Solution of the Nonlinear Self-congruent Problem of an Electron in a Cluster Placed in a Strong Magnetic Field

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Abstract. The solutions of the nonlinear Schrodinger equation of an electron in a cluster placed in a strong magnetic field were studied. It was shown that there is a minimal cluster radius at which a localized solution of the one-dimensional nonlinear Schrodinger equation exists. With larger cluster radii, there emerge two, three, and more solutions of the equation. For the solutions found, the energies, the total energies, and the electron radii were numerically calculated. The possibility of experimentally checking the results obtained is discussed.
Key words: nonlinear Schrodinger equation, electron, cluster, magnetic field

1. INTRODUCTION

We have earlier [1] considered the states of an electron in a cluster consisting of polar molecules in a superstrong magnetic field. To describe these states, a polaron model has been used. According to [1], a superstrong magnetic field leads to the stabilization of the electron states in the cluster and to the possibility of formation of electron states where the number of molecules is smaller than the critical one. The approximate equations for an electron in the cluster in the limit of a superstrong magnetic field are [1]

$$\chi''(Z) + \frac{\pi\mu e^2}{\hbar^2 \varepsilon}(\chi^2(Z) - \chi^2(R))\,\chi(Z) + \frac{2\mu}{\hbar^2} W\chi(Z) = 0\,,$$
$$|Z| \le R, \tag{1.1}$$
$$\chi''(Z) + \frac{2\mu W}{\hbar^2}\chi(Z) = 0\,, \quad |Z| > R\,.$$

Here, e and μ are the electron charge and weight, respectively; $\hbar$ is Planck's constant; ε is the effective dielectric permittivity of the cluster; W is the electron energy; and R is the cluster radius. Equations (1.1) are the nonlinear Schrodinger equations for the wave function $\chi(Z)$, which obeys the norming condition

$$\int_{-\infty}^{\infty} \chi^2(Z) = 1. \tag{1.2}$$

Earlier [1], only one of the solutions of equations (1.1) has been investigated in detail, namely, that giving the lowest electron state in the cluster. The purpose of this work was to examine the properties of other solutions of problem (1.1) and to consider their role in studying the electron states in the cluster.

2. BASIC RELATIONS

Among the most important characteristics of electron states in clusters are the electron energy W determined from equation (1.1) and the total energy F of an electron in the cluster [1]:

$$F = \frac{\hbar^2}{2\mu}\int_{-\infty}^{\infty}\chi'^2(Z)\,dZ - \frac{\pi}{4}\frac{e^2}{\varepsilon}\int_{-R}^{R}\chi^4(Z)\,dZ + \frac{\pi}{4}\frac{e^2}{\varepsilon}\chi^2(R)\int_{-R}^{R}\chi^2(Z)\,dZ. \tag{2.1}$$

The energy and the total energy of an electron in the cluster can be conveniently computed as in [1], viz., through changing from ÷(Æ) and **Z** to new variables defined from the relations

$$\chi(Z) = \sqrt{\frac{2\varepsilon|W|}{\pi e^2}}\,y(z), \qquad Z = \sqrt{\frac{\hbar^2}{2\mu|W|}}\,z. \tag{2.2}$$

Then, instead of (1.1), we obtain

$$\begin{gathered} y''(z) + [y^2(z) - y^2(a)]\,y(z) - y(z) = 0, \qquad |z| \le a, \\ y''(z) - y(z) = 0, \qquad |z| > a \end{gathered} \tag{2.3}$$

where

$$a = R\sqrt{\frac{2\mu|W|}{\hbar^2}}. \tag{2.4}$$

In terms of these dimensionless variables, proceeding from the norming condition (1.2) and relations (2.2), the electron energy can be derived:

$$W = -\frac{\pi^2}{2\Gamma^2}\frac{e^4\mu}{\varepsilon^2\hbar^2}, \qquad \Gamma = \int_{-\infty}^{\infty} y^2(z)\,dz. \tag{2.5}$$

From (2.1) and (2.2), the total energy ***F*** is found:

$$F = \frac{\pi^2}{2}\frac{e^4\mu}{\varepsilon^2\hbar^2}\frac{\overline{F}}{\Gamma^3}, \tag{2.6}$$

where

$$\overline{F} = \int_{-\infty}^{\infty} y'^2(z)\,dz - \frac{1}{2}\int_{-a}^{a} y^4(z)\,dz + \frac{1}{2}y^2(a)\int_{-a}^{a} y^2(z)\,dz. \tag{2.7}$$

