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THEORY OF HYPERFINE ANOMALIES IN MUONIC ATOMS

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Abstract

Negative muon spin precession experiments by Yamazaki, et al. have found giant hyperfine anomalies in muonic atoms ranging from a few percent up to 36%. In order to understand their results, we present Breit interaction calculations based on atomic self-consistent unrestricted Dirac-Fock solutions which explicitly include all electrons and the negative muon. The Breit interaction results (including the relativistic correction for the bound muon g-factor), vary from near zero for μ^- O/N to -5% for μ^-Pd/Rh; this latter is much larger than the calculated muonic or nuclear Bohr-Weisskopf anomalies and much smaller than the 36% measured value. For μ^-Ni/Co we find a calculated range of results (depending on assumed electronic configurations) of -2.3 to -2.7% in excellent agreement with recent measurements of the Yamazaki group. This excellent agreement in μ^-Ni/Co provides strong support for the earlier suggestions that the discrepancy in the case of μ^-Pd/Rh is due to experimental factors.

I. INTRODUCTION

The development of negative-muon spin precession techniques for measurement of electron spin distributions in solids by Yamazaki and co-workers [1] has led to great interest in the negative muon as a sensitive probe of magnetic structure. It was immediately clear after the dramatic announcement of a very large hyperfine anomaly in μ^{-}Pd vs. Rh[1], that the development of a rigorous theoretical treatment was necessary to explain these new results. Such a theory would have to (a) treat in a fully self-consistent way all particles in the system, (b) treat the muon not as a point charge, but as a "heavy electron", with its own single particle wave function, (c) obtain highly accurate electron spin distributions, and (d) include all relativistic effects. Recognizing that although the measurements were in solids (negative muon spin precession in Pd and Knight shift measurements in Rh), the hyperfine anomaly was (to first approximation) an atomic-like effect, we set out to modify Dirac-Fock theory in order to include the muon self-consistently with the electrons. In particular, we turned to Unrestricted Dirac-Fock theory in order to treat electron spin induced effects correctly; i.e. to include core polarization, the "driving force" behind the anomaly. Our results [2,3] showed that the anomalies were quite large (several percent) as compared to electron-nuclear (Bohr-Weisskopf) hyperfine anomalies (fractions of a percent), but much smaller than experiments [1] had indicated.

In the following sections of this paper we review the Unrestricted Dirac-Fock theory for muonic atoms, and present new results of calculations of the hyperfine anomaly for transition metal systems.

II. Unrestricted Dirac-Fock Theory for Muonic Atoms

In Dirac-Fock theory for ordinary atoms, we write the Hamiltonian as:

$$H = \sum_j [\vec{\alpha}\cdot cp_j + \beta E_0 + V_n(r_j)] + \sum_{i<j} [\frac{1}{r_{ij}} + H_B(i,j)] \qquad (1)$$

The terms in the first summation are the kinetic and rest energies and the nuclear potential $V_n(r_j)$, which may be varied in form, depending on our choice of nuclear model. (We have performed calculations for various models, and have seen no dependence on this choice. The results we report here are for a constant-charge-density hard-sphere nucleus.)

The terms in the second summation include the Coulomb interaction between electrons, and the Breit interaction H_B. This latter is actually calculated not self-consistently, but as a perturbation. The energy eigenvalue equation (without H_B) $H_1\Psi = E\Psi$ is then solved self-consistently, for Ψ a Slater determinant of one-electron wave functions of the form

$$U_{n\kappa}^{m_j}(\vec{r}) = 1/r \begin{pmatrix} P_{n\kappa}^{m_j}(r)\, X_{\ell m_j}(\Theta,\phi) \\ i\, Q_{n\kappa}^{m_j}(r)\, X_{\bar{\ell} m_j}(\Theta,\phi) \end{pmatrix} \qquad (2)$$

Here n is the principal quantum number, κ the angular quantum number, and m_j the magnetic quantum number. Unlike the usual Restricted Dirac-Fock Theory, in which the large and small parts of the radial function, P and Q respectively, are independent of m_j, here we allow the radial terms to differ for different m_j. This leads to spin polarization of the core electrons [4] which gives the spin density which interacts with the probe (nucleus or muon).

The Dirac-Fock equations are a coupled set of integro-differential equations, and are solved by a self-consistent field procedure. Details of this procedure may be found in several references [5,6]. In order to include the muon we introduce a one-muon wavefunction $U^{m_j}_{n\kappa}(r_\mu)$ and add to the Hamiltonian of Eq. (1) the muonic terms:

$$H_\mu = \alpha\cdot c\vec{p}_\mu + \beta E_o(U) + V_n(r_\mu) + \sum_k \frac{1}{r_{\mu k}} \quad (3)$$

where the summation is over the k electrons. The muon is then treated self-consistently as a "heavy electron" with no exchange interactions with other electrons; viz., as a distinguishable particle.

