . Let us consider the simplest example setting  $F_k = F_3 = D_3$ , where  $D_3$  is the rotation symmetry group of equilateral triangle. The group  $D_3$  has two one-dimensional irreducible representations and one two-dimensional irreducible representation. We denote their types by  $\tau_1, \tau_2, \tau_3$  respectively. Then

$$\begin{aligned} d(\tau, \tau'_0) &= \frac{|\tau|}{6} && \text{if } \tau'_0 = \tau_1, \tau_2 \text{ and} \\ d(\tau, \tau'_0) &= \frac{|\tau|}{3} && \text{if } \tau'_0 = \tau_3. \end{aligned}$$

As justification of such situation one can add that similar lack of the determination is present in the all known results on the spectrum structure of PR and NR many particle hamiltonians with symmetry account. It is generated by the absence of any results on the hierarchy (subordination) of the operators lower bounds in the symmetry spaces depending on the symmetry types.

3. Theorem 4 gives only leading term of spectral asymptotics similar to the cases, where we took into account the symmetry with respect to groups  $S_n$  [5] or  $S_n \times O^+(3)$  or  $S_n \times O^+(3) \times W$  [3]. The main reasons of the second term absence are the same, as in [5]. Namely, to get the second term of spectral asymptotics (using geometrical methods similar to [8]) it is necessary to know the summability with suitable weight of the eigenfunctions of the discrete spectrum PR operator  $H_n^{(\sigma)}$ . Unfortunately such results are absent for  $n \geq 2$ .

## References

1. Lieb E., Yau H.-T. The stability and instability of relativistic matter // *Comm. Math. Phys.* 1988. V. 118. P. 177–213.
2. Lewis R. T., Siedentop H., Vugalter S. The essential spectrum of relativistic multiparticle operators // *Ann. Ins. Henri Poincare, Phys. Theor.* 1997. V. 67, No 1. P. 1–28.
3. Zhislin G.M. On the spectrum of pseudorelativistic electrons hamiltonian in the spaces of given symmetry functions // *Dokladi Russian Academy of Science.* 2004. V. 397, No 1 (Russian).
4. Zhislin G.M., Mandel E.L. On the spectrum of the molecular electrons energy operator in the spaces of given symmetry functions // *Theor. and Math. Phys.* 1969. V. 1, No 2. P. 295–301 (Russian).
5. Zhislin G.M. On the discrete spectrum of pseudorelativistic hamiltonians of the identical particles in the spaces of functions, having fixed type of permutational symmetry // preprint No 473 Radiophysical Research Institute. — Nizhny Novgorod: NIRFI, 2002. 16 p. (Russian).
6. Zhislin G.M., Vugalter S.Á. On the discrete spectrum of Hamiltonian for pseudorelativistic electrons // *Izvestiya: Mathematics.* 2002. V. 66, No 1. P. 71–102.
7. Vugalter S. A., Zhislin G. M. Spectral properties of a pseudorelativistic system of two particles with finite masses // *Theor. and Math. Phys.* 1999. V. 121, No 2. P. 1506–1515.
8. Vugalter S. A., Zhislin G. M. On the asymptotics of the discrete spectrum of a given symmetry of multiparticle Hamiltonians // *Trans. Moscow Math. Soc.* 1993. P. 165–189
9. Wigner E. P. Group theory and its applications to the quantum mechanics of atomic spectra. — New York: Academic Press, 1959.

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