Normalized shell model alpha decay theory applied to unfavored decay

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A shell model α decay theory is presented which uses correctly antisymmetrized and normalized wave functions. Numerical calculations are performed for the α decay constants for unfavored decay of ^{211}Po and ^{211}Bi and for hindrance factors of excited ^{212}Po states. The results are compared with those of the conventional shell model α decay theory.

[NUCLEAR STRUCTURE α decay rate theory, ^{211}Bi, ^{211,212}Po. Calculations of rates by conventional and by revised shell model theory.]

I. INTRODUCTION

Shell model α decay theory has over the years enjoyed considerable success in calculations of relative transition probabilities. However, there has been some uncertainty as to whether the theory, even using the best configuration-mixed wave functions, could satisfactorily explain absolute rates.

In the usual theory a channel radius R_0 is chosen and the shell model wave function of the parent nucleus is projected on the product of the daughter nucleus and α-particle wave functions. The resulting projection amplitude $G(R_0)$ is regarded as the α wave function boundary condition for propagation outward through a barrier derived from Coulomb and nuclear optical model potentials.

The absolute rate agreement has remained uncertain largely because of the great sensitivity of the penetrability to the optical potential defining the barrier. Furthermore, to make α cluster projection practicable it has been necessary to use harmonic oscillator nucleon wave functions, and the Gaussian-like tails of such wave functions are known not to be a valid approximation in the tail region. In spite of these uncertainties it seems that simple shell model theory falls short by at least an order of magnitude on absolute rates.

It was only recently that a careful reexamination[1,2] focused on the problems connected with the antisymmetrization of the product wave function of the α particle and the daughter nucleus. This antisymmetrization was usually taken into account in the shell model theory of α decay.[3] It enforces the requirements of the Pauli principle, preventing double occupation of states. However, antisymmetrization between two composite particles leads to non-normalized states. The proper normalization may be hidden in the function of relative motion between the α particle and the daughter nucleus. We are not able to calculate this function (including the normalization) exactly; instead we introduce a distorted wave approximation for the wave function of relative motion, and then it is vital to take the proper normalization explicitly into account.

This normalization results[2] in a considerable enhancement of the reduced width for α decay. Reduced width means here $\delta^2 = \hbar/(P\tau)$, with τ the mean lifetime and P the barrier penetration factor.

Since the new theoretical absolute ground-to-ground state decay widths are strongly enhanced[2] over the previous version of the theory, we felt it important to check also on various cases of hindered α decay to see to what extent relative α transition rates would be affected by the normalization.

II. THEORY

Let us give a short review of the formalism. The conventional reduced width amplitude is given by

$$G(R) = \left\langle \mathcal{A} \frac{1}{R^2} \delta(R - R_\alpha) [\, y_l(\hat{R}_\alpha) \chi_\alpha \phi_A^j]^J \right| \phi_{A+4}^J \Big\rangle , \tag{2.1}$$

where χ_α is the internal α-particle wave function, ϕ_A^j and ϕ_{A+4}^J are shell model states for the daughter and parent nucleus, respectively. All states χ_α, φ_A^j, and ϕ_{A+4}^J are normalized and antisymmetrized. $\vec{R}_\alpha$ is the center-of-mass coordinate of the α particle. The spherical harmonic is denoted by $y_l(\hat{R}_\alpha)$. The square brackets in (2.1) denote the coupling of the α-particle angular momentum l and the daughter nucleus spin j to the total spin J. The antisymmetrization operator

is given by

$$\mathcal{A} = \left(\frac{A}{4}\right)^{1/2} \left(\frac{1}{(A+4)!} \sum_P (-)^P P\right), \tag{2.2}$$

where the sum runs over all $(A+4)!$ possible permutations P.

The normalization of the state $|\mathcal{A}(1/R^2)\delta(R-R_\alpha)[y_l(\hat{R}_\alpha)\chi_\alpha\phi_A^j]^J\rangle$ in (2.1) defines the operator $K_l(R,R')$

$$\frac{1}{R^2}\delta(R-R') - K_l(R,R') = \left\langle \mathcal{A}\frac{1}{R^2}\delta(R-R_\alpha)[y_l\chi_\alpha\phi_A^j]^J \,\middle|\, \mathcal{A}\frac{1}{R'^2}\delta(R'-R_\alpha)[y_l\chi_\alpha\phi_A^j]^J\right\rangle. \tag{2.3}$$

Since these states are not normalized to $(1/R^2)\delta(R-R')$ the function $G(R)$ is not a wave function and $|G(R)|^2$ cannot be interpreted as a probability density. In order to define such a probability density we introduce an operator $N(R,R')$ which normalizes these states to $(1/R^2)\delta(R-R')$ by

$$\int\int R_1^2 R_2^2 dR_1 dR_2 N(R,R_1)\left[\frac{1}{R_1^2}\delta(R_1-R_2) - K_l(R_1,R_2)\right]N(R_2,R') = \frac{1}{R^2}\delta(R-R'). \tag{2.4}$$

This means we introduce the inverse square root of the operator $1-\hat{K}_l$ as $N(R,R') = [(1-\hat{K}_l)^{-1/2}]_{R,R'}$.

