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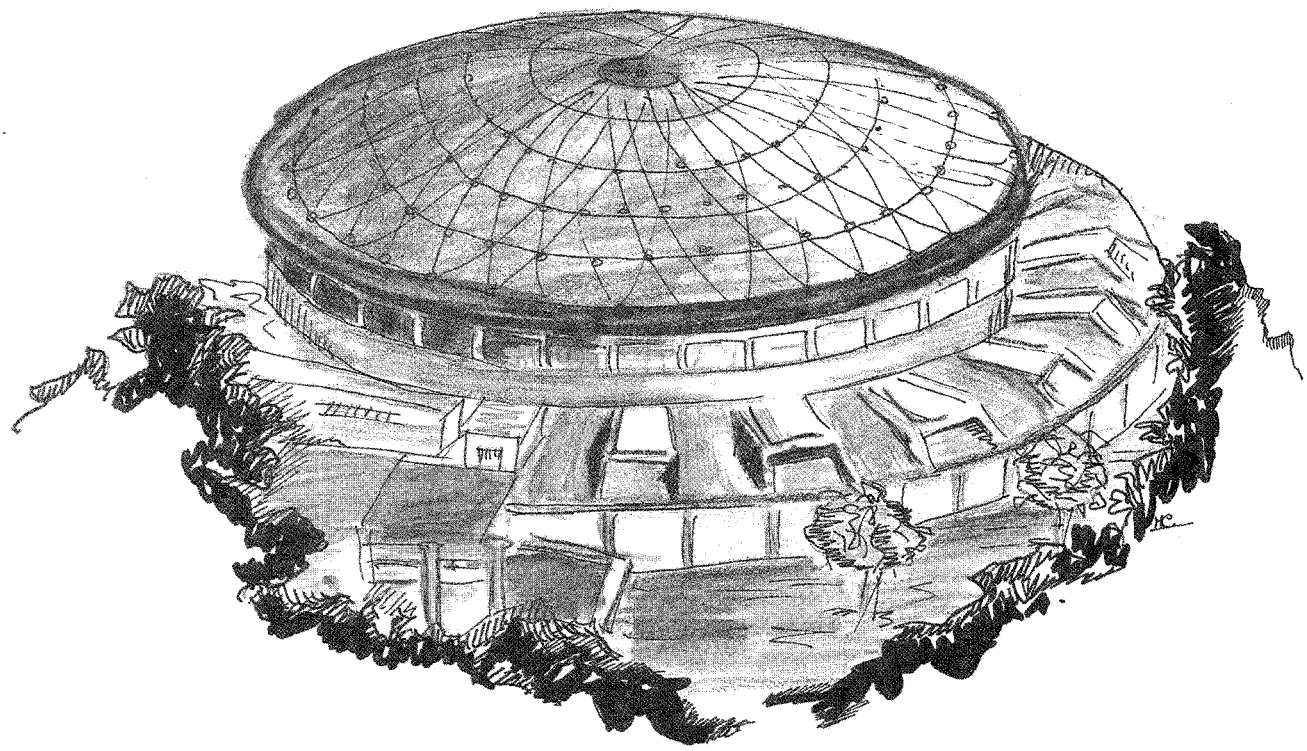

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EXCITATION AND IONIZATION IN LOW Z ATOMS BY SLOW MAGNETIC MONOPOLES

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ABSTRACT

We discuss the atomic excitation induced in atomic media by the passage of a slow monopole. We give a method for computing the Drell effect in low Z atoms that reproduces known results about the He case and gives new results for the Neon atom. An estimate of the velocity threshold for the process in Argon atom is also given.

ABSTRACT

Viene discussa la ionizzazione indotta in un mezzo atomico dal passaggio di un monopolo lento. Si presenta un metodo di calcolo per l'effeto Drell in atomi leggeri che riproduce risultati noti nel caso dell'atomo di He e ne fornisce di nuovi nel caso dell'atomo di Neon. Viene inoltre fornita una stima della minima velocita' del monopolo che puo' innescare tale processo in Argon.

1. - INTRODUCTION

In recent years there has been a renewed interest in the experimental search for magnetic monopoles. Also for the very first time an experiment will make it possible to explore the cosmic monopole flux well below the Parker limit[1] (the MACRO experiment at the Gran Sasso Laboratory [2]). This occasion has stimulated the investigation of those features of monopole interactions with matter that are specifically related to experimental detection, such as energy loss, ionization and excitation power.

