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Discrete Spectrum of Schrödinger Operators with Non-Constant Magnetic Fields

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In this note we discuss the discrete spectrum of the Schrödinger operator $H_{N,Z}(b)$, defined as below, for an atomic system in a magnetic field. Let $x = (x^1, ..., x^N) \in \mathbf{R}^{3N}$, each $x^j \in \mathbf{R}^3$ $(1 \le j \le N)$ and ∇_j being the gradient in $\mathbf{R}^3$ with respect to x^j $(1 \le j \le N)$. Then we consider the following operator :

$$H_{N,Z}(b) = \sum_{j=1}^{N} \left(T_j(b)^2 - \frac{Z}{|x^j|} \right) + \sum_{1 \le i < j \le N} \frac{1}{|x^i - x^j|}, \tag{1.1}$$

as a self-adjoint one in $L^2(\mathbf{R}^3)$, where $Z > 0$, $N \in \mathbf{N}$, $b \in C^1(\mathbf{R}^3)^3$ being real-valued and

$$T_j \equiv T_j(b) = -i\nabla_j - b(x^j) \quad (1 \le j \le N).$$

This operator $H_{N,Z}(b)$ is the atomic Hamiltonian with a nucleus, that is assumed to be infinitely heavy, with charge Z and N electrons of charge 1 and mass 1/2, and with the magnetic vector potential b.

The problem is the finiteness or the infiniteness of the discrete spectrum of $H_{N,Z}(b)$, which is one of the characteristic spectral properties. This problem in the case that $b = 0$ was studied by Zhislin [9],[10], Yafaev [2] and others. The following theorem, which is obtained by combining with [9],[10] and [2], gives the necessary and sufficient condition, which is the relation between Z and N, for the finiteness of the discrete spectrum of $H_{N,Z}(0)$.

Theorem 0.1 ([2],[9],[10]). *The number of the discrete spectrum of $H_{N,Z}(0)$ is finite if and only if $Z \le N - 1$.*

On the other hand, in the case of uniform magnetic fields, Avron-Herbst-Simon [1] and Tamura [7], and Vugal'ter-Zhislin [8] gave a necessary and a sufficient condition, respectively, for the finiteness of the discrete spectrum of the atomic Hamiltonians.

Theorem 0.2 ([1],[8]). *The number of the discrete spectrum of $H_{N,Z}(b_c)$ is finite if and only if $Z < N - 1$.*

Here $b_c(y) = (0,0,B/2) \times y \ (y \in \mathbf{R}^3)$, which satisfies $rot\,(b_c) = (0,0,B)$, B is a positive constant and $rot(\cdot)$ denotes 3-dimensional rotation. We remark that, comparing Theorem 0.2 with Theorem 0.1, the difference between the presence and the absence of uniform magnetic fields appears only in the delicate case that $Z = N - 1$.

Then our concern is the case of non-constant magnetic fields. Some different phenomena are expected to occur in non-constant magnetic fields. In fact, we have the following theorem.

Theorem 1.1. *For any positive constant Z, there exists a vector potential $b_Z \in C^1(\mathbf{R}^3)^3$, which is independent of N, such that the number of the discrete spectrum of $H_{N,Z}(b_Z)$ is always finite for $N \geq 2$.*

In other words, any atomic system has only finitely many bound states in a suitable magnetic field. Also we have the following result.

Theorem 1.2. *There exists a vector potential $b_0 \in C^1(\mathbf{R}^3)^3$, which is independent of N and Z, such that the number of the discrete spectrum of $H_{N,Z}(b_0)$ is infinite for any N and any Z.*

In other words, any atomic system has infinitely many bound states in a suitable magnetic field. So, as a consequence, the finiteness or the infiniteness of the number of bound states generically depends on magnetic fields.

Besides, it follows from Theorem 1.2 that the discrete spectrum of $H_{N,Z}(b_0)$ is not empty. This is related to the problem of the presence or the absence of the discrete spectrum. This problem was studied by Ruskai [4],[5], Sigal [6], Lieb [3] and others. Ruskai and Sigal proved that there is no very negative ions and Lieb [3] improved their results as follows.

Theorem 0.3 ([3]). *If $N \geq 2Z + 1$, then $H_{N,Z}(0)$ has no discrete spectrum.*

As a consequence of the above theorem, the number of electrons that a nucleus of charge Z can bind is less than $2Z + 1$. In view of Theorem 1.2, the presence or the absence of the discrete spectrum depends on magnetic fields. Also, even if there is no very negative ions in a fixed magnetic field, the maximal number of electrons that a nucleus can bind depends not only on the charge of the nucleus but also on the magnetic field.

At the end we roughly explain the vector potentials in Theorems 1.1 and 1.2. First $b_Z(y) = f_Z(\rho)(-y_2, y_1, 0)$, where $y = (y_1, y_2, y_3)$, $\rho = \sqrt{y_1^2 + y_2^2}$, and f_Z is larger than $B/2$ and converges to $B/2$ of the order $\rho^{-1/2}$ as $\rho \to +\infty$. Further the height $B/2$ is sufficient small and dependent of Z (Figure 1). Next $b_0(y) = f_0(r)(-y_2, y_1, 0)$, where $r = |y|$, and f_0 is smaller than $B/2$ and converges to $B/2$ of the order $r^{-1/2}$ as $r \to +\infty$. Further the height $B/2$ is sufficient large and independent of N and Z (Figure 2). We note that these are perturbations of constant magnetic fields.

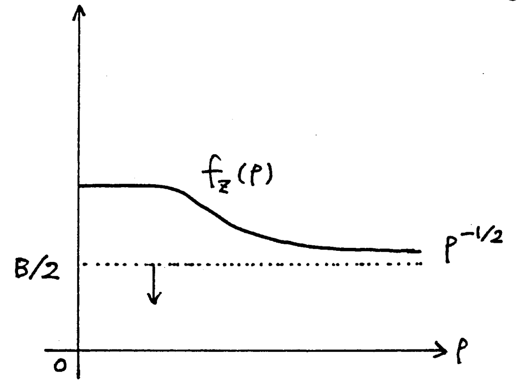

Figure 1

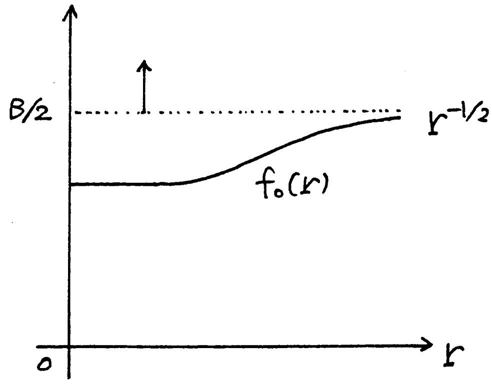

Figure 2

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