Once the Dirac-Fock calculations for the muonic Z atom and the ordinary (Z-1) atom have been completed, it remains only to compare magnetic interactions to obtain the hyperfine anomaly. For the muonic atom, the magnetic interaction is given by the unretarded part of the Breit interaction between the muon which is in the 1s state, and the electrons. This takes the form

$$\iint P^\mu(r_1)\, Q^\mu(r_1)\, P^e_i(r_2)\, Q^e_i(r_2)\, \frac{r_<}{r_>^2}\, dr_1\, dr_2 \quad (4)$$

where $r_>$ and $r_<$ are respectively the greater and smaller of r_1 and r_2. The hyperfine interaction energy W, is a summation over electrons of these integrals. For the muonic atom, therefore, the muon acts as a probe of the electron spin distribution according to the Breit interaction. For the ordinary atom, the nucleus acts as the probe. The usual expression for ordinary atoms is the Bohr-Weisskopf approximation [7]:

$$W \alpha \sum_{\text{electrons}} s_z c_i \int_{\text{probe}} w(r)\, d^3r \int_r^\infty \frac{P^e_i(r)\, Q^e_i(r) dr}{r^2} \quad (5)$$

where $w(r)$ is the spin density of the probe, s_z is the spin and c_i is the weighting coefficient for the i^{th} electron. For the very compact nucleus, this approximation is adequate, and we use it for the ordinary atoms of charge (Z-1). For the rather diffuse muon, we found that the Bohr-Weisskopf approximation seriously underestimates the effect: thus, we use the full Breit interaction for the muonic atom of charge Z.

In the non-relativistic limit, the magnetic interaction reduces to

$$\int_{\text{probe}} w(r)\ [\rho_e(r)\uparrow - \rho_e(r)\downarrow]\ r^2 dr \qquad (6)$$

where the bracketed term is the density of spin-up (↑) electrons minus the density of spin-down (↓) electrons; namely, the core-polarization [8]. We must emphasize that this difference of densities in no way resembles either density separately.

The hyperfine anomaly is defined as

$$\frac{W\ (\mu^-(Z))\ -\ W(Z-1)}{W(Z-1)} \qquad (7)$$

The non-relativistic approximation (Eq. 6) helps provide a visual understanding of the size of the anomaly. This is shown in Figure 1. (Note that the electron spin density scale is given on the left hand side, and is compressed compared to the other densities; in fact, it would appear much flatter if the scale were expanded.) We see from the figure that the muon density is much more diffuse than the nuclear density; we might then expect an anomaly of some tens of percent. Somewhat surprisingly, however, this does not turn out to be the case. Figure 2 is a plot of the integrands of Eq. 6 for nucleus and muon. Although they are very different, the areas under the respective curves, representing the integrals themselves, differ by only a few percent. Thus, the anomaly is in fact expected to be of the order of a few percent.

Table I lists the results of various calculations of hyperfine interaction energies from which the anomaly is determined for $\mu^- Pd^+$ (Z = 45) vs. Rh (Z-1 = 44).

Table I. Hyperfine interaction energies (in MHz)

	Calculation	$\mu^- Pd^+$	Rh
1.	Breit interaction	388.11	——
2.	Bohr-Weisskopf	392.68	399.17
3.	"Point probe"	399.93	399.81

We compare the hyperfine interaction energies calculated by three independent methods: (1) The Breit interaction between the muon and the electrons, (2) the Bohr-Weisskopf effect, and (3) the "point probe", in which the magnetization density $w(\vec{r})$ of the probe (muon or Rh nucleus) is given by $w(\vec{r}) = \delta(\vec{r})$. The muonic hyperfine anomaly is the percent difference between the Breit interaction for $\mu^- Pd^+$ and the Bohr-Weisskopf approximation for Rh:

$$\frac{W(\mu^- Pd^+) - W(Rh)}{W(Rh)} = \frac{388.11 - 399.17}{399.17} .$$

This value is -2.8%. Note that if we use the Bohr-Weisskopf value for the muon we obtain an anomaly of -1.8%, about 1/3 too low. The two "point probe" results, in which the muon is treated as a point charge at the Pd nucleus, are extremely close, differing by 0.03%. This is a measure of the difference in core polarization between the electrons in $\mu^- Pd^+$ and in Rh, and, as we see, is very small.

Similar calculations on μ^-Ni^+ vs. Co lead to an anomaly of -1.3 to -1.7%. The variations in the values are due to different choices of electron configurations. These variations are clearly very small. Recent experimental results [9] give an anomaly of -2.7%, in excellent agreement with our results, if we include the -1% bound-muon g-factor correction included in the experimental analysis. This striking agreement between theory and experiment in this latest measurement indicates that the earlier disagreement for μ^-Pd vs. Rh may well be due to as yet not well-understood experimental factors in that highly sensitive experiment.

