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BOUND ELECTRON STATES IN CLUSTERS OF INERT ATOMS IN A MAGNETIC FIELD

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ABSTRACT

An external magnetic field is shown to stabilize negatively charged clusters of inert atoms. In an external magnetic field the critical number of atoms in a cluster, necessary to bound an excess electron to a neutral cluster, is less than that in the absence of a field. General conditions for creation of electron bound states in a cluster in a magnetic field are considered.

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We witness an increased interest in the study of charged clusters of inert gases [1 – 3]. The critical number of atoms at which an electron can be trapped by a cluster were found in [2] for $(Ar)_n$, $(Kr)_n$, $(Xe)_n$, clusters. These charged clusters are difficult to observe near the critical size because the electron wave function is highly diffuse and the bound state energy is close to zero. The formation of deeper electron levels requires clusters with the number of atoms by an order of magnitude greater than their critical values.

In this work electron states are examined in the clusters of inert gases placed in a magnetic field. In the case of an external magnetic field the electron level becomes deeper, thus, the charged cluster is stabilized and the critical number of atoms in a cluster necessary to bound an electron is less than that without a magnetic field.

According to the simple continuum model [2], the potential energy of an electron in a cluster is defined by the relation

$$U = V_0 + \frac{1}{2}\cdot\frac{e^2}{R}\left(1-\frac{1}{\varepsilon_0}\right),\ r < R;\ U = 0,\ r > R, \tag{1}$$

where V_0, is the energy of the bottom of the band of a quasifree electron in continuum media with dielectric permittivity ε_0, and R is the cluster radius.

The condition at which a bound state is formed in a spherically-symmetric well is given by

$$|U| \geq \frac{\pi^2\hbar^2}{8mR^2}, \tag{2}$$

where m is the electron mass. According to (1) and (2) the critical size of a negatively charged Xe_n^-, cluster is about R_c = 6.7 Å. Using (1) authors of [2] obtain R_c = 10.8 Å. This great difference is due to the more rough inequality $U > \hbar^2/2mR^2$ used in [2] instead of exact inequality (2). The detailed calculation of R_c, which takes into account the electrostatic image-force potential introduced in the continuum cluster model yields $R_c \approx 5 \div 5.4$ Å. The electron-atom pseudopotential was used in [3] to calculate the binding energy of xenon cluster anions Xe_n^- by the diffusion Monte carlo method. In that paper R_c, was calculated as: $R_c \approx 5$ Å. So we can expect that even the simplest model potential (1) can give results close to those, obtained by more sophisticated models.

According to [3] a cluster may be approximated by a continuum model if the cluster is small enough, so that the associated electron state is very diffuse, extending to large radial distances from the cluster and therefore has small amplitude in the interatomic spaces. It was shown in [3] that in this case the continuum model, which ignores the detail of the electron-atom potential, agrees with the microscopic model.

Let us consider clusters for which $U(r < R) < 0$, but inequality (2) does not hold. Physically, this means that the potential well in the cluster is not sufficiently deep to form a bound state. According to [4] any potential well, including the small-depth one, being placed in an external magnetic field H leads, to the formation of a bound state with the energy

$$\varepsilon = -\frac{me^2H^2}{8\pi^2\hbar^4c^2}\left[\int U d\upsilon\right]^2. \tag{3}$$

The physical reason for the existence of a bound state in a magnetic field is the effectively one-dimensional character of the electron motion along magnetic lines. According to quantum mechanics, in one-dimension a particle has a bound state for arbitrary shallow well.

Magnetic field H in (3) is considered to be weak: $\rho_0 >> R$, where $\rho_0 = \sqrt{c\hbar / eH}$ is the magnetic length. Integration in (3) is performed over the whole volume and in the above case gives the following value of the electron energy ε

$$\varepsilon = -\frac{2}{9}\cdot\frac{mR^2}{\hbar^2}\left(\frac{R}{\rho_0}\right)^4\left[V_0 + \frac{1}{2}\cdot\frac{e^2}{R}\left(1-\frac{1}{\varepsilon_0}\right)\right]^2. \tag{4}$$

It follows from the condition $\rho_0 >> R$ that $|\varepsilon| << |U|$ that is the electron level lies at the top of a potential well (1). From (4), it follows that an electron in the external magnetic field forms a bound state for clusters with the radius larger than R_{c1}, where R_{c1} is deduced from the condition that the potential energy U has to be negative inside the cluster

$$R_{c1} = \frac{1}{2}\cdot\frac{e^2}{|V_0|}\left(1-\frac{1}{\varepsilon_0}\right). \tag{5}$$

The effective radius of the electron state r_z along the magnetic field can be evaluated from the relation $|\varepsilon| \cong \hbar^2 / 2mr_z^2$. It is evident from (3) that the characteristic size of the localized electron state r_z in a magnetic field is equal to

$$r_z \approx R\frac{\hbar^2}{mR^2\left|V_0+\frac{1}{2}\cdot\frac{e^2}{R}\left(1-\frac{1}{\varepsilon_0}\right)\right|}\left(\frac{\rho_0}{R}\right)^2. \tag{6}$$

and far exceeds the cluster size.

Notice, that the electron energy for $R < R_c$ is very small even in very strong magnetic fields. For example, for cluster $(Xe)_n$ the potential energy U may be calculated using $V_0 = -0.65$ eV, $\varepsilon_0 = 1.71$ [5, 6] (Table and (10) for ε_0 in [2]). According to (2) the critical value of cluster radius R, for which the bounding energy of electron equals zero is $R_c = 6.7$Å. By (1), this leads to $U(R=R_c) = -0.2$ eV. If the magnetic field intensity is $H = 5\times10^5$ Oe the bounding energy of an electron is, by (4), equal to $\varepsilon = -0.6\times10^{-4}$ eV. The corresponding magnetic length is equal to $\rho_0 = 3.5\times10^{-7}$ cm and the condition $\rho_0 >> R$ used in deriving (3) is fulfilled well.

The characteristic size of the state, calculated from (6) is equal to $r_z = 165$ Å.

It should be pointed out that for numerical calculations the value $V_0 = -0.65$ eV was used which was measured for liquid bulk *Xe*. This value can drastically change for solid bulk media. For example, for *Ar* $V_0 < 0$ for liquid media, and $V_0 > 0$ for solid media [5-7]. Thus, the results are valid for clusters in the liquid state and may be inappropriate for the solid state.

If $V_0 > 0$ the accuracy of continuum model (1) can be insufficient since the potential energy of electron-cluster attraction $\sim -\frac{1}{2}e^2\alpha f(r)/r^4 < 0$ is not taken into account when the electron is outside the cluster. This attractive potential arises due to electrostatic image-force interaction. It can be shown that the electron bound state can be formed in a cluster if

$$\int U d\upsilon < 0 . \tag{7}$$

To test this condition a detailed microscopic model is required which is beyond the scope of this paper. The consideration of the electrostatic image-force potential may also be of importance if $R < R_{c1}$. In this case the electron bound state can also be formed in a cluster as a result of the electrostatic image-force potential alone.

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