The wave function of the α particle is then given by

$$G_N(R) = \int R'^2 dR' N(R,R')G(R'). \tag{2.5}$$

It is this wave function which enters instead of G into the calculation of the reduced width

$$\delta^2 = \frac{\hbar^2}{2M_\alpha}\frac{k(R_0)}{2}\left((R_0G_N)^2 + \frac{R_0^2}{k^2(R_0)}[G_N'(R_0)]^2\right). \tag{2.6}$$

The conventional theory used G in this formula. The details of the derivation of (2.6) may be found elsewhere.[1,2] For the evaluation we need an α-nucleus potential $V(R)$, first for $k(R_0)$ in (2.6)

$$\frac{\hbar^2}{2M_\alpha}k^2(R_0) = E_\alpha - V(R) \tag{2.7}$$

and, more importantly, for the penetrability P. The decay constant λ is then

$$\lambda = \delta^2(P/\hbar). \tag{2.8}$$

This result is still channel-radius dependent. We will also use the channel-radius-independent formulation

$$\lambda = \lambda_{s.p.} S \tag{2.9}$$

using a spectroscopic factor

$$S = \int R^2 dR[G_N(R)]^2 \tag{2.10}$$

and a single-particle decay constant[2] $\lambda_{s.p.}$, derived from a one-body Schrödinger equation.

Originally, these results were derived[1] in a reaction theory for one open channel and one bound state. In the following we will apply (2.8) and (2.9) in cases with different final states ϕ_A^j, which means with more than one open channel. This implies neglect of the coupling between these channels.

III. MODEL ASSUMPTIONS

A. Wave functions

For the application of the normalized shell model α decay theory to unfavored decays we have taken three dimensional harmonic oscillator wave functions with size parameter $\alpha = 0.17$ fm^{-2}. The corresponding size parameter β for the α cluster is taken as 0.47 fm^{-2}. For the odd mass nuclei the wave functions have been taken as purely the main shell model configuration with no configuration mixing. For these near-closed shell nuclei this approximation should be reasonable.

To check the effects of configuration mixing we did the calculation also for the two-proton configuration[4] $0.943(h_{9/2})^2_0 + 0.101(f_{7/2})^2_0 - 0.317(i_{13/2})$ for ^{211}Po, and for the two-neutron configurations[5] $0.935(g_{9/2})^2_0 + 0.325(i_{11/2})^2_0 + 0.141(d_{5/2})$ for ^{211}Bi. These configurations were actually calculated[4,5] for ^{210}Po and ^{210}Pb. For ^{212}Po ground and excited states we have taken the configuration-mixed wave function of Glendenning and Harada,[6] including all configurations with greater than 1% admixture.

B. Channel radius

The expressions (2.6) and (2.8) are still channel-radius dependent. In a previous work we showed that we have to take a channel radius at the nuclear surface where G_N (or G) usually has its outer maximum. Indeed we found a region 6 to 7 fm where the result (2.6) is approximately channel-radius independent.[2]

In (2.6) $k(R_0)$ is related to the velocity of an α particle in the potential $V(R)$. If the theory

leading to (2.6) is valid, we may as well derive this velocity from the curvature of the interior solution $G_N(R)$ [or $G(R)$ in the old theory]. At the surface this yields typically a value $k(R_0)\simeq 2$ fm^{-1}, corresponding to a kinetic energy of the α particle of about 20 MeV.

To simplify the calculation we used (2.6), unless otherwise stated, at a channel radius R_m at the position of the outer maximum of $|G_N|^2$ (or $|G|^2$). Then we have

$$\delta^2\simeq 5\ \text{MeV}[R_m G_N(R_m)]^2. \tag{3.1}$$

C. α-nucleus potential

We still have to choose an α-nucleus potential for the calculation of the penetrability P:

$$P=\exp\left[-2\int_{R_i}^{R_f}\left(\frac{2M_\alpha}{\hbar^2}[E_\alpha - V(R)]^{1/2}dR\right)\right]. \tag{3.2}$$

Here R_f and R_i are the outer and inner classical turning points, respectively. M_α is the reduced α-particle mass. The energy E_α is the measured α decay energy plus the screening corrections as given in Ref. 7.

