SPECTRAL PROPERTIES OF HAMILTONIANS WITH A MAGNETIC FIELD AT A FIXED PSEUDOMOMENTUM. III

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The general results (see previous Part II) on the structure of the discrete spectra of energy operators of neutral systems in a homogeneous magnetic field at a fixed pseudomomentum are proved to be applicable to Hamiltonians of arbitrary atoms. Asymptotic expressions for the discrete spectra of Hamiltonians in the presence of a homogeneous magnetic field are found for arbitrary atoms. This paper completes the investigation of the spectral properties of Hamiltonians of neutral systems in a homogeneous magnetic field at a fixed pseudomomentum. The essential and discrete parts of the spectrum for such systems were found previously; however, whether the theorems in Part II were valid for actual n-particle systems remained an open question for the case n > 3.

Introduction

This paper completes the series of papers in which geometric methods are used to study the spectra of energy operators of neutral systems with a homogeneous magnetic field at a fixed pseudomomentum. The theorem on localization of the essential spectrum of such operators [1], the conditions for the discrete spectrum to be finite [2], and the asymptotic behavior of the spectrum [2] were previously obtained. However, all results in [2] concerning the discrete spectrum were based on the assumption that the boundary of the essential and discrete spectrum of the system is completely determined by splitting the system into two stable subsystems, $Z_2 = (A_1, A_2)$, where the subsystems $A_1$ and $A_2$ are such that the lower bound of the essential spectrum of the corresponding Hamiltonian $H_0(Z_2)$ is a point of its discrete spectrum. Such an assumption is customary when investigating discrete spectra of Hamiltonians in both the presence and the absence of a magnetic field; however, verifying its validity for actual systems is far from trivial even in the simplest cases. In [2], it was proved only for atoms of hydrogen and helium, while the question whether it is true for more complicated systems remained open.

Later, S. A. Vugal’ter proved the validity of this condition for arbitrary atoms; these results were announced in [3] (but have not yet been published).

In the present paper, we prove the validity of the assumptions that ensure the applicability of asymptotic spectral expressions found in [2] to Hamiltonians of arbitrary atoms, which thus proves the results in [3]. We formulate the results for atomic Hamiltonians following from [2] with the Pauli exclusion principle taken into account (this symmetry was lacking in [3]).

Essentially, the proof consists in studying the spectral properties of the lower boundary of the spectrum of the Hamiltonian of a positive ion. This Hamiltonian can be obtained from the atomic Hamiltonian after fixing the pseudomomentum of the system. This is done in Sec. 2, where we also show that the discrete spectrum is not empty (this ensures the applicability of the results in [2] to the atomic Hamiltonian) as soon as the ion Hamiltonian satisfies the conditions of the Hunziker–van Winter–Zhislin theorem. We prove this theorem for the energy operators of positive ions in Sec. 3 using special partitions of the configuration space introduced in [4]. For simplicity, we neglect the permutation symmetry in the proof, but all its technical constructions are such that they preserve the permutation symmetries of all the subsystems.
involved. Therefore, we can take the permutation symmetry into account by merely adding the "symmetry reasonings."

1. Main definitions and results

1.1. Let \( Z_1 = \{1, 2, \ldots, N\} \) be an arbitrary neutral system of the atomic type embedded in a homogeneous magnetic field \((0, 0, B)\) directed along the \( z \) axis; let \( m_i, e_i, \) and \( r_i = (x_i, y_i, z_i) \) be the respective mass, charge, and radius vector of the \( i \)th particle; and let \( e = e_2 = e_3 = \cdots = e_N, e_1 = -(N - 1)e, m = m_2 = m_3 = \cdots = m_N, \) and \( M = m_1 + (N - 1)m, \)

\[
q_i = (q_{i1}, q_{i2}, q_{i3}) = (q_{j1}, q_{j2}, q_{j3}) = r_j - \sum_{t=1}^{N} m_tr_tM^{-1}, \quad q = (q_1, \ldots, q_N).
\]

After separating the center-of-mass motion along the \( z \) axis and restricting the consideration to the subspace of states with the fixed component values \( \nu_1 \) and \( \nu_2 \) of the pseudomomentum, we can represent the Hamiltonian of the system \( Z_1 \) as

\[
H_0 = T_{0.1} + T_{0.3} + F + V(q), \quad (1.1)
\]

where

\[
T_{0.1} = \sum_{t=1}^{N} m_t \sum_{p=1}^{2} \left( \frac{1}{i} \nabla_{tp} - D_{tp} \right)^2, \quad T_{0.3} = \sum_{t=1}^{N} m_t \left( \frac{1}{i} \nabla_{t3} \right)^2,
\]

\[
\nabla_{tp} = \frac{1}{m_t} \frac{\partial}{\partial q_{tp}} - \frac{1}{M} \sum_{j=1}^{N} \frac{\partial}{\partial q_{jp}}, \quad p = 1, 2, 3, \quad (1.2)
\]

\[
D_{tp} = \nu_p \left( \frac{1}{M} - \frac{1}{Nm_t} \right) + (-1)^{p+1} \sum_{j=1}^{N} (q_{jp} - q_{tp}) (\frac{e_t - e_j}{Nm_t} + \frac{2e_j}{M}), \quad p = 3 - p,
\]

\[
F = (\nu_1 + \nu_2)^2 + (\nu_2 - \nu_1)^2, \quad \nu_j = 2B \sum_{i=1}^{N} e_i q_{ij}, \quad V(q) = \sum_{s<t} V_{st}(|q_s - q_t|) \quad (1.3)
\]

\[
V_{st}(|q_s|) = e_se_t|q_t|^{-\gamma}, \quad 0 < \gamma < 2.
\]

For simplicity, we call this system the atom, particle number 1 the nucleus, and particles number 2, 3, \ldots, \( N \) the electrons, although only the case where \( \gamma = 1 \) corresponds to actual atoms whereas we permit \( \gamma \in (0, 2). \)

1.2. Let

\[
R_0 = \left\{ q \mid q = (q_1, \ldots, q_N) \mid q_i = r_i - \sum_{j=1}^{N} m_j r_j M^{-1}, \quad i = 1, 2, \ldots, N \right\}.
\]

In the space \( \mathcal{L}_2(R_0) \), we expand the operator \( H_0 \) from the domain \( \mathcal{D}(H_0) \equiv C^2_0 \) to the self-adjoint operator and preserve the same notation \( H_0 \) and \( \mathcal{D}(H_0) \) for the latter operator and its domain of definition. We let \( S_p \) denote the group of permutations of \( p \) identical elements and \( \alpha_k(p), 0 \leq k \leq p/2, \) denote the types of irreducible representations of this group, which correspond to decomposing the number \( p \) into \( k \) pairs and \( p - 2k \) singles, i.e., to one- (for \( k = 0 \)) or two-column Young schemes. Let \( S = S_{N-1} \) and \( \alpha = \alpha_k(N-1), 0 \leq k \leq (N-1)/2. \) Because of the Pauli principle, only the coordinate wave functions possessing a symmetry \( \alpha = \alpha_k \) may describe states of a quantum system. We let \( P^{(\alpha)} \) denote the projection