In this paper we study the excitation induced in noble atoms by the passage of a slow ($\beta < 10^{-3}$) GUT monopole[3]. This investigation is of interest also from an experimental point of view, since the active media of several particle detectors are gases such as Helium or Argon.

The typical physical processes involved have atomic scales, so the much shorter GUT structure of the monopole can safely be neglected. Thus our calculation for a Dirac[4] massive monopole interacting in an atomic medium applies to any supermassive, singly-charged monopole.

This paper consists of five sections. In the second we give a picture of that part of the Drell effect (D.E.) theory that is of interest for our work and in the third we give the extension to the case of an atom with many electrons. The fourth section reports the applications to the already known He case and to the uninvestigated Neon case. In the fifth section we present an estimate for the impact velocity threshold for the D.E. in Argon.

2. - DRELL EFFECT

The study of the monopole energy loss has revealed a characteristic feature: cosmic monopoles are supposed to have impact velocities with the Earth in the range $10^{-3} < \beta < 10^{-4}$ and, in this range, the adiabatic principle strongly suppresses the usual atomic ionization mechanism. In other words, in order to have electronic transitions, the interaction time Δt and atomic excitation frequency ω must verify the relation $1/\Delta t >> \omega$, so that usual atomic transitions are forbidden between levels whose energies differ by more than $2 \cdot 10^3 \beta$ eV. On the other hand, the strong interaction between the magnetic field of the monopole and the electronic magnetic moments substantially shifts the atomic levels as the pole approaches the atom. If the closest approach distance is much less than a_0, an occupied state may become quasi degenerate with an excited level, allowing non adiabatic transitions. It follows that, in order to evaluate the excitation rate, it is important to study the system made up of an atom and a pole at very short distance on the atomic scale.

As the impact velocities lie in the range $10^{-4} < \beta < 10^{-3}$, the characteristic interaction time and the typical time scale of the proton motion are much longer than the electron orbital period. Thus a non relativistic quantum mechanical description for the electron can be used and the nuclear coordinate can be regarded as a classical parameter in the Schrodinger equation for the electron wave-function.

Drell and co-workers treated the case of a H atom closely interacting with a Dirac monopole[5]. When the impact parameter b is much less than a_0 they approximated the Hamiltonian of the system with the Hamiltonian of an H atom with a pole on top of it plus a dipole perturbation term that depends linearly on the proton-monopole distance.

In the Hydrogen case the Schrodinger equation for the Hamiltonian without the perturbation term is separable and has analytic solution. Eigenfunctions and eigenvalues[5,6,7] are labeled by four quantum numbers: n,|J|,J_z and Q, where **J** is the total electron angular momentum, n is the

radial quantum number and Q = 0,1 is a new quantum number related to the spin-magnetic field coupling, whose introduction removes the usual atomic spin degeneracy.

The total electron angular momentum is:

$$\mathbf{J}^{tot} = \mathbf{r} \times (\mathbf{p} - e\mathbf{A}) + 1/2\,\mathbf{s} - (eq)\,\mathbf{n} = \mathbf{J}^{el} - (eq)\,\mathbf{n} \qquad (2.1)$$

where **r** is the electron coordinate relative to the proton fixed at the origin , **n** is the unit vector from the monopole to the electron, q and e are the magnetic and electric charge. The term **r** x (**p** - e**A**) represents the orbital angular momentum **L** and the term - (eq) **n** is the e.m. angular momentum (associated with electron's electrostatic field crossed with the magnetic field of the pole).

Only the angular momentum multiplets [n,J,Q], where non adiabatic transitions can occurr, are relevant for D.E. For example, in the Hydrogen case the multiplet of interest is [0,1,0].

The transition amplitudes are computed in the following way. Consider an electron with the pole on top of the nucleus to be described by a generic eigenfunction $\Psi^{n,Q}_{J,m}$ of H_0 . Owing to the presence of V_{dip} in the Hamiltonian the same electron is described, during the interaction, by a time varying linear combination of the unperturbated wave functions of all the magnetic substates in the multiplet:

$$\Psi(t) = \Sigma_m A_m(t)\,\Psi_m \qquad m = -J\,,\,-J+1\,,\ldots,\,J-1\,,\,J \qquad (2.2)$$

The origin of the time axis coincides with the moment of closest approach. The initial conditions (no interaction yet) are $A_{m'}(-\infty) = 1$; $A_{m\neq m'}(-\infty) = 0$. Since the different substates of the multiplet connect different atomic levels as the interaction is switched off, the transition rate to the atomic level linked to the $t = 0, J_z = m$ level is given by $|A_m(+\infty)|^2$. These mixing coefficients can be computed in the framework of time-dependent, degenerate perturbation theory[5,8].