In Table I we give the parameters for several potentials. The first potential[8] $V1$ has the advantage that it is consistent with the kinetic α-particle energy at the nuclear surface calculated from G_N (see Sec. III B). The second potential $V2$ is the Set A recommended by Barnett and Lilley[9] for α decay calculations. The third potential[10] is Igo's best fit Woods-Saxon potential for $\alpha+{}^{208}$Pb; it gives a very low penetrability which may be considered as a limiting case. Similarly Igo's exponential potential gives a penetrability which may be regarded as an upper limit.

The tabulated results in Sec. IV are calculated with $V1$. The penetrabilities calculated with $V1$ and $V2$ happen to be very close to one another; $V2$ gives typically a 5 to 10% higher penetrability.

IV. RESULTS

Tables III–V give the results for relative and absolute α decay rates for ^{211}Po and ^{211}Bi. Owing to an approximation (Appendix A) in the calculation of $N(R,R')$, the accuracy of the results containing G_N is at least ±5% (or perhaps a little better).

TABLE I. α-nucleus potential parameters for various Woods-Saxon potentials $V(R)=V_0/\{1+\exp[(R-r_0A^{1/3})/a]\}$.

	V_0 (MeV)	r_0 (fm)	a (fm)	Ref.
$V1$	−58.8	1.454	0.56	Satchler Ref. 8
$V2$	−96.44	1.376	0.625	Barnett *et al* Ref. 9
$V3$	−35	1.47	0.6	Igo Ref. 10

The relative rates r_i for the decay to a particular daughter nucleus ϕ_A^i are given by

$$r_i=\left(\sum_l \delta_{i,l}{}^2P_l\right)\Big/\left(\sum_{l,i'}\delta_{i',l}{}^2P_l\right). \tag{4.1}$$

The sums run over all possible angular momenta l, the sum in the denominator running also over i'.

The relative amplitudes $A(l)$ for different angular momenta are given by

$$A(l_1):A(l_2):\ldots = \pm(\delta_{i,l_1}{}^2P_{l_1})^{1/2}:\pm(\delta_{i,l_2}{}^2P_{l_2})^{1/2}:\ldots . \tag{4.2}$$

The sign is determined by the sign of G_N (or G) at the nuclear surface.

The relative ratios are also calculated with the spectroscopic factor (2.10). For this δ^2 has to be replaced by the corresponding S in (4.1) and (4.2). The absolute values are calculated by formula (3.1).

The results for ^{212}Po are given in a different form: In Table V we listed the spectroscopic factors and the hindrance factors (reciprocal of S normalized to the ground state transition). In Figs. 1 and 2 we show $G(R)$ and $G_N(R)$ for the first and second 0^+ states of ^{212}Po.

V. DISCUSSION

A. ^{211}Po and ^{211}Bi

From examination of Table II it appears that the α branching ratios by the old and new theory

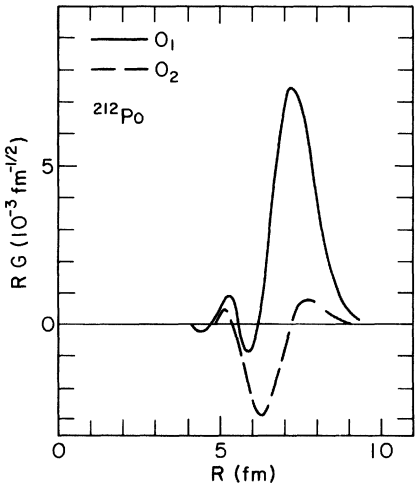

FIG. 1. The reduced amplitude G of the old theory versus the radius for the first and second 0^+ state of ^{212}Po.

are not much different. That is, the substantial enhancement of α decay rates by the new theory applies rather uniformly to the various state combinations of ^{211}Po and ^{211}Bi decay. This result is reassuring in that it suggests that extensive previous calculations in the literature with the old shell model α decay theory are not all invalidated. Likewise, in Table III we see that the relative amplitudes for various l values are not much altered; also there seems to be some systematic lowering of higher l values by a few percent.

From Table IV we see that the absolute decay widths are increased by two orders of magnitude in the new theory, giving good agreement with experiment. The ratio of widths for the two nuclei differs by a considerable amount for the old and new theories, with the result of the new theory in better agreement with experiment.