Another important characteristic of electron states in a cluster is the effective radius of a state:

$$<r> = \int_{0}^{\infty} Z\chi^2(Z)\,dZ, \tag{2.8}$$

which can be calculated with the use of (2.2) and (2.8):

$$\langle r\rangle = \frac{\varepsilon\hbar^2}{\pi\mu e^2}\Gamma_1, \qquad \Gamma_1 = \int_{0}^{\infty} z y^2(z)\,dz. \tag{2.9}$$

Thus, the computation of the energy, the total energy, and the radius of the states is related to solving equations (2.3).

states tend to infinity as $\boldsymbol{R} \to \infty$.
Knowing the asymptotic behavior of the solutions of the reduced problem as $\boldsymbol{a} \to 0$ and as $\boldsymbol{a} \to \infty$, one can predict the asymptotics of $\langle \boldsymbol{r} \rangle$ when $\boldsymbol{R} \to \infty$. We shall make only one note. Let $\boldsymbol{n} > 1$, and let the internal states be considered. Then, as $\boldsymbol{R} \to \infty$, $\boldsymbol{W} \to$ const, and substitution (2.2) is changed into a scaling transformation that is independent of $\boldsymbol{R}$. In this case, the solutions take the form of several peaks (with almost invariable heights and shapes) that drift apart with increasing R. Evidently, $\langle \boldsymbol{r} \rangle \to \infty$.

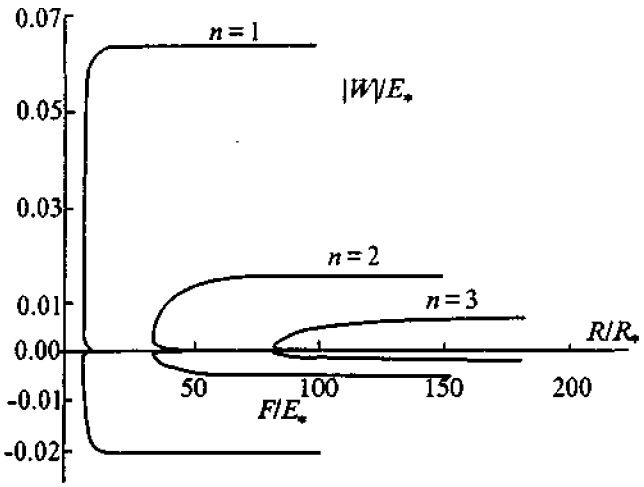

Fig. 2. Eigenvalues **W** and total energies $\boldsymbol{F}$ versus $\boldsymbol{R}$; $E_* = \dfrac{\pi^2 e^4 \mu}{2\varepsilon^2 \hbar^2}$; $R_* = \dfrac{\varepsilon \hbar^2}{\pi \mu e^2}$.

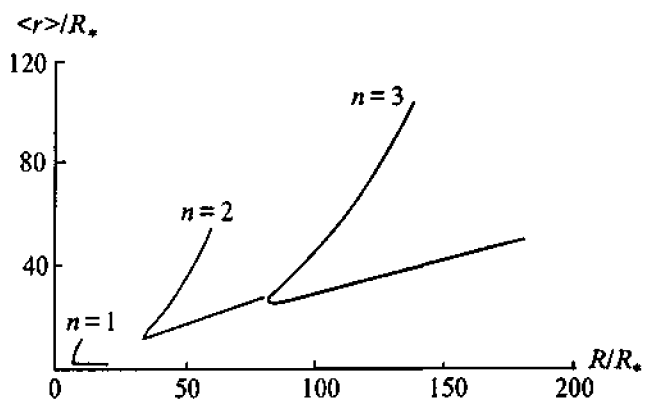

Fig. 3. Radii $\langle \boldsymbol{r} \rangle$ of the electron states for various solutions of problem (1.1) as dependent on $\boldsymbol{R}$; $R_* = \dfrac{\varepsilon \hbar^2}{\pi \mu e^2}$.