Moreover, as the atom gets closer to the monopole, the shift of the levels stores part of the kinetic energy in the spin-magnetic field coupling, therefore raising the value of the binding energy of the atom. So a threshold impact velocity β_t follows from the energy conservation :

$$\frac{\beta_t}{\sqrt{2}} = \left(\frac{E_0 - E_\infty}{M_{atom}} \right)^{\frac{1}{2}} \qquad (2.3)$$

The results of Drell et al. for H atom were[5] $\beta_t = 9.310^{-5}$

$$\sigma = 37\,\beta_4 \left(1 - \frac{\beta_t^2}{\beta^2} \right)^{\frac{3}{2}} 10^{-18}\ cm^2 \qquad \text{where } \beta_4 \text{ stands for } 10^4\,\beta.$$

3. - MANY ELECTRON ATOMS

When we tackle the problem of Z electron atom closely interacting with a monopole, we choose to study the interaction in the center of mass frame, because in this frame, during the interaction time, the origin coincides with the center of the monopole to a very good approximation.

We assume that the atom impinges upon the pole along the z axis with small but non zero impact parameter. From now on we will refer to the state with the atom very far from the pole and with the atom on the top of it, as the $z_n=\infty$ and $z_n=0$ state, respectively.

Our attempt to extend the basic D.E. theory runs into two main complications, namely the more complex procedure needed to connect the $z_n=0$ and the $z_n= \pm\infty$ electron levels, and the necessity of solving a many body problem in evaluating the wave function of the $z_n=0$ system.

In analogy with the H case we approximate the Hamiltonian with the one describing a Z electron atom with a pole on top of it, plus a perturbation term linearly dependent upon the nucleus-monopole distance:

$$H = \sum_i^{1,Z} \left(\frac{(\mathbf{p}_i - e\mathbf{A}_i)^2}{2m} - \frac{e}{2m}\sigma_i \mathbf{B}_i - \frac{Z\,e^2}{r_i} + \frac{1}{2}\sum_k^{1,Z} \frac{e^2}{r_{ik}} \right) + Ze^2 \sum_i^{1,Z} \frac{\mathbf{r}_i \mathbf{R}_{nucl}}{r_i^2}$$

$$\mathbf{B} = g\frac{\mathbf{r}}{r^3} \qquad \mathbf{A} = \frac{-g\,\mathbf{v}\wedge\mathbf{r}}{r(r - \mathbf{n}\mathbf{r})} \qquad \mathbf{R}_n = b\,\mathbf{x} + \beta t\,\mathbf{z} \qquad b \ll a_0 \tag{3.1}$$

where **x** and **z** are the unit vector along the x and z axis, **r** is the electron coordinate, **B** and **A** are the magnetic field and the vector potential induced by the pole, **v** is the unit vector that indicates the direction of the monopole string[4] and the σ are the Pauli matrices.

The choice of **v** orientation is arbitrary and is equivalent to fixing the e.m. gauge. Obviusly, this arbitrarieness does not affect our results, but for the sake of definiteness we have chosen to follow Wu and Yang[6] adopting the concept of "section" for the electron wave function. In particular we choose for our calculation the gauge in which the string lies along the positive z axis.

The problem we have to face when we increase the number of electrons in the $z_n=0$ system has the same features as that of the passage from Z=1 to Z>1 atoms in atomic physics. Actually, both in atomic physics and in our case, the single electron Hamiltonian has analytic solutions and the many electron Hamiltonian has the structure:

$$H = \sum_i^{1,Z} H_i + \frac{1}{2}\sum_i^{1,Z} \sum_{k\neq i}^{1,Z} \frac{e^2}{r_{ik}} \tag{3.2}$$

Therefore we adopt a method of solution very similar to the one used by Roothan[9] in atomic and molecular physics.