As far as the absolute decay widths are concerned there is still a considerable uncertainty in the theory. This is mainly due to the sensitivity of the penetrability of the α-nucleus potential. For Igo's exponential potential[10] the values would be enhanced by about a factor of 2; for Igo's best fit ($V3$ in Table I) they would be reduced by about a factor of 5. The inclusion of configuration mixing (see Sec. III A) results in an enhancement by a factor of 3 for ^{211}Po and a factor of 1.5 for ^{211}Bi. Even taking these uncertainties into account (a factor of 5 up or down) the old theory is obviously unable to reproduce the absolute decay width.

It is interesting to see that there is not much difference between the values from the channel-radius-dependent equation (2.8) and from the spectroscopic factor. The main reason for this seems to be that the radial shapes of G_N (or G)

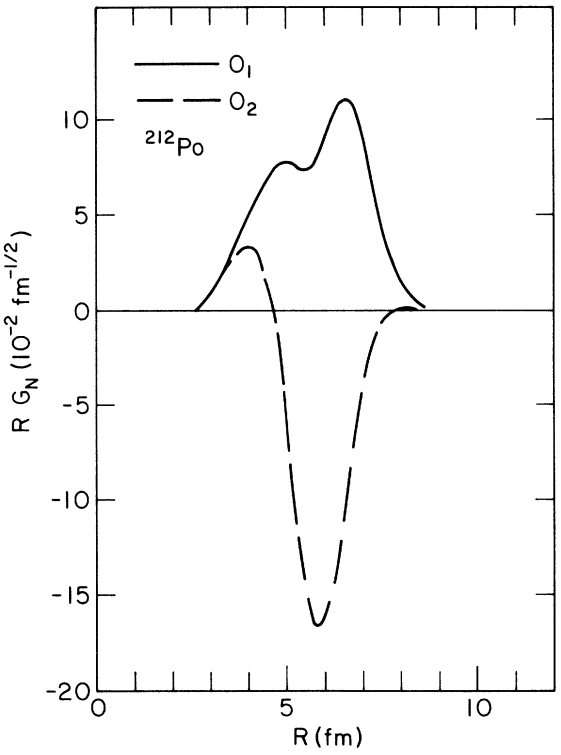

FIG. 2. The reduced amplitude G_N of the new theory versus the radius for the first and second 0^+ state of ^{212}Po.

are not too different for various decays. G_N (or G) usually has a large maximum at the nuclear surface at about 7 fm. It may be also noted that the relative values calculated with the old theory and a 7 fm radius here are in good agreement with the literature values of Mang for a 9 fm channel radius.

TABLE II. α branching ratios for ^{211}Po and ^{211}Bi. The results of the old and new theory are displayed versus the experiment. The numbers in the upper line are from the channel-radius-dependent formula (2.8); the lower line is calculated with spectroscopic factors.

Parent nucleus	Daughter nucleus	α branching ratios Experiment	Old theory	New theory
^{211}Po	$p_{1/2}$	99	98.0 98.0	96.8 97.8
	$f_{5/2}$	0.5	1.6 1.6	2.7 1.7
	$p_{3/2}$	0.5	0.4 0.4	0.5 0.5
^{211}Bi	$s_{1/2}$	83	82 82	78 81
	$d_{3/2}$	17	18 18	22 19

TABLE III. Relative angular momentum mixing amplitudes. The numbers in the upper line are from the channel-radius-dependent formula (2.8); the lower line is calculated with spectroscopic factors.

Parent nucleus	State of daughter nucleus	Relative angular momentum mixing amplitudes Experiment	Old theory	New theory
^{211}Po	$f_{5/2}$	1 : −0.96 : 0.55	1 : −0.88 : 0.58 1 : −0.88 : 0.58	1 : −0.85 : 0.52 1 : −0.85 : 0.56
	$p_{3/2}$	1 : −0.14	1 : −0.33 1 : −0.33	1 : −0.32 1 : −0.33
^{211}Bi	$d_{3/2}$	1 : −0.27	1 : −0.33 1 : −0.33	1 : −0.32 1 : −0.33

B. ^{212}Po

It is when we come to the spectroscopic factors for ^{212}Po in Table V that we find striking differences between the old and new theory. In particular the considerable hindrance factors predicted for the second 0^+ and second and third 2^+ states are lowered by an order of magnitude in the new theory. To understand this effect we plotted the reduced amplitudes of the old theory (Fig. 1) and the new theory (Fig. 2) for the first 0_1^+ and second 0_2^+ states. Obviously, the 0_2^+ state has a configuration mixing which leads to destructive interference for the amplitude G in the nuclear surface. In the outer nuclear surface $R>7$ fm this effect is still preserved in G_N. Since $N(R, R')$ is more important the larger the overlap between the α cluster and the daughter nucleus, the inner maximum of $|G|^2$ at 5.2 fm is relatively strongly enhanced, resulting in a large contribution to the spectroscopic factor. Since various parts of G are differently enhanced, the results for G_N are probably very sensitive to the details of the wave function.

