MONOPOLE CHEMISTRY

Th.W. RUIJGROK, J.A. TJON
Instituut voor Theoretische Fysica, Utrecht, The Netherlands

and

Tai Tsun WU [1]
Deutsches Elektronen-Synchroton DESY, Hamburg, Germany

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Possible chemical binding of the magnetic monopole is discussed. The interaction of a monopole with a hydrogen atom is investigated in the Born–Oppenheimer approximation with the electron described by the Dirac equation. The effective potential between the monopole and the proton is determined together with the resulting bound states.

Over a half century ago Dirac [1] invented the magnetic monopole on theoretical grounds.

Recently the interest in this object has been intensified for two reasons: Cabrera's experimental observation [2] of a candidate for the monopole and Rubakov's theoretical analysis [3] of monopole catalysis of proton decay.

In order to have additional methods for detecting magnetic monopoles it is natural to investigate the possibility of binding such a monopole to an atomic nucleus or to a molecule. Thirty years ago a preliminary investigation was performed by Malkus [4] who suggested that chemical binding might be possible, but a definite conclusion was not reached. Because of the work of Yang and his collaborators [5]–[8], this possibility can now be studied in detail and the main objective of this letter is to present a quantitative investigation of the simplest monopole–atom system, namely the one consisting of one monopole, one proton and one electron. This molecule is of atomic size (~ 1 Å) and has atomic binding energy (~ 1 eV). We investigate the bound states of this system by using the Born–Oppenheimer approximation [9].

[1] On leave from Harvard University, Cambridge, MA, USA. Work supported in part by the US Department of Energy Contract No. DE-AS02-76ER03227.

Thus both the monopole and the proton are considered to be fixed with a distance R between them.

The Dirac equation for the four-component electron wave function can be written as $H\psi = E\psi$, where the hamiltonian has the form

$$H = \boldsymbol{\alpha}\cdot(-\mathrm{i}\,\boldsymbol{\nabla} - eA) + \beta m - \kappa q\beta(\boldsymbol{\sigma}\cdot\boldsymbol{r})/2mr^3 - e^2/|\boldsymbol{r} - \boldsymbol{R}|\,. \tag{1}$$

The number $q = eg$ has the Dirac-value $q = \frac{1}{2}$, while A is the vector potential for the magnetic field of the monopole. In eq. (1) m is the mass of the electron and $(e/2m)(1 + \kappa)$ its magnetic moment, where eventually $\kappa \to 0$ in accordance with the Kazama–Yang–Goldhaber prescription [7].

With the monopole at the origin and the proton on the positive z-axis, we restrict ourselves to the states with $m_z = 0$, so that the electron wave function is of the form {see eqs. (5) and (6) of ref. [8]}

$$\psi = \frac{1}{r}\begin{pmatrix} v_1(r)\eta_{00} \\ -\mathrm{i}v_2(r)\eta_{00} \end{pmatrix} + \frac{1}{r}\sum_{j=1}^{\infty}\begin{pmatrix} v_{4j-1}(r)\xi_{j0}^{(1)} + v_{4j+1}(r)\xi_{j0}^{(2)} \\ -\mathrm{i}s\,[v_{4j}(r)\,\xi_{j0}^{(1)} + v_{4j+2}(r)\,\xi_{j0}^{(2)}] \end{pmatrix}, \tag{2}$$

in which $s = \mathrm{sign}\,(\kappa)$. By substituting this form of the wave function into the eigenvalue equation $H\psi = E\psi$

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and using lemmas 1 and 2 of ref. [7], the final equations for the radial functions $v_n(r)$ ($n = 1, 2, ...$) become

$$\begin{aligned}
dv_1/dr &= (m+E+V_0)v_2 \\
&\quad + s\sum_{j'=1}^{\infty}(V_{0j'}^{01}v_{4j'} + V_{0j'}^{02}v_{4j'+2}) , \qquad (3)\\
dv_2/dr &= (m-E-V_0)v_1 \\
&\quad - \sum_{j'=1}^{\infty}(V_{0j'}^{01}v_{4j'-1} + V_{0j'}^{02}v_{4j'+1}) ,
\end{aligned}$$