According to the exclusion principle the wave function is a Slater determinant made of Z single electron orbitals, each one defined by means of the expansion:

$$U_i(\xi_i, \theta_i, \phi_i, s_i^3) = S^{Q_i}_{J_i, m_i}(\theta_i, \phi_i, s_i^3) \sum_p^{1,N} C^i_p R^i_p(wr_i) \qquad (3.3)$$

The $S^Q_{J,m}$ are angular eigenfunctions of the single electron Hamiltonian, $R^i_p(wr)$ are an appropriate basis for the radial functions defined in the appendix and the constant w is a variational parameter that has the meaning of a scale length.

Appropriate angular eigenfunctions were chosen for each U_i in order to satisfy the total angular momentum conservation:

$$\sum_{i=1}^{Z} (J^{el}_i)_z \Big|_{zn=-\infty} - eg \sum_{i=1}^{Z} (n_i)_z \Big|_{zr=-\infty} = \sum_{i=1}^{Z} (J^{tot}_i)_z \Big|_{zn=0} \qquad (3.4)$$

A standard variational procedure was used to obtain the set of C^i_p that minimize the configuration energy and keep the U_i orthonormalized (see appendix).

In this way we obtained Z coupled matrix equations for the C^i_p :

$$M^i_{kp} \; C^i_p = E^i \; C^i_k \qquad\qquad i = 1,..,Z$$

$$M^i_{nk} = H^i_{nk} + e^2 \sum_{j \neq i}^{1,Z} \sum_{p,q}^{1,N} C^j_p C^j_q \sum_{l=0}^{lmax} \{ A^l_{ij} F^l_{ij}(n,k,p,q) - B^l_{ij} G^l_{ij}(n,p,k,q) \} \qquad (3.5)$$

where $lmax = 2\,|\,(J^z_i)_{max}\,|$ and the matrices H^i_{nk} , A^l_{ij} , $F^l_{ij}(n,k,p,q)$, B^l_{ij} , $G^l_{ij}(n,p,k,q)$ are defined in the appendix.

The solutions were obtained numerically with an iterative method[10]. It should be noticed that these equations are cubic in the C^i_k coefficients since each electron interacts both with the nuclear charge and with other electrons' charge densities, which in turn are proportional to $C^{j*}_p C^j_q$.

Electronic excitations can take place if in the z_n=0 configuration there are partially filled multiplets. In this case, in fact, the non adiabatic transitions can be induced by the perturbation term in the Hamiltonian. The related transition coefficients are computed by means of the system of equations[11]

$$i\frac{\partial A_m}{\partial t} = \gamma \beta_0 t\, m\, A_m +$$

$$+ \gamma \frac{b_0}{2} \left(A_{m+1} \sqrt{(J-m)(J+m+1)} + A_{m-1} \sqrt{(J+m)(J-m+1)} \right) \qquad (3.6)$$

where β_0 and b_0 are the velocity and the impact parameter at the distance of closest approach.

The factor

$$\gamma = \frac{Ze^2}{J(J+1)}\, eg \left\langle \frac{1}{r^2} \right\rangle \qquad (3.7)$$

scales roughly inversely with the cross section and takes into account the properties of the $z_n=0$ state of the electron. In particular the mean value $< 1/r2 >$ is taken over this "unperturbed" wave function.

The accuracy of the method depends crucially on the number of terms we use in the radial expansion, but, as it increases, the number of the F and G matrix elements grows with the fourth power of it. It follows that the computer memory capacity puts a severe constraint on the precision. Moreover the larger the electronic number is, the more problematic the situation gets, since the number of F and G matrix elements depends quadratically on the atomic number.

After the determination of the $z_n=0$ configuration the next step is to make the connections to the $z_n=\pm\infty$ levels. We developed this procedure for low Z atoms ($Z < 20$), for which we can assume that the $(J^{tot}_i)_z$ is a good quantum number and connect the $z_n=0$ and the $z_n=\pm\infty$ levels with the same value of $(J^{tot}_i)_z$.

However this rule is not yet sufficient to thoroughly define the connections between all levels. We need two more prescriptions. First we assume with Kroll[11] that the levels with the same $(J^{tot}_i)_z$ do not cross, then we consider the case of two degenerate atomic levels wich have the same $(J^{tot}_i)_z$ .We establish which one of the two levels has lower energy in the $z_n = 0$ system by considering that for $| z_n | >> a_0$ the generic single electron Hamiltonian can be approximated

$$H_i (z_n >> a_0) \approx H_i (z_n = -\infty) + V_{pert}$$

$$V_{pert} = \pm \frac{eg}{2m(z_n)^2} \left\{ (J^{tot}_i)_z + 1/2(s_i)_z \right\} - \frac{eg}{4m(z_n)^2} \qquad (3.8)$$

The upper sign refers to the nucleus on the negative z axis and the lower to the nucleus on the positive z axis.

