GENERALIZED BETHE-NEGELE INEQUALITIES FOR EXCITED STATES IN MUONIC ATOMS

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IPNO-TH-76-49
FR7700257

- November 1976 -

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Abstract :

Rigorous upper and lower bounds are derived for the Bethe logarithms in excited states of muonic atoms. Comparison with previous empirical estimates shows that the latter are inadequate in certain cases.

The Bethe logarithm $\ln k_0(n,\ell)$, which enters the lowest order expression of the Lamb shift, is defined by a sum over states belonging to the whole non-relativistic energy spectrum (discrete and continuous) of the atomic system. This sum is very difficult to calculate in muonic atoms with correct account of the extended nuclear charge distribution.

It has been suggested[1,2] that, at least in the case of heavy atoms, k_0 may be simply approximated by the binding energy B of the corresponding muonic state, with limits of uncertainty given by the empirical prescription $B/2 < k_0 < 2B$. However, for the ground state rigorous lower and upper bounds may be also readily obtained from sum rules, as shown by Bethe and Negele[3]. In this note we discuss an extension of their method to the case of excited states.

Since all the energies here are non-relativistic it is convenient to express them in units $Z^2 Ry_\mu$, where $Ry_\mu = \mu c^2 \alpha^2/2$ is the "muonic" Rydberg ($Ry_\mu = 2.81325$ keV). Next we introduce the sums-over-states

$$S_p(n,\ell) = \sum_{n'\ell'} f\,\omega^p \quad , \qquad (1)$$

where f is the oscillator strength for the transition $|n,\ell\rangle \to |n',\ell'\rangle$, and $\omega = E_{n'\ell'} - E_{n\ell}$ the corresponding change in energy (the selection rules restrict, of course, the summation over ℓ' to $\ell' = \ell \pm 1$).

For a given muonic state $|n,\ell\rangle$ one has, by definition,

$$\ln k_0(n,\ell) = S(n,\ell)/S_2(n,\ell) \quad , \qquad (2)$$

where

$$S(n,\ell) = \sum_{n'\ell'} f\ \omega^2 \ell n|\omega| \qquad (3)$$

is the famous Bethe sum.

Many of the sums S_p may be calculated explicitly on starting from first principles (commutation relations and closure). In particular the following sum rules hold :

$$S_o(n,\ell) = 1 \quad , \qquad (4)$$

$$S_1(n,\ell) = 4\langle E-V\rangle_{n\ell}/3 \quad , \qquad (5)$$

$$S_2(n,\ell) = 2(\lambda\!\!\!^{-}_\mu\ /\alpha Z)^2\langle\nabla^2 V\rangle_{n\ell}/3 \ , \qquad (6)$$

$$S_3(n,\ell) = 4(\lambda\!\!\!^{-}_\mu\ /\alpha Z)^2\langle(\nabla V)^2\rangle_{n\ell}/3 \ , \qquad (7)$$

where V is the potential energy (also in units $Z^2 Ry_\mu$), and $\lambda\!\!\!^{-}_\mu = \hbar/\mu c$ is the reduced Compton wavelength of the muon.

The Bethe-Negele inequalities for the ground state read :

$$K_a < k_o(1,0) < K_b \quad , \qquad (8)$$

where

$$K_a = S_2(1,0)/S_1(1,0) \qquad (9)$$

and

$$K_b = S_3(1,0)/S_2(1,0) \quad . \qquad (10)$$

A simple proof[4] of Eq. (8) rests upon the following general property of convex functions : if $\varphi(x)$ is convex for $a < x < b$, then

$$\varphi(\Sigma\lambda_i x_i) \leq \Sigma \lambda_i \varphi(x_i) \qquad (11)$$

where x_i are arbitrary points in $[a,b]$ and λ_i positive numbers subject only to $\Sigma \lambda_i = 1$.[5)]

Since f and ω are positive quantities for all possible transitions from the ground state, all one has to do is to apply Eq. (11) to the convex function $\varphi = \ln(1/x)$ with $\lambda = f\omega^2/S_2(1,0)$, and either $x = \omega$ or $x = 1/\omega$.