We conclude by reporting results of calculations of one additional quantity using our Dirac-Fock wavefunctions; namely $\langle r^{-3}\rangle$ values for the valence d electrons. Not only is this number important for obtaining relaxation times of the atom after absorption of the muon; it can also give an estimate of the core polarization due to orbital angular momentum rather than to spin alone. The m_j-UDF scheme includes both possibilities; thus, if $\langle r^{-3}\rangle$ differed significantly for μ^-Pd^+ vs. Rh or for μ^-Ni^+ vs. Co, this would mean that orbital core-polarization was important. In fact, this is not the case: $\langle r^{-3}\rangle$ for the 3d electrons in μ^-Ni^+ and Co is identical to five places; the same is true for the 4d electrons in μ^-Pd^+ and in Rh.

In the m_j-Unrestricted Dirac-Fock scheme, each electron has a different wavefunction; thus, there is a range of values for quantities such as $\langle r^{-3}\rangle$. For simplicity, we list in Table II the mean for the $d_{3/2}$ and the $d_{5/2}$ electrons in each case.

Table II. $\langle r^{-3} \rangle$ values in atomic units

	$\mu^{-}Pd^{+}$ and Rh (4d)	$\mu^{-}Ni^{+}$ and Co (3d)
$d_{3/2}$	5.8	4.9
$d_{5/2}$	5.4	4.7

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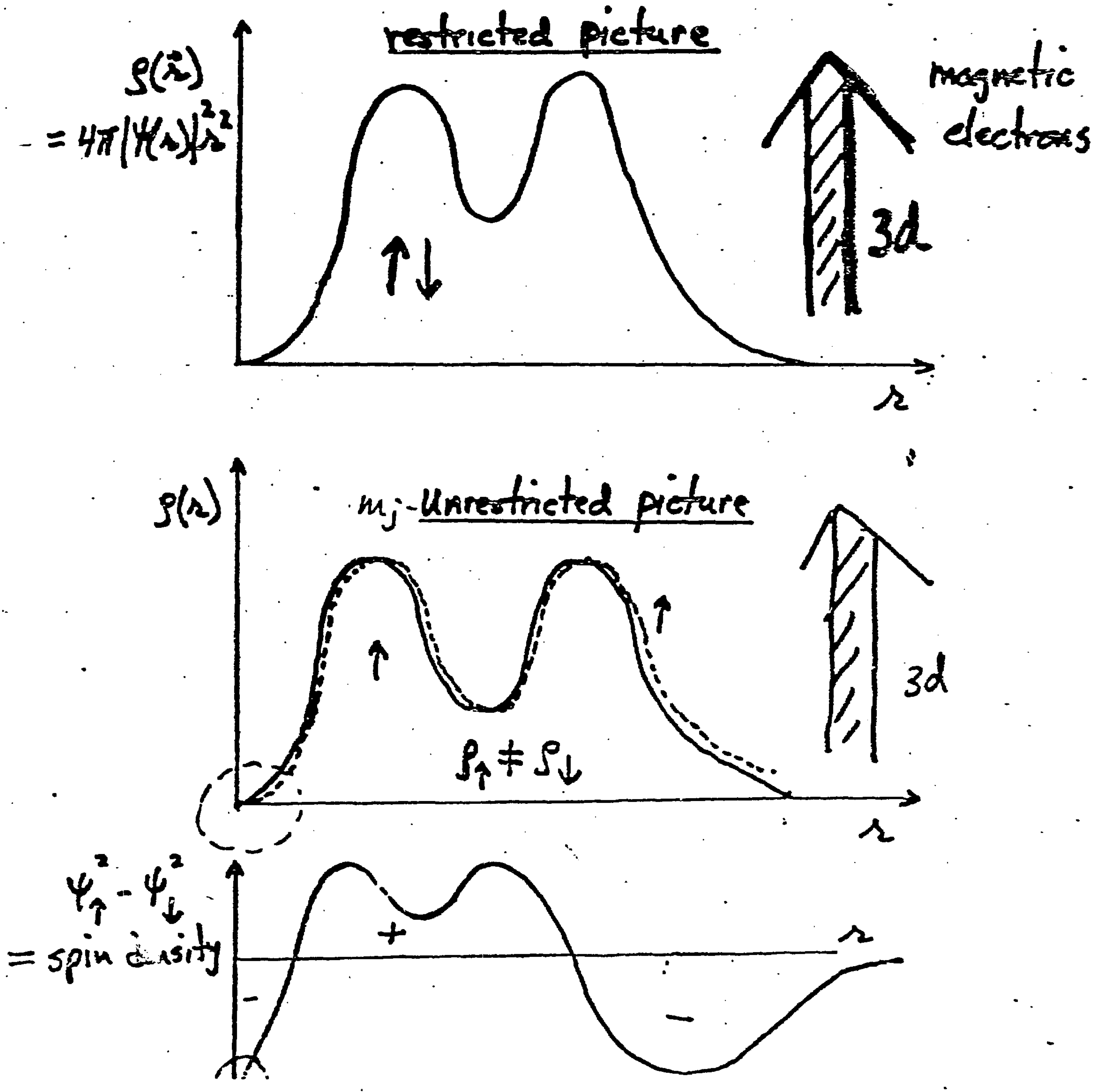
Figure 1