It follows that the spin up levels are lowered in comparison to the spin down ones as the atom approaches the pole and vice versa when the atom moves away from the pole. In this way we are able to define completely the level connections.

Finally it must be noted that in many electrons atoms (like Ne or A) "off- center" crossings may be present. An "off-center" crossing occurrs when two energy levels with different $(J^{tot}_i)_z$ cross for a value of z_n different from 0. It can be shown[10] that these crossings induce level transitions only if the z component of the total angular momentum of the two levels satisfies the condition : $\Delta(J^{tot}_i)_z = \pm 1$. The actual evaluation of the effectiveness of these crossings as a possible source of excitation would require the knowledge of the $z_n \neq 0$ wave functions. However in this work we will not take into account these transitions and as a consequence our results are to be considered as lower bounds for cross sections and energy loss (unless otherwise stated).

4. - APPLICATIONS

In order to test the accuracy of this method we applied it to a case that was already studied in literature[11], the D.E. in the Helium atom.

The calculation of the excitation cross section follows the same steps of the H case and gives:

$$\sigma(\beta_4) = 3.8\ 10^{-14}\ \beta \left(1 - \frac{\beta_t^2}{\beta^2} \right)^{\frac{3}{2}} \text{cm}^2 \qquad \beta_t = 9.3\ 10^{-5}$$

It must be noticed that, due to the lack of off-center crossings, these results are not to be considered as lower bounds and coincides, within the 10% level, with the result quoted by Kroll et al[11].

The second application we made consisted in computing the cross section and the energy loss due to D.E. in Neon atoms.

This system has a z component of the total angular momentum ($J^{tot})_z = 5$. We stress that a $(J^{tot})_z=5$ configuration is an highly excitated state of the $z_n=0$ system; in fact two electrons that in the ground state would be in the [1,1,0] and [0,1,1] shell are forced in the [0,2,0] multiplet in order to mantain the $(J^{tot})_z=5$ condition. It follows that D.E. transitions can take place not only in the outer partially filled [0,2,0] shell, but also in the inner [0,1,1] and [1,1,0] incomplete shells.

We report in Fig. 1 and in Fig. 2 the connections and the quantum numbers of the levels that are occupied in the lowest energy, $(J^{tot})_z=5$ configuration.

In the derivation of the $z_n= 0$ wave function we used an 8-term expansion for each radial orbital in the Slater determinant. The minimum energy was obtained for the value of the variational parameter w=3 and this value indicates that, on the average, the electronic charge densities are much more confined near the nucleus than in the H or He case.

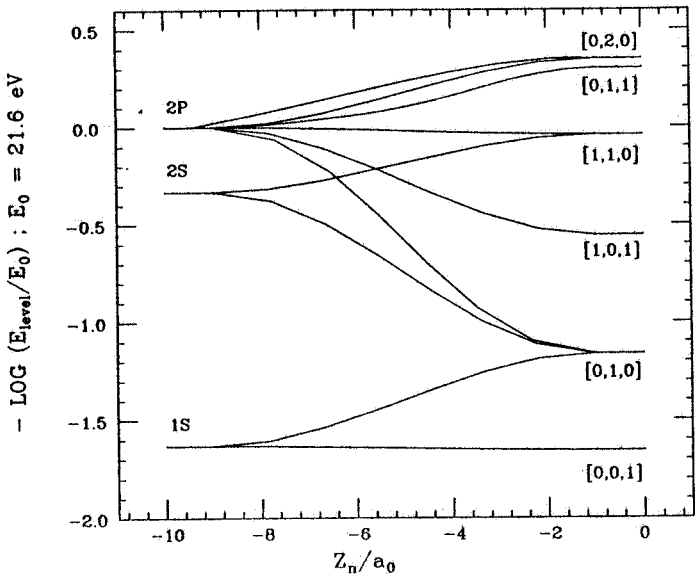

FIG. 1 - Level connections at $t < 0$.

