Lawrence Berkeley National Laboratory

LBL-11893 c.2
Preprint

Lawrence Berkeley Laboratory
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Submitted to Physics Letters

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May 1981

NUCLEAR SCIENCE DIVISION

Prepared for the U.S. Department of Energy under Contract W-7405-ENG-48

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LBL-11893

Calculation of Muon Final Probabilities After Muon-Induced Fission in Four-State Basis

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Abstract

Our earlier theoretical work on the relative muon capture between heavy and light fission fragments is extended by including $2p\sigma$ states as well as $1s\sigma$. We calculate about 0.8% population of the 2p state in the heavy fragment with negligible change from our earlier two-state basis regarding the 1s population of light and heavy fragments.

This work was supported by the Chinese Academy of Science and by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract W-7405-ENG-48.

I. Introduction

As a negative muon captured by a heavy atom cascades down to the 1s state through the atomic orbitals, it may excite the nucleus by inverse conversion, that is, by so-called radiationless excitation. The transition energies in actinides exceed the fission barrier height, so that prompt fission becomes possible.(1) The probabilities of this radiationless process have been investigated theoretically.(2) Since the mean lifetime of a negative muon in the 1s orbital is much longer than the mean lifetime of the coupled system of muon and fissioning nucleus, it is possible to follow the μ^- as a probe and to investigate the fission dynamics. Recently the mean lifetimes of muons bound to the fission fragments of actinide nuclei have been measured.(3) The measurements show that the muon is predominantly captured by the heavy fragment with less than ten percent probability that the muon is captured by the light fragment. In another report(4) the probability was reported as about 8%. The dynamics of the coupled system composed of muon and fissioning nucleus can give rise to the excitation of the muon. Thus, the comparison of the theoretical calculation with experiments may give some information about the fission dynamics.

Demkov *et al*(5) applied the Landau method of complex trajectories to update earlier work, and they obtained a result of 1% binding to the light fragment.

Recently some theoretical work addressed this problem by solving the time-dependent Schroedinger equation in the Coulomb field of two separate point charges(6) and extended charges(7) and obtained the relative probabilities of the muon binding to the light and heavy fragments.

These calculations[6,7] were made with two basis states, using linear combinations of the 1s atomic orbitals (LCAO) on the two fragments. In a recent study Maruhn, et al[8] have made large numerical integrations of the muon wave function in the Coulomb field of spherical uniformly charged fragments. They have expanded their wave functions to extract p-state as well as s-state probabilities.

II. Formulation of Four-State Basis Calculations

We have thought it worthwhile to expand the two-state basis to a four-state basis by including two $2p_z$ states. We have investigated the μ dynamics problem in the Coulomb field of two separate exponential charges by the same method as in ref. (7) The four eigenvalues of the stationary Schroedinger equation at each instant of time are obtained by the LCAO method, and the time-dependent Schroedinger equation is solved by the PSS method (perturbed stationary states).

Since the mass of the muon is much larger than the mass of an electron, it is not reasonable to treat the nucleus as a point charge. In order to get analytical expressions, we treat the nucleus as having an exponential charge distribution. The results show that this assumption is reasonable for this problem.

$$\rho = \rho_0 e^{-r/r_0} \tag{1}$$

The range constant r_0 of the charge distribution is chosen to match the root-mean-square charge distribution of the nucleus. The trial wave functions of muonic 1s and 2p states are chosen to have exponential form:

$$\phi_{1s} = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}$$

$$\phi_{2p} = \frac{1}{\sqrt{\pi b^5}} z e^{-r/b} \tag{2}$$

The constants a and b are fixed by the variational equations so as to minimize the orbital energies in the field of the isolated fission fragments.

$$\frac{\hbar^2}{me^2}\frac{1}{Zr_o} = \left(\frac{\xi}{\xi+2}\right)^4 (\xi + 8) \qquad (3a)$$

$$\frac{\hbar^2}{4mZe^2 r_o} = \zeta\left[\frac{1}{8} - \frac{2}{(\zeta+2)^4} - \frac{8}{(\zeta+2)^5} - \frac{20^{\ 2}}{(\zeta+2)^6}\right] \qquad (3b)$$

where $\xi = \frac{a}{r_o}$, $\zeta = \frac{b}{r_o}$. The variational energy levels are then

$$E_{1s} = \frac{\hbar^2}{2ma^2} - \frac{Ze^2}{(a+2r_o)^3}\left[a^2 + 6ar_o + 4r_o^2\right] \qquad (4a)$$

$$E_{2p} = \frac{\hbar^2}{2mb^2} - \frac{4Ze^2}{b}\left[\frac{1}{8} - \frac{2r_o^4}{(b+2r_o)^4} - \frac{4br_o^4}{(b+2r_o)^5}\right] \qquad (4b)$$