$$\begin{aligned}
(d/dr - \mu_j/r)v_{4j-1} &= -V_{j0}^{20}v_2 - (m+E)sv_{4j+2} \\
&\quad - s\sum_{j'=1}^{\infty}(V_{jj'}^{21}v_{4j'} + V_{jj'}^{22}v_{4j'+2}) ,\\
s(d/dr - \mu_j/r)v_{4j} &= V_{j0}^{20}v_1 - (m-E)v_{4j+1} \\
&\quad + \sum_{j'=1}^{\infty}(V_{jj'}^{21}v_{4j'-1} + V_{jj'}^{22}v_{4j'+1}) ,\\
(d/dr + \mu_j/r)v_{4j+1} &= -V_{j0}^{10}v_2 - (m+E)sv_{4j} \\
&\quad - s\sum_{j'=1}^{\infty}(V_{jj'}^{11}v_{4j'} + V_{jj'}^{12}v_{4j'+2}) , \qquad (4)\\
s(d/dr + \mu_j/r)v_{4j+2} &= V_{j0}^{10}v_1 - (m-E)v_{4j-1} \\
&\quad + \sum_{j'=1}^{\infty}(V_{jj'}^{11}v_{4j'-1} + V_{jj'}^{12}v_{4j'+1}) ,
\end{aligned}$$

$$j = 1, 2, ... ,$$

with $\mu_j = [j(j+1)]^{1/2}$. The matrix elements of the Coulomb interaction are defined by:

$$V_0(r,R) = \int \eta_{00}^{*}\eta_{00}\frac{e^2}{|r-R|}\,d\Omega , \qquad (5)$$

$$V_{j0}^{\alpha 0}(r,R) = V_{0j}^{0\alpha}(r,R) = \int \xi_{j0}^{(\alpha)*}\eta_{00}\frac{e^2}{|r-R|}\,d\Omega , \qquad (6)$$

$$V_{jj'}^{\alpha\beta}(r,R) = \int \xi_{j0}^{(\alpha)*}\xi_{j'0}^{(\beta)}\frac{e^2}{|r-R|}\,d\Omega . \qquad (7)$$

By expanding $1/|r-R|$ in Legendre polynomials these integrals can be calculated explicitly.

In order to find bound states we must impose the usual boundary conditions on the functions $v_3, v_4, ...$,

$$\lim_{r\to 0} v_n(r) = \lim_{r\to\infty} v_n(r) = 0 \quad \text{for } n \geqslant 3 . \qquad (8)$$

Furthermore, in the limit of $\kappa \to 0$ the correct boundary conditions for v_1 and v_2 are given by [7]

$$\lim_{r\to 0} v_1(r)/v_2(r) = -s = -\kappa/|\kappa| . \qquad (9)$$

To solve numerically eqs. (3) and (4) with sufficient accuracy a variation of the Numerov method has been employed [10].

Consider the equation $\varphi' = A\varphi$, where $\varphi(r) = (\varphi_1, ..., \varphi_N)$ and $A(r)$ is a given $N \times N$ matrix. Let $w(r) = \varphi(r) - \frac{1}{2}h\varphi'(r)$, where h is the step length. The integration was then done by the repeated application of

$$w(r+h) = w(r) + hA(1+\tfrac{1}{2}hA)w(r) + O(h^3) , \qquad (10)$$

and using

$$w(r+h) = (1+\tfrac{1}{2}hA)\varphi(r) + O(h^3) \qquad (11)$$

for the first step. Experience shows that this is a stable integration procedure.

The numerical results for the effective potential in the sense of the Born–Oppenheimer approximation, both for positive and for negative κ ($s = +1$ and $s = -1$), are shown in fig. 1. Note that this effective potential is much less attractive than the rough estimate of Malkus [4]. For large proton–monopole separations the electron feels a field which is almost pa-

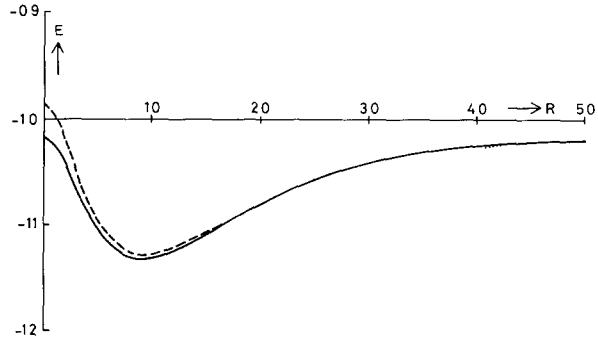

Fig. 1. Effective monopole–atom potential for κ negative (full line) and κ positive (dashed line). Also shown (dotted curve) is the result of eq (12). The energy unit is $e^2/2a_0 = 13.6$ eV. The distance is measured in units of a_0.