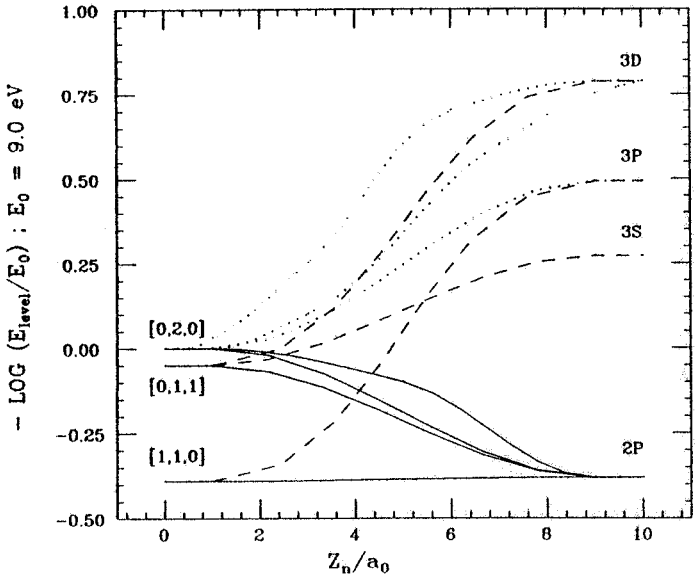

FIG. 2 - Level connections at $t>0$ dashed and dotted lines indicate links to atomic excited levels.

The results are:

multiplet [n,J,Q]	$E_{ionization}$ (Hartree)	$<\frac{1}{r^2}>(a_0)^{-2}$
[0,0,1]	-33.4	$2.4\ 10^2$
[0,1,0]	10.7	$4.3\ 10^1$
[1,0,1]	-2.65	$1.0\ 10^1$
[1,1,0]	-0.81	2.1
[0,1,1]	-0.37	$8.0\ 10^{-1}$
[0,2,0]	-0.33	$7.5\ 10^{-1}$

$E_{Zn=0} = -118$ Hartree $\quad \beta_t = 1.8\ 10^{-4}$

In the Table above the values of the quantities $E_{ionization}$ and $<1/r2>$ for the outer incomplete shells are the mean values of the multiplet. The splitting of these values for the different substates is due to the angular asymmetry of the system ($J^{tot}\neq 0$) and the variations are at most 5% of the values shown (for the outer [0,2,0] level).

The excitation cross section for each incomplete multiplet resulted to be:

$$\sigma_{[1,1,0]} = 0.22\ K \qquad \sigma_{[0,1,1]} = 0.58\ K \qquad \sigma_{[0,2,0]} = 3.2\ K$$

$$K = 10^{-18}\ \beta_4 \left(1 - \frac{\beta_t^2}{\beta^2} \right)^{\frac{3}{2}} cm^2 \qquad \beta_4 = 10^4 \beta \tag{4.1}$$

It should be noticed that the cross sections are inversely proportional to the mean value of the operator $< 1/r2 >$ over the multiplet so that, the wider is the charge density spread, the easier it is for the electrons to get excited.

We obtain the following energy loss per unit density:

$$\frac{1}{\rho}\frac{dE}{dx} = 2.3\ \beta_4 \left(1 - \frac{\beta_t^2}{\beta^2} \right)^{\frac{3}{2}} MeV\frac{cm^2}{g} \tag{4.2}$$

We point out that out of the several off-center crossings that occurr for $z_n>0$ only one can contribute to the atomic excitation. Indeed the only crossing between an occupied level and an excited one that satisfies the $\Delta J_z = \pm 1$ requirement is the one between the [0,2,0],J_z=-1 and the [0,1,1],J_z=0 levels. Our neglect of this possible source of transitions implies that our results are lower bounds.

Let us consider an application of these results to detection of a slowly moving monopole. We consider the typical 3x3 cm^2 streamer tube[2,12,13] detector of the dedicated MACRO experiment. We assume a mean track length of 5 cm and a gas mixture of 20% of Neon and 80% of quencher gas inert to D.E.

One condition must be fulfilled to have ionization via Penning Effect[14]: the Neon atom must be excited to a metastable level with higher energy than the ionization threshold of the quencher. Since even the first excitated level of Neon is higher than the ionization threshold of any commonly used quenching gas, to get the metastable cross section it is enough to consider all those transitions that force the electron to change the third component of the spin, so at $z_n=+\infty$ the total spin results to be $(S^{tot})_z = \pm 1$.