The comparison of variational energy levels in the Coulomb field of the exponential charge distribution and in that of the point charge with the exact solutions(9), where the Dirac equation with Woods-Saxon charge distribution is used, is given in Table I. It is noted that the Bohr formula point nucleus energies for the 1s state are far from the exact solution, but the point-charge approximation for the 2p state is rather good. It is evident that the variational energy levels with exponential charge distribution and exponential trial wave functions both for 1s and 2p are fairly good approximations. The constants a, b, r_o and variational energy levels for the fission fragments in our calculation are listed in Table II and compared with that of the point charge lower numbers).

We first solve the stationary problem of a muon in the Coulomb field of two centers by the LCAO method. We have chosen four nonorthogonal basis functions, i.e., the wave functions from eqs. (2) of 1s and 2p states for light and heavy fragments. The Hamiltonian matrix in this basis set can be obtained analytically. Then the generalized eigenvalue problem is solved numerically. The eigenvalue as a function of the separation distance R between the two charge centers for the most probable asymmetric case is shown in fig. 1. When $R \to \infty$, the four energy levels and wave functions correspond to the one-center asymmetric solutions for heavy and light fragments. The dashed line in the figure is for the case of two 1s basis states. The energy levels for the two cases almost overlap except for the region of R < 20 fm.

The time-dependent solution for the muon can be expressed by

$$\Psi = \sum_{\alpha=1}^{4} a_\alpha(t)\psi_\zeta \, e^{-\frac{i}{\hbar}\int^t E_\alpha dt'} \tag{5}$$

Substitution of (5) into the time-dependent Schroedinger equation gives the coupled equations,

$$a_\alpha(t) = -\sum_{\beta=1}^{4} a_\beta \left\langle \psi_\alpha \middle| \frac{\partial}{\partial t} \middle| \psi_\beta \right\rangle e^{-\frac{i}{\hbar}\int^t (E_\beta - E_\alpha) dt'} \qquad \alpha = 1,2,3,4 \tag{6}$$

The time differential can be expressed as $d/dt = \mathring{R} \frac{d}{dR}$, where $\mathring{R}$ is fragment separation speed. Let $Q_{\alpha\beta} = \left\langle \psi_\alpha \middle| \frac{d}{dR} \middle| \psi_\beta \right\rangle$; the transition matrix Q is an antisymmetric matrix. The $\left| a_\alpha^{(\infty)} \right|^2$ represent the final probabilities of the muon being in the 1s or 2p states of heavy or light fragments as $R \to \infty$. We have solved the coupled equations (eight, including real and imaginary parts)[6] numerically by the improved Euler method.[7] Nix has estimated,[10] based on the liquid drop model of fission, that the time for a fissioning nucleus to go from saddle point ($\sim$9.5 fm) to scission point ($\sim$23 fm) is about 3.7×10^{-21} sec. Hence, we assumed that the two parts of the fissioning nucleus move with uniform speed (3×10^{8} cm/sec) from saddle point to scission point and then are accelerated in a pure Coulomb field. Our starting point is chosen as 11 fm, at which point the muon is assumed lying entirely in the ground state. The two parts of the fissioning nucleus are accelerated in a pure Coulomb field from 18 fm. This distance was chosen in order to match the final kinetic energy to the experimental 170 MeV.

The results for the most probable asymmetric case are shown in fig. 2. The solid line represents the final occupation probability of the muon on the light fragment; the dash-dot line is for the case of the 2-state basis. The lowest line shows the probability of the muon lying in the 2p state of the heavy fragment. It shows that the final occupation probability of the muon on the light fragment is about 3.5% and the probability for the 2p state of the heavy fragment is about 0.8%. The population of the 2p level in the light fragment is negligibly small, and the dominant $1s_h$ population can be determined by difference.

