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FILLING OF ELECTRON SHELLS OF COMPRESSED ATOMS IN THE STATISTICAL MODEL

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A statistical analysis of the electrons of the atom makes it possible to show sufficiently simly that at high pressures the electrons with given quantum number l can first appear in elements whose atomic numbers are smaller than the atomic numbers of the periodic system.

In the simple Thomas-Fermi (TF) model, it is most convenient to solve the problem with the aid of the Lenz-Jensen variational method [1], since the existing solution of the TF equation for the compressed atom [2] does not make it possible to vary its radius continuously. On the other hand, in a model in which quantum corrections are taken into account [3], the general solution of the problem is possible only with the aid of a variational method. By virtue of the normalization condition for the compressed atom, the electron-density distribution function can be chosen only in the zeroth approximation.

In the TF model for a compressed atom we have

$$\rho = (Z\lambda^3/16\pi)[e^{-\Lambda}/\Lambda^3(1 - \gamma)] \tag{1}$$

where $\Lambda = (\lambda R)^{1/2}$, λ is a variational parameter determined from the condition that the total energy of the atomic numbers be minimal, $\gamma = (1 + \Lambda + \Lambda^2/2)e^{-\Lambda}$ is a correction term, and Z is the atomic number of the element.

Starting from the simplified Sommerfeld condition [4], we can show that for a compressed atom the first appearance of s-, p-, d-, and f-electrons will be determined by the formula

$$Z_l = 1.26(1 - \gamma)(l + \tfrac{1}{2})^3 \quad (2)$$

The factor $(1 - \gamma)$ in (2) will decrease with increasing pressure, and consequently, the atomic number Z of the element in which the electrons with given quantum number l first appear will also decrease. It is easy to determine the factor $(1 - \gamma)$, meaning also the parameter Λ.

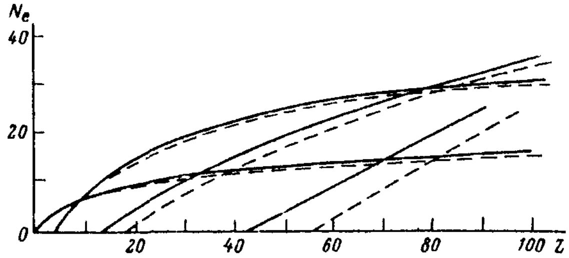
Following Fermi [5], we can show that formation of electronic groups in a compressed atom depends essentially on the pressure and is determined with the aid of the following relation

$$N_l = [2.13Z^{1/3}(l + \tfrac{1}{2})(1 - \gamma)^{-1/3}\int_{x_1}^{x_2}[e^{-2x/3}x^2 - \alpha]^{1/2}\frac{dx}{x} \quad (3)$$

where

$$\alpha = (16/3\pi Z)^{2/3}(1 - \gamma)(l + \tfrac{1}{2})^2$$

The results of the calculation for $\Lambda = \infty$ ($P = 0$) and $\Lambda = 4$ ($P = 2.37 \times 10^2 Z^{10/3}$ atm) are shown by the dashed and continuous lines in the Figure, respectively. It is seen from the figure that the number of the d- and f-electrons increases appreciably in atoms with increasing pressure, and g-electrons also appear; on the other hand, the number of s- and p-electrons increases very little. It follows also from the figure that the first appearance of electrons with a given quantum number shifts towards the elements whose atomic numbers are smaller than atomic numbers corresponding to the periodic table.



An analogous calculation was carried out for a compressed atom in the statistical model with account of quantum corrections [3] that have the same order of magnitude. In this model, the electron density function must be chosen in the form

$$\rho = [Z\lambda'^3/20\pi 14!][e^{-\Lambda'}/(1 - \gamma')], \quad \Lambda' = (\lambda' R)^{1/5}, \quad \gamma' = e^{-\Lambda'}\sum_{k=0}^{14}(\Lambda^k/k!) \quad (4)$$

For Z_l and N_l the following relations were obtained

$$Z_l = 1.38(1 - \gamma')(l + \tfrac{1}{2})^3 \quad (5)$$

$$N_l = [1.12Z^{1/3}(l + \tfrac{1}{2})10^{-3}(1 - \gamma)^{-1/3}\int_{x_1'}^{x_2'}[e^{-2x'/3}x'^{10} - \alpha']\frac{dx'}{x'} \quad (6)$$

$$\alpha' = [(10 \times 14!)/3\pi' Z]^{2/3}(1 - \gamma')^{2/3}(l + \tfrac{1}{2})^2$$

In the model with the corrections, the dependence of the energy of the atomic shell on the radius is such that one can speak of its finite dimensions in the absence of pressure. This makes it impossible to determine for several elements the pressure at which the electrons with a given quantum number first appear. On the other hand, the dependence of N_l on the pressure is the same as in the TF model.

Element	Atomic number	First appearance of electron number	Pressure, atm	
			TF model	Model with corrections
K	19	2	1.57×10^5	-
Ca	20	2	1.91×10^4	-
Sn	50	3	1.54×10^7	1.03×10^7
Te	52	3	6.32×10^6	2.08×10^6
Ba	56	3	1.57×10^5	3.17×10^3

The table lists for several elements the calculated pressures in the TF model and in the model with the quantum corrections.

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CONCERNING THE QUANTIZATION OF THE ENERGY LEVELS OF ELECTRONIC EXCITATIONS IN THE INTERMEDIATE STATE OF A SUPERCONDUCTOR

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The transition of a metal into an intermediate state is accompanied by a sharp decrease in the thermal conductivity of the electronic excitation [1], thus evidencing their reflection from the boundary between the normal and superconducting phases. It was shown in [2] that the excitations suffer a strict reversal of the motion upon reflection. As a result, motion of the excited normal phase sets in between its boundaries, leading to quantization of the energy levels with characteristic energy $\epsilon_0 = \hbar v/a$, where v is the velocity of the electrons on the Fermi surface and a is the dimension of the regions of the normal phase of the intermediate state [3].

Quantization of the energy levels should lead to a change in many characteristics of the normal phase, particularly to a decrease in the specific heat C in the temperature region $kT < kT_0 = \epsilon_0$. The present investigation was undertaken to ascertain the extent to which this decrease actually takes place.