Hyperfine Interaction - core polarization

Dominant role of core polarization in transition metal systems



Rh/pd

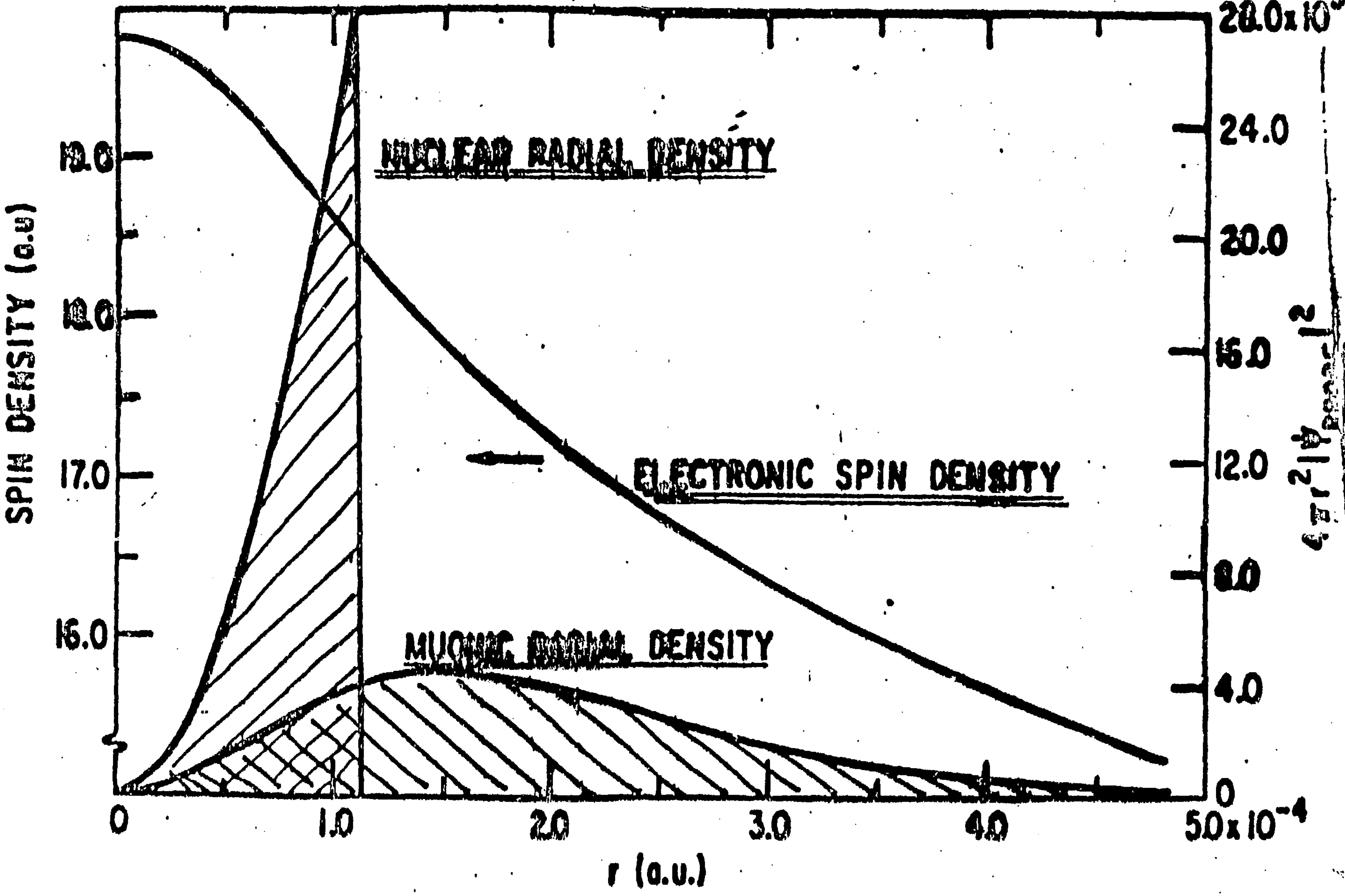


Figure 2
Muon, electron-spin and nuclear ~~radial charge~~ densities

Product of probe & electron densities