The results show that the inclusion of the two 2p orbitals along with the 1s did not make much change for final 1s populations of fission fragments, compared with the case of two 1s states as basis.[7]

We should comment about the oscillation on the $2p_h$ probability of large separation distance. This oscillation is not physical and represents a small numerical instability in the calculations giving transitions between 1s and 2p states in the separated fragment. The reason is that some transition matrix elements in our model become constant when $R \to \infty$. For instance,

$$\lim_{R\to\infty} \langle\psi_2\left|\frac{d}{dR}\right|\psi_4\rangle = \langle\psi^H_{1s}\left|\frac{d}{dR}\right|\phi^H_{2p}\rangle = -\frac{8(a_H b_H)^{3/2}}{(a_H+b_H)^4}\frac{M_L}{M_L+M_H}$$

these terms cause transition oscillations between 1s and 2p states of each fragment. We think this is due to a spurious state of the motion of the center-of-mass. It is still an open question how to remove such spurious state. But we also notice that the amplitude of the oscillation in our case is very small and will not influence our main conclusions.

Our result of 0.8% for the heavy fragment 2p final state probability is a bit lower than that of Maruhn, et al.,[8] who found 1.7-2% probability. Given the many different assumptions and methods in our and their calculations the agreement seems satisfactory. The percentage of p state unfortunately seems so low as to make experimental detection unlikely.

This work was supported by the Chinese Academy of Science and by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract W-7405-ENG-48.

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TABLE I

Calculated Muonic Atom Binding Energies

nuclei	I		II		III	
	E_{1s}(Mev)	E_{2p}(MeV)	E_{1s}(MeV)	E_{2p}(MeV)	E_{1s}(MeV)	E_{2p}(MeV)
$^{68}_{30}Zn$	-2.223	-0.632	-2.531	-0.633	-2.219	-0.633
$^{80}_{34}Se$	-2.755	-0.812	-3.252	-0.813	-2.755	-0.814
$^{88}_{38}Sr$	-3.336	-1.013	-4.062	-1.015	-3.332	-1.017
$^{98}_{42}Mo$	-3.936	-1.235	-4.962	-1.241	-3.931	-1.242
$^{108}_{46}Pd$	-4.560	-1.479	-5.952	-1.488	-4.552	-1.490
$^{120}_{50}Sn$	-5.194	-1.742	-7.033	-1.758	-5.182	-1.759
$^{132}_{54}Xe$	-5.843	-2.026	-8.202	-2.051	-5.823	-2.048
$^{142}_{58}Ce$	-6.514	-2.328	-9.463	-2.366	-6.485	-2.359
$^{152}_{62}Sm$	-7.197	-2.648	-10.81	-2.703	-7.155	-2.689
$^{164}_{66}Dy$	-7.876	-2.985	-12.25	-3.063	-7.818	-3.037

I: exponential charge distribution, exponential wave function, variational method eqs. (4a) and (4b)

II: point charge non-relativistic Bohr formula

III: Fermi charge distribution, Dirac level energy[9]

TABLE II
Muonic Orbital Size Parameters and Energies used in Dynamic Calculation

	r_o(fm)	a(fm)	b(fm)	E_{1s}(MeV)	E_{2p}(MeV)
$^{84}_{34}Se$	1.18	9.24	15.1	2.75	0.812
	0	7.53	15.1	3.25	0.813
$^{98}_{40}Zr$	1.24	8.29	12.9	3.62	1.12
	0	6.40	12.8	4.50	1.13
$^{116.4}_{45}Rh$	1.31	7.75	11.5	4.36	1.42
	0	5.69	11.4	5.70	1.42
$^{121.6}_{47}Ag$	1.33	7.56	11.1	4.67	1.54
	0	5.45	10.9	6.21	1.55
$^{140}_{52}Te$	1.39	7.17	10.1	5.45	1.88
	0	4.92	9.84	7.61	1.90
$^{154}_{58}Ce$	1.44	6.75	9.12	6.45	2.33
	0	4.41	8.83	9.46	2.37

Definition of parameters: $\rho = \rho_o e^{-\frac{r}{r_o}}$ $\qquad$ $r_o \to \infty$: point charge

$$\phi_{1s} = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$$

$$\phi_{2p} = \frac{1}{\sqrt{\pi b^5}} z e^{-\frac{r}{b}}$$

Figure Captions

Fig. 1. Calculated four lowest energy ($1s\sigma h$, $1s\sigma \ell$, $2p\sigma h$, and $2p\sigma \ell$ in increasing order of energy) levels of the muon for most probable fission asymmetry. The dashed line shows the earlier result[7] for the two-state basis. An exponential nuclear charge distribution matchin g experimental r.m.s. charge radii was used.