The cross section for excitation at metastable levels is :

$$\sigma_{metastable} = 1.8\ K \tag{4.3}$$

If we take into account that for a wide range of quencher percentage the efficiency of the conversion in ionization is roughly equal to 80 %, we obtain the plot in fig.3 for the number of primary ionizations.

This result confirms that it should be possible to use the neon gas as active medium in the mixture of the MACRO streamer tubes to detect slowly moving monopoles with impact velocity $\beta \geq 2 \cdot 10^{-4}$.

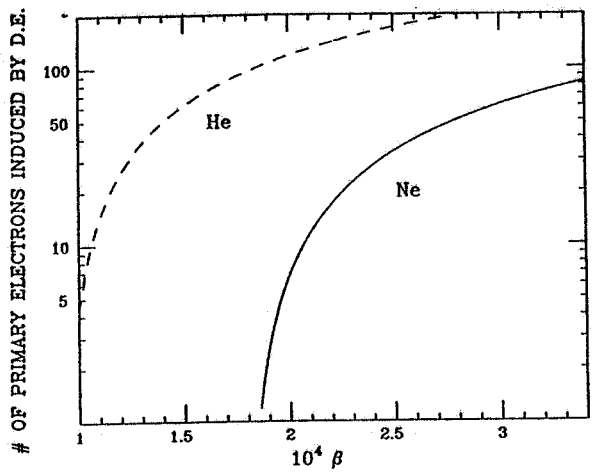

FIG. 3 - Number of primary electrons induced by Drell Effect with a Ne or He concentration of 20%.

5. - ARGON THRESHOLD

The excitation induced in Ar by the passage of a monopole is of major interest for the detection because this gas is mostly used as active medium in several ionization detectors.

Unfortunately our calculation method is ineffective to describe such a process because the configuration of the Argon $z_n=0$ system is a highly excited state; indeed the total angular momentum conservation states that for the z component :

$$(J^{tot})_z = \sum_{i=1}^{18} (J_i^{el} - eg\, n_i)_z = 18\, eg = 9 \qquad (5.1)$$

As a matter of fact such a high angular momentum forces the system to have a large number of holes in the inner shells so that we can no longer use the angular part of the $z_n=0$ Hydrogen eigenfunctions as angular part of the orbitals.

Nevertheless we can give an estimate of the monopole velocity threshold for the D.E. in Ar. We start from the consideration that the atomic binding energy is proportional to Z^2 if the atomic number is in the range $10 < Z < 20$; afterwards we compare the single electron Hamiltonian of a many electron atom with that of the same system with a pole in the center. As can be seen in the appendix, the expression of the eigenvalues and of the radial part of the eigenfunctions are very similar in the two cases. Furthermore, (3.1) indicates that the structure of the complete many body Hamiltonians is the same; so it is quite safe to assume that, in the $10 < Z < 20$ range, the binding energies of the two systems roughly have the same scaling property with respect to Z. Since the mass scales approximatively as the atomic number for $Z < 20$, we extrapolate a square root scaling for the D.E. threshold and a value for this quantity in Argon:

$$\beta_t^{Ar} \approx 2.4\ 10^{-4}$$

This value turns out to be quite satisfactory when compared to the impact velocity threshold of the most suitable active media for the monopole detection, that is the D.E. threshold in He ($\beta_t \approx 10^{-4}$) and the conventional energy loss threshold in scintillator[15] ($\beta_t \approx 5 \cdot 10^{-4}$).

I am deeply indebted to Prof. A.F.Grillo for many enlightening discussions and for his continuous interest and encouragement. I wish to thank Prof E.Iarocci for calling my attention to this problem and for many useful suggestions. I am also grateful to Prof. Y.Srivastava who kindly revised the manuscript.

APPENDIX

In this section we define the radial part of the single electron orbitals and the matrix elements involved in the variational calculation for the z_n=0 wave function.

The basis functions of the radial expansion are defined by:

$$R_p^i (w r_i) = \left(\frac{(2w)^{2L_i+3} (p!)}{\Gamma(2L_i + 3 + p)} \right)^{\frac{1}{2}} \exp(-w r_i) \; r^{L^i} \; L_p^{2L^i+2} \left(2 w r_i \right) \qquad \text{(A1)}$$

$$L^i = \sqrt{J_i (J_i + 1) + Q_i} - 1$$

The functions $L^a_b (x)$ are the generalizated Laguerre functions[16] and the Γ functions are the usual Euler gamma functions[17].