6. DISCUSSION

Currently, there is no experimental data on the properties of charged clusters in strong magnetic fields. The condition of quantizing magnetic field: $\hbar \omega_c \gtrsim |W|$, where $\boldsymbol{\omega_c}$ is the cyclotron frequency, is obeyed more readily by the branches of the found solutions that describe the external states. For example, according to [1], the external electron state corresponding to the solution with $\boldsymbol{n} = 1$ can be observed at $\boldsymbol{R} < \boldsymbol{R_c}$ in fields with $H \gtrsim 10^5$ Oe. Here, $\boldsymbol{R_c}$ is the least possible cluster radius in the absence of magnetic field. Therefore, below, we dwell briefly only on the external states with $\boldsymbol{n} \geq 2$.

In a $(NH_3)_m$ cluster, the bound states with $\boldsymbol{n} = 2$ are possible only at $\boldsymbol{R} > 10.7$ Å (see Fig. 2, the values of the physical parameters are the same as those in [2]). As noted, the absolute values of the energies and the total energies of the external states with $\boldsymbol{n} = 2$ are higher than those at $\boldsymbol{n} = 1$, and a

(2) The relative positions of maxima and minima of a solution on the segment [-***a***, ***a***] are independent of ***a***. For example, at ***n*** = 2, there are one mini-mum at ***z*** = 0 and two maxima at ***z*** = ±2/3*a*.

3) The peak-to-peak amplitude of a solution is independent of ***á*** and ***n***:

$$M_n(a) - m_n(a) = \sqrt{2}.$$

(4) As ***a*** →0, the amplitude $\mathbf{M_n}(\boldsymbol{a})$ at a maximum increases without limit:

$$M_n(a) \approx \frac{C_n}{a}, \qquad C_n = \frac{\pi(2n-1)}{2\sqrt{2}}.$$

(5) As ***a*** → ∞, the solutions with ***n*** = 1 tend to the "soliton" solution

$$\bar{y}(z) = \frac{\sqrt{2}}{\cos h\, z}. \tag{4.2}$$

The solutions with ***n*** = 2, 3, ... take the form of several peaks, each resembling the graph of function (4.2), which are separated by portions where the solutions are close to zero.

5. WHAT IS KNOWN ON THE SOLUTIONS OF INITIAL PROBLEM (1.1)?

Numerical computation of **Ã** enables one, at given a and ***n*** = 1, 2, 3, ..., to find the normalized solution $\div_n$(Æ, ***a***) of equation (1.1), the eigenvalue $\mathbf{W_n}(\boldsymbol{a})$, and the radius $\boldsymbol{R_n(a)}$. In this computation, the following results were obtained.

(1) The function $\boldsymbol{R_n(a)}$ has a single minimum; as ***a*** →0 and as ***a*** → ∞, $\boldsymbol{R_n(a)}$ increases, tending to infinity. Thus, at large ***R*** values, for each ***n*** there are two types of states, one of which corresponds to large ***a***; and the other, to small ***a***.

(2) There exists a critical value $\boldsymbol{R} = \boldsymbol{R_{min}}$. At $\boldsymbol{R} < \boldsymbol{R_{min}}$, problem (1.1) has no solutions. At all $\boldsymbol{R} > \boldsymbol{R_{min}}$, there are two solutions with ***n*** = 1 (i.e., possessing one maximum). One of these solutions describes the "internal" states [the function $\chi_1(Z)$ is mainly localized within the region Z < R], and the other characterizes the "external" states. At large ***R***, the internal and external states correspond to large and small ***a***, respectively.

When ***R*** → ∞, the solutions of the first type tend to soliton solutions [derived from (4.2) by a scaling transformation], and their total energy tends to a constant value; whereas the maxima of the solutions of the second type diminish, and their total energy approaches zero.

(3) At $\boldsymbol{R_{min}}^{(2)} > \boldsymbol{R} > \boldsymbol{R_{min}}$, two different solutions, each having two maxima, become possible; and on the interval $\boldsymbol{R_{min}}^{(2)} < \boldsymbol{R} < \boldsymbol{R_{min}}^{(3)}$ the initial problem has four solutions. At $\boldsymbol{R} > \boldsymbol{R_{min}}^{(3)}$, solutions with ***n*** = 3 arise, etc.