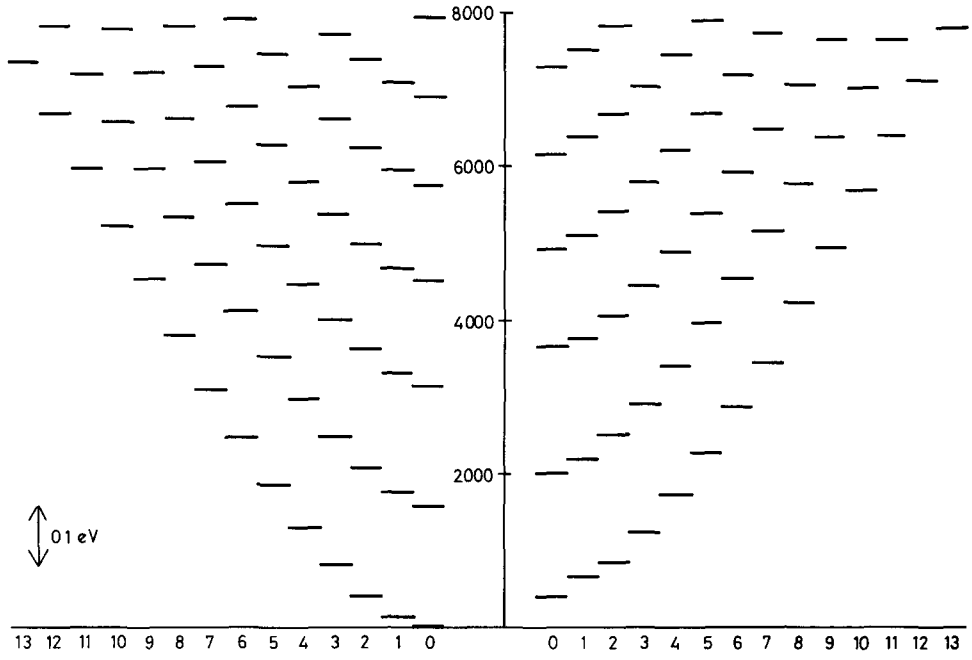

Fig. 2. Level scheme of monopole–atom bound states for κ negative (on the left) and κ positive (on the right). The energy units are in cm^{-1}. The values of the angular momentum are shown along the horizontal axis, which lies 1.646 eV below the energy of the free atom.

rallel to the z-axis. The paramagnetic and diamagnetic energy of the electron in the ground state of the H-atom is easily calculated and found to be

$$E_{pd} = -(e^2/2a_0)\,[1 \pm \tfrac{1}{2}(a_0/R)^2 - \tfrac{1}{8}(a_0/R)^4 + \ldots]\,, \quad (12)$$

where a_0 is the Bohr radius. The upper sign in $\pm$ applies when the magnetic moment of the electron is parallel to the field. For large R the energy calculated in this way is also shown in fig. 1 and smoothly joins the results of the numerical calculation.

With this effective potential, the Schrödinger equation for the proton wave function is solved numerically to give the lower lying energy levels as shown in fig. 2. It should be noted that since the potential has an $(a_0/R)^2$-tail it supports an infinite number of bound states [11].

In this part of the considerations the Schrödinger equation is used instead of the Dirac equation and the direct proton interaction with the magnetic field of the monopole is small and hence neglected.

We have shown here the existence of a number of bound states of a Dirac monopole and an hydrogen atom. This may be viewed as a modest initial investigation of monopole chemistry. If monopoles do exist in nature, their rarity will undoubtedly demand novel physical and chemical methods of experimental investigation. While systems consisting of a monopole with a Li, Na, K, Rb or Cs atom can be treated approximately by the method used here, other atomic and molecular systems would need generalizations of methods such as molecular orbitals [12].

A related problem is the lifetime of the bound states. While the decay of the higher levels in fig. 2 to the lower ones can be treated by usual perturbation methods, there is an interesting problem of the decay of the lowest level listed there to Kazama–Yang [8] type of states, if present. Such decays are expected to be rather slow, because of the small overlap of wave-functions, but an actual computation is highly desirable.

A further point to be investigated deals with capture cross sections. If monopoles are slow or are slowed down by, for example, the mechanism discussed recently by Drell et al. [13], then the capture cross

sections are expected to be rather large, i.e. roughly of the order of atomic capture cross sections.

Finally we mention that the boundary conditions of Kazama et al. [7] may not be the only possible ones. The dependence of the level structures on the additional parameters [14] may lead to insight into monopole chemistry and experimental determination of the parameters.

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