The mean energy of the configuration is given by:

$$H = \sum_{i=1}^{Z} < u_i | H_i | u_i > + \frac{e^2}{2} \sum_{i=1}^{Z} \sum_{j \neq i}^{1,Z} \left(< u_i , u_j | \frac{1}{r_{ij}} | u_i , u_j > - < u_i , u_j | \frac{1}{r_{ij}} | u_j , u_i > \right)$$

(A2)

The single hamiltonian matrix elements are defined by :

$$< u_i \mid H_i \mid u_i > \quad = \sum_{n,k}^{1,N} C_n^i C_k^i H_{nk}^i$$

$$H_{nk}^i = \int_0^\infty dr\ r^2\ R_n^i(r) \left\{ -\frac{1}{2}\frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{Z}{r} + \frac{L^i(L^i+1)}{2r^2} \right\} R_k^i(r) \qquad \text{(A3)}$$

We also need to evaluate the matrix elements of the Coulomb and exchange interactions. We have for the Coulomb part :

$$< u_i, u_j \mid \frac{1}{r_{ij}} \mid u_i, u_j > = \sum_{n,k,p,q}^{1,N} C_n^i C_k^i C_p^j C_q^j \sum_{l=0}^{lmax} A_{ij}^l\ F_{ij}^l\ (n,k,p,q) \qquad \text{(A4)}$$

the A^l_{ij} matrix take care of the angular properties of the orbitals while the F^l_{ij} are mostly related with the radial part of the U_i .The lmax in the summation is the biggest value of l which satisfies the triangular relation $| J_i - J_j | \le lmax \le | J_i + J_j |$ .The definition of the angular matrix is:

$$A_{ij}^l = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} \int d\Omega_i\ Y_l^m \mid S^{Q_i}_{J_i, m_i} \mid^2 \int d\Omega_j\ Y_l^{m*} \mid S^{Q_j}_{J_j, m_j} \mid^2 \qquad \text{(A5)}$$

The radial matrix can be written as:

$$F_{ij}^l\ (n,k,p,q) = N_n^i N_k^i N_p^j N_q^j \int_0^\infty dr\ r^{2L^i} \exp(-2wr)\ L_n^{2L^i+2}(2wr)\ L_k^{2L^i+2}(2wr) \quad x$$

$$x \left\{ r^{l+2} \int_r^\infty dy\ y^{2L^j+1-l} \exp(-2wy)\ L_p^{2L^j+2}(2wy)\ L_q^{2L^j+2}(2wy) \right. +$$

$$\left. + \quad r^{1-l} \int_0^r dy\ y^{l+2L^j+2} \exp(-2wy)\ L_p^{2L^j+2}(2wy)\ L_q^{2L^j+2}(2wy) \right\} \qquad \text{(A6)}$$

This integral can be solved analytically in terms of Hypergeometric Gauss functions[17].
In the same way we obtain for the exchange matrix elements:

$$< \psi_i, \psi_j | \frac{1}{r_{ij}} | \psi_j, \psi_i > = \sum_{n,k,p,q}^{1,N} C_n^i C_k^i C_p^j C_q^j \sum_{l=0}^{lmax} B^l_{ij} G^l_{ij} (n,p,k,q) \qquad (A7)$$

The angular part B^l_{ij} is given by:

$$B^l_{ij} = \frac{4\pi}{2l+1} \left| \sum_{m=-l}^{l} \int d\Omega_i \; Y^m_l \; S^{Q_i *}_{J_i, m_i} \; S^{Q_j}_{J_j, m_j} \right|^2 \qquad (A8)$$

and the radial part is defined by:

$$F^l_{ij} (n,k,p,q) = N^i_n N^i_k N^j_p N^j_q \int_0^\infty dr \; r^{L^i + L^j} \exp(-2wr) \; L_n^{2L^i+2}(2wr) \; L_p^{2L^j+2}(2wr) \quad x$$

$$x \left\{ r^{l+2} \int_r^\infty dy \; y^{L^j+L^i+1-l} \exp(-2wy) \; L_q^{2L^j+2}(2wy) \; L_k^{2L^i+2}(2wy) \; + \right.$$

$$\left. + \; r^{1-l} \int_0^r dy \; y^{l+L^j+L^i+2} \exp(-2wy) \; L_p^{2L^j+2}(2wy) \; L_k^{2L^i+2}(2wy) \right\} \qquad (A9)$$

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