In order to generalize this to an excited state $|n,\ell\rangle$ of the muon, we now split the sums $S_p = S_p(n,\ell)$ in two parts, say $S_p = S_p^+ + S_p^-$, corresponding respectively to transitions into higher states ($f > 0$), and to transitions into lower states ($f < 0$). Similarly we write $S = S^+ + S^-$ for the Bethe sum $S = S(n,\ell)$. Obviously the sums S_p^-, S^-, consist only of a few terms, and are therefore easily evaluated.

Applying again Eq. (11) one readily gets

$$K_a < k_c(n,\ell) < K_b \quad , \qquad (12)$$

where K_a and K_b are now given by

$$\ln K_a = (S_2^+ \ln K_a^+ + S^-)/S_2 \quad , \quad K_a^+ = S_2^+/S_1^+ \quad , \qquad (13)$$

and

$$\ln K_b = (S_2^+ \ln K_b^+ + S^-)/S_2 \quad , \quad K_b^+ = S_3^+/S_2^+ \quad . \qquad (14)$$

From here one clearly recovers Eqs. (8)-(10) for the ground state.

In order to apply these results to some specific cases we consider a spherically symmetric nuclear charge distribution of the form

$$\rho(r) = \rho_0 \, f_\beta(x) \quad , \qquad x = r/r_0 \quad , \qquad (15)$$

where r_o is a range parameter (defining the "radius" of the nucleus) β a collective name for other possible parameters, and ρ_o is obtained from the normalization condition

$$4\pi r_o^3 \rho_o \, I_\beta = Ze, \qquad I_\beta = \int_0^\infty dx \; x^2 f_\beta(x) \; . \tag{16}$$

The potential energy (in units $Z^2 Ry_\mu$) may be written as

$$V(r) = -\,(2/\gamma) U(x) \quad , \tag{17}$$

where $\gamma = \alpha Z r_o / \lambda_\mu$, and

$$U(x) = \left[(1/x) \int_0^x d\xi \; \xi^2 f_\beta(\xi) + \int_x^\infty d\xi \; \xi \, f_\beta(\xi) \right] / I_\beta \; . \tag{18}$$

The three sum rules in Eqs. (5)-(7) then become

$$S_1 = (4/3) \left[E_{n\ell} + (2/\gamma) \int_0^\infty dx \; x^2 U(x) R^2_{n\ell}(x) \right] , \tag{19}$$

$$S_2 = (4/3\gamma^3 I_\beta) \int_0^\infty dx \; x^2 \; f_\beta(x) \; R^2_{n\ell}(x) \quad , \tag{20}$$

$$S_3 = (16/3\gamma^4) \int_0^\infty dx \; x^2 \; U'^2(x) \; R^2_{n\ell}(x) \; , \tag{21}$$

where $R_{n\ell}(x)$ is the radial wave function of the muonic bound state $|n,\ell\rangle$, normalized according to

$$\int_0^\infty dx \; x^2 \; R^2_{n\ell}(x) = 1 \quad . \tag{22}$$

On the other hand, the oscillator strength for the transition $|n,\ell\rangle \rightarrow |n',\ell'\rangle$ has the expression

$$f = [\max(\ell,\ell')/3(2\ell+1)]\ \gamma^2\omega\ (R_{n\ell}^{n'\ell'})^2 \quad , \qquad (23)$$

where $\ell' = \ell \pm 1$, $\omega = E_{n'\ell'} - E_{n\ell}$, and

$$R_{n\ell}^{n'\ell'} = \int_0^\infty dx\ x^3 R_{n\ell}(x)\ R_{n'\ell'}(x) \qquad (24)$$

is the dipole radial integral.