Fig. 2. Calculated muon orbital occupation probabilities as a function of fission fragment separation energies. The upper curves refer to the 1s level of the light fragment, the solid curve being present results for the 4-state basis and the dash-dot line for the 2-state basis. The lowest (dashed) line is the probability for being in the state that correlates with the 2p level of the heavy fragment. The system shown is $^{98}Zr + ^{140}Te$.

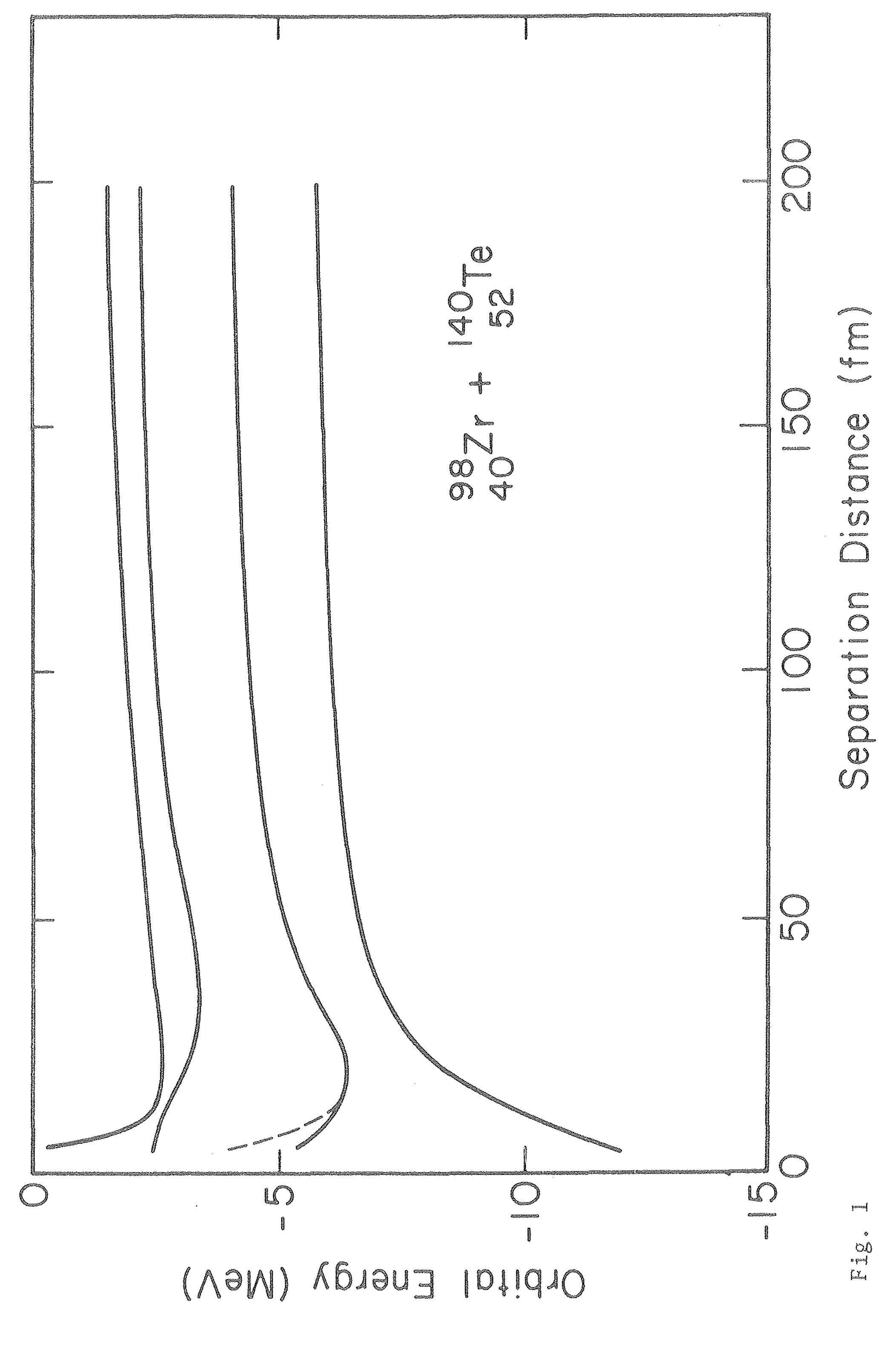

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Fig. 1

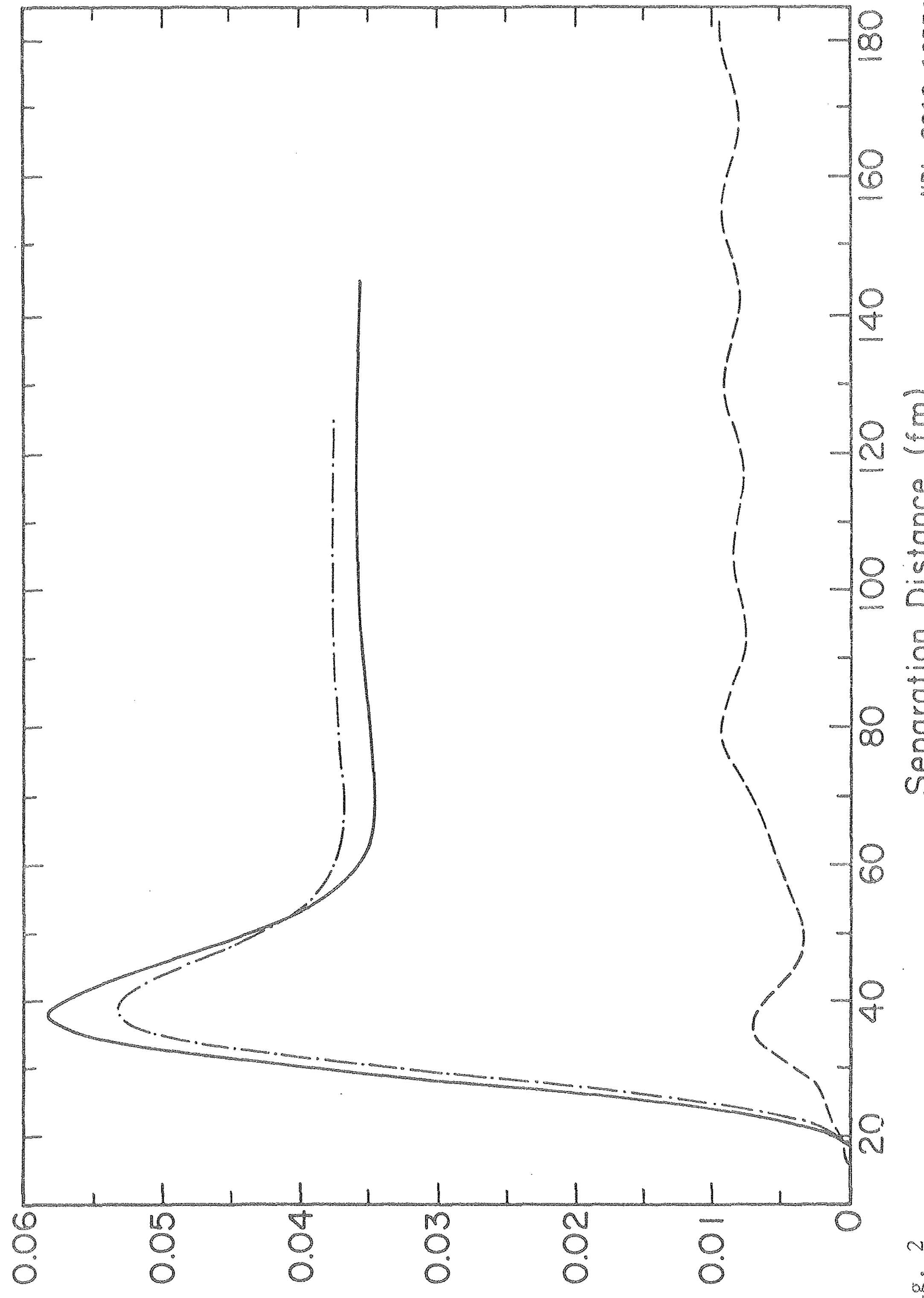

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Fig. 2