The question of whether the enhancement of the 0_1^+ over the 0_2^+ in G_N in the outer surface is relevant, or whether we may consider the spectroscopic factor as more important, is open. The answer may be found in a better reaction theory. We might also hope to get some answer from the experimental side. Newer experiments and the analysis of deVries *et al.*[11] indicate the possibility of deriving the absolute α width for the excited states as well, by doing transfer experiments.

As far as the absolute decay widths are concerned, the new theory can reproduce the ground state decay width (see also Ref. 2); the old theory falls short by two orders of magnitude. The ratio $\Gamma(18^+$, assumed to be the isomer at 2930 keV)/$\Gamma(0_1^+)$ comes out too large by a factor of 30 in the new theory and a factor of 150 in the old one.

TABLE IV. α decay width in 10^{-22} MeV [calculated with (3.1)]. The last line gives the ratio of the total decay width for ^{211}Po and ^{211}Bi.

α emitter	α decay width (10^{-22} MeV) Experiment	Old theory	New theory
^{211}Po	8.8	9×10^{-2}	12
^{211}Bi	3.5×10^{-2}	5.4×10^{-4}	4.4×10^{-2}
Γ_{Po}/Γ_{Bi}	250	167	273

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APPENDIX A

We consider the ground state transition of ^{211}Po. The exact operator $1-\hat{K}_l$ has to be calculated with $\phi_A^j = a(p_{1/2})|^{208}\mathrm{Pb}\rangle$, where $a(p_{1/2})$ is the annihilation operator for a neutron in the $3p_{1/2}$ state. In the calculation of $1-\hat{K}_l$ we use the following two alternative approximations for this state:

(1) $|\phi_A\rangle \simeq |^{208}\mathrm{Pb}\rangle$,

(2) $|\phi_A\rangle \simeq [a(p_{1/2})a(p_{1/2})]_0|^{208}\mathrm{Pb}.\rangle$.

According to Ref. 2 $K(R, R')$ is given in the form

$$K_l(R, R') = \sum_i g_i^{l\,*}(R) g_i^l(R'), \tag{A1}$$

where i runs over all sets of four particles which contain at least one in a ϕ_A occupied level. $g_i^l(R)$ is the overlap of an α cluster at R with the product of the four single-particle functions.

From the structure of $\hat{K}_l$ it is clear that the error in $N(R, R') = (1-\hat{K}_l)_{R,R'}^{-1/2}$ is positive semidefinite for approximation (1) and negative semidefinite for (2). Therefore, the exact spectroscopic factor has to be between the two approxi-

TABLE V. α decay theoretical properties from ground and excited states of ^{212}Po.

State of ^{212}Po	Spectroscopic factors S Old theory ($\times 10^{-5}$)	New theory ($\times 10^{-2}$)	Ratio new to old ($\times 10^{2}$)	Hindrance factors $[S(0_1)/S(\text{excited})]$ Old theory	New theory
0_1	6.0	2.6	4	1	1
0_2	0.71	3.1	44	8	0.8
0_3	0.17	0.16	9	35	16
2_1	1.6	0.56	3.5	4	5
2_2	0.09	0.40	44	66	7
2_3	0.17	0.47	3	35	6
2_4	0.08	0.04	5	71	68
2_5	1.6	0.29	2	4	9
4_1	0.79	0.20	2.5	8	13
10_1	2.8	0.76	3	2	3
16_1	0.79	0.39	5	8	7
18_1	6.0	0.50	1	1	5

mate values

$$S[\text{approx.}(2)] \leq S(\text{exact}) \leq S[\text{approx.}(1)]. \quad \text{(A2)}$$

From the calculation of the approximate values and from (A2) we find

$$S(\text{exact}) = S[\text{approx.}(1)](1 - 0.05) \pm 5\%. \quad \text{(A3)}$$

The error is probably smaller than 5%. The evaluation with formula (3.1) yields a somewhat smaller difference between the two approximations.

As a generalization we employed (A3) for all ^{211}Po and ^{211}Bi transitions.

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