The two-parameter Fermi-type charge distribution is widely used in both muonic X-ray and electron scattering data analysis. The Fermi shape is characterized by the density

$$f_\beta(x) = 1/[1 + e^{\beta(x-1)}] \quad , \qquad (25)$$

and one has

$$I_\beta = (1 + \pi^2/\beta^2)/3 + O(e^{-\beta}) \quad . \qquad (26)$$

The β parameter is related to r_o and to the skin-thickness t (defined as the 90-10 % fall-off distance) by $\beta = (4\ln 3)r_o/t$. We adopt here the values $r_o = 1.13\ A^{1/3}$ fm, $t/4\ \ln 3 = 0.5$ fm, which are often quite close to actual situations.

Non-relativistic binding energies for states 1s through 3d, calculated with the above charge distribution, are given in Table I for several representative muonic atoms , and numerical values of the bounds K_a and K_b computed from Eqs.(13), (14), are displayed in Table II.

It may be noticed that for all the states the bounds become looser when Z decreases. On the other hand, for a given atom the bounds are better for s-states than for p-states, but they worsen rapidly with increasing excitation energy.

In spite of this bad quality, it is apparent that in some cases the empirical bounds mentioned at the beginning are definitely wrong. For instance, twice the binding energy of states 2s and 3s (see Table I) is less than the lower bound K_a in ^{96}Mo and in ^{40}Ca. The same occurs for the 3s state in ^{120}Sn.

More generally, it may be seen that for the 2s and 3s states in all the atoms considered K_a represents an improved lower bound as compared to half their binding energy. This is true also for the 2p and 3p states in ^{238}U, ^{208}Pb, and ^{182}W.

Finally, all this only stresses with more acuity the necessity of an accurate evaluation of the Bethe logarithms in muonic atoms.

References

1) R.C. Barrett, S.J. Brodsky, G.W. Erickson and M.H. Goldhaber, Phys. Rev. 166 (1968) 1589.

2) R.C. Barrett, Phys. Lett. 28B (1968) 93

3) H.A. Bethe and J.W. Negele, Nucl. Phys. A117 (1968) 575

4) This proof is due to R.C. Barrett (private communication to J.W. Negele).
I am indebted to Dr. Negele for kindly informing me about it.

5) For a discussion of Eq. (11), known as Jensen's inequality, see, for instance, E.F. Beckenbach and R. Bellman, Inequalities, Springer-Verlag, Berlin (1965), Chapter 1.

Table captions

Table I Non-relativistic binding energies (in MeV) for a Fermi-type nuclear charge distribution with parameters $r_o = 1.13\ A^{1/3}$ fm, $t/4\ell n3 = 0.5$ fm.

Table II Upper and lower bounds (in MeV) for Bethe's average excitation energy $k_o(n,\ell)$. Missing entries were completely out of order.

Table I

	^{238}U	^{208}Pb	^{182}W	^{146}Nd	^{120}Sn	^{96}Mo	^{40}Ca
1s	12.121	10.450	9.126	6.766	5.136	3.904	1.057
2p	5.597	4.532	3.739	2.497	1.747	1.237	0.281
2s	4.195	3.480	2.941	2.059	1.498	1.098	0.273
3d	2.642	2.100	1.711	1.125	0.781	0.551	0.125
3p	2.527	2.036	1.674	1.113	0.777	0.550	0.125
3s	2.087	1.708	1.426	0.979	0.702	0.508	0.122
$Z^2 Ry_\mu$	23.811	18.916	15.405	10.128	7.033	4.963	1.125

Table II

	^{238}U	^{208}Pb	^{182}W	^{146}Nd	^{120}Sn	^{96}Mo	^{40}Ca
1s	10.49 8.30	10.44 7.91	10.45 7.58	10.19 6.70	9.95 5.91	9.82 5.20	8.43 2.36
2s	8.85 3.62	8.50 3.38	8.50 3.20	8.31 2.82	8.28 2.52	8.41 2.27	7.95 1.12
3s	8.45 2.09	8.11 1.99	7.99 1.91	7.86 1.73	7.93 1.59	8.16 1.46	7.99 0.79
2p	11.87 3.47	12.80 2.72	14.20 2.08	19.21 1.01	31.14 0.41	72.06 0.11	* *
3p	11.98 1.71	13.16 1.32	14.84 0.99	20.63 0.44	34.17 0.15	80.59 0.03	* *