(4) At a given ***R***, in a rise in n, the absolute value of the energy of the internal states decreases, and that of the external states increases. In Fig. 2, the energy ***F***

and the eigenvalue **W** are normalized to $E_* = \dfrac{\pi^2 e^4 \mu}{2\varepsilon^2 \hbar^2}$, and the radius ***R*** is normalized to $R_* = \dfrac{\varepsilon \hbar^2}{\pi \mu e^2}$

(5) Figure 3 presents the radii ⟨***r***⟩ of the electron states for various solutions of problem (1.1) as dependent on ***R***. At ***n*** = 1, for ***R*** → ∞, the radius of the internal state tends to a constant value, and that of the external state rises, tending to infinity. For the states with ***n*** > 1, the radii of both internal and external

3. ON THE RELATIONSHIP BETWEEN THE INITIAL AND REDUCED PROBLEMS

The transition from the initial problem (1.1) to the "reduced" one (2.3) is not only a mere (conventional) introduction of dimensionless variables: transformation (2.2) depends on the eigenvalue **W** to be found. At a given ***R***, for each of the solutions of equation (1.1) that decreases as $\mathbf{Z} \to \infty$, solution of equation (2.3) at a certain a. And vice versa, for each (decreasing) solution of reduced problem (2.3) at a given a, there is a corresponding (normalized) solution of the initial problem at a certain ***R***. To find this solution, one needs to calculate the integral $\tilde{\mathbf{A}}$ and the **W** value from (2.5), and, next, compute ***R*** from (2.4).

Thus, there is an exact correspondence between the set of all (normalized) solutions of initial problem (1.1) at various R and the set of all solutions of reduced problem (2.3) at various a.

4. WHAT IS KNOWN ON THE SOLUTIONS OF THE REDUCED PROBLEM?

The analytical investigation of problem (2.3) (see [2]) leads to the following conclusions.

(1) At any positive ***a***, this problem has an infinitely large (denumerable) number of solutions, with the ***n***th solution possessing ***n*** maxima (Fig. 1) and having the form of a segment of a periodic function with the period

$$T = 4a/(2n-1). \tag{4.1}$$

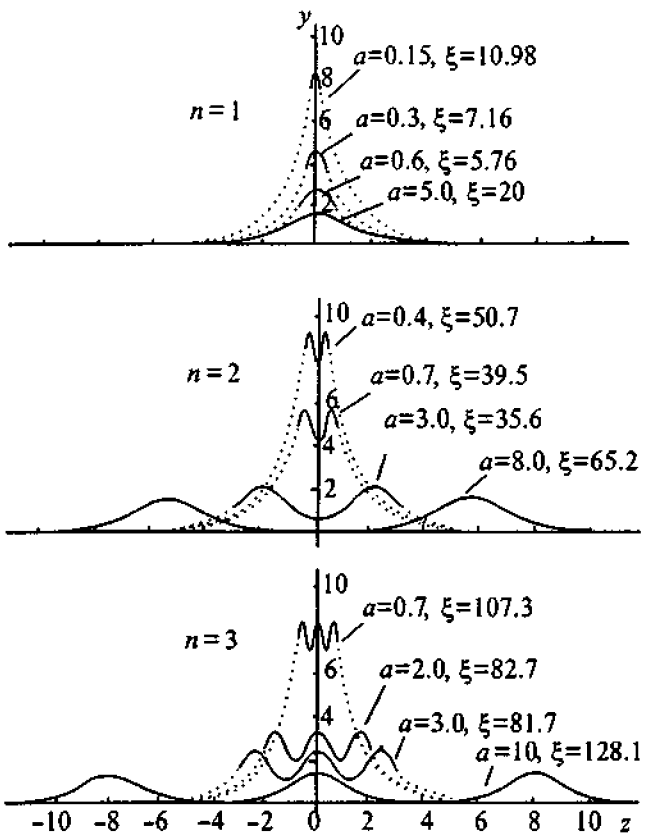

Fig. 1. Solutions of reduced problem (2.3); $\hat{\imath} = R/R_*$; $R_* = \dfrac{\mathfrak{E}\hbar^2}{\pi\mu e^2}$.

stronger magnetic field is necessary for them to be observated. On the other hand, the external states with $n = 2$ are more stable and more easily observable at finite temperatures. The main difficulty in observing the states with $n \geq 2$ is that they are possible only in clusters with $R > R_c$, and in this instance, bound states may occur in the absence of magnetic field as well [3-6].

In conclusion, let us note that the studied equations (1.1) are among the simplest nonlinear Schrödinger equations. We hope that the results obtained can be useful for solving other problems as well. At the same time, it should be emphasized once again that the physical pattern described follows from the analysis of equations (1.1), which themselves are approximate. The question of how this pattern can change after the initial problem will have been solved exactly (see [1]) is the subject of our further investigations.

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