Evaluation of the newly developed pocket-type dynamical double-folding potential: Systematic calculations of α-decay half-lives and nuclear charge radii

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Abstract

The α-nucleus interaction is crucial in the deet al. ., Phys. Rev. C 109, L011301 (2024)]. This potential results in a pocket geometry within the nuclear surface region, which is consistent with the α-clustering characteristics predicted by microscopic calculations. In this study, the accuracy of the pocket-type DDFP was validated via systematic calculations of α-decay half-lives and an extended evaluation of the nuclear charge radii of the daughter nuclei. The results demonstrate good agreement with the experimental data for both quantities, thereby confirming the reliability of the DDFP model. Compared with calculations that use α-nucleus interactions derived from conventional double-folding procedures, DDFP employs fewer adjustable parameters to achieve a more accurate description of the charge radii based on the experimental α-decay energies.

Full Text

Evaluation of the Newly Developed Pocket-Type Dynamical Double-Folding Potential: Systematic Calculations of α-Decay Half-Lives and Nuclear Charge Radii

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The α-nucleus interaction is crucial for describing α decay. Recently, we developed a pocket-type dynamical double-folding potential (DDFP) that effectively

incorporates both the surface-medium effect and interior Pauli repulsion in α decay [H. Zheng *et al.*, Phys. Rev. C 109, L011301 (2024)]. This potential produces a pocket geometry within the nuclear surface region, consistent with α-clustering characteristics predicted by microscopic calculations. In this study, we validate the accuracy of the pocket-type DDFP through systematic calculations of α-decay half-lives and an extended evaluation of nuclear charge radii for the daughter nuclei. The results demonstrate good agreement with experimental data for both quantities, thereby confirming the reliability of the DDFP model. Compared with calculations using α-nucleus interactions derived from conventional double-folding procedures, DDFP employs fewer adjustable parameters to achieve a more accurate description of charge radii based on experimental α-decay energies.

Keywords: α decay, nuclear charge radii, α-clustering effect

Introduction

Nucleon clustering is fundamental to the study of nuclear structure and reactions [1–4]. In particular, the clustering effect plays a crucial role in understanding cluster radioactivity and α decay in both heavy and superheavy nuclei. Although α decay has been observed in laboratories for over a century, recent experiments have directly demonstrated the formation of α clusters at the surface of heavy nuclei using (p, pα) knockout reactions [5]. This clustering feature in heavy nuclei has long been a key assumption in various cluster model theories of α decay, where it is attributed to enhanced α correlation in the surface region [6–10].

Studies on few-body correlations in nuclear matter have demonstrated that α correlation is highly sensitive to nucleon density due to the Pauli exclusion principle [4, 11–16]. This α correlation becomes prominent only when the medium density is below a critical threshold of approximately one-fifth the saturation density, known as the Mott density. Above this density threshold, α correlation is suppressed due to antisymmetrization of the many-body wave function for the entire fermion system [12, 16]. Consequently, α cluster formation in a finite nucleus is confined to the nuclear surface, where nucleon density is relatively low. As the α cluster moves from the surface toward the residual daughter nucleus, it experiences increasing Pauli blocking from surrounding nucleons (see Eq. (45) in Ref. [12]). This Pauli blocking weakens the binding of the α-like quartet (α correlation), resulting in cluster expansion—a phenomenon referred to as the medium effect. When the medium density exceeds the Mott density, the α correlation vanishes and the quartet transitions from a bound α-cluster state to single-nucleon states [12, 13, 16]. Therefore, α clusters rarely form in the interior of heavy nuclei.

Based on these experimental and theoretical findings, the α cluster in the α-daughter configuration of an α emitter is expected to experience a pocket-like potential at the nuclear surface during its center-of-mass motion [12, 17–20]. Our

recent study investigated the correlation between this pocket structure and the α-clustering effect [21]. We developed a pocket-type dynamical double-folding potential that incorporates both the surface-medium effect and interior Pauli repulsion for α decay. The improved α-nucleus potential produces a surface pocket geometry beyond the critical radius that marks the Mott density, thereby concentrating the α-cluster wave function at the nuclear surface beyond this radius in a self-consistent manner.

In this study, we further assess the reliability of the pocket-type DDFP model by extending α-decay half-life calculations to a broader range of even-even nuclei with $60 \leq \mathrm{Z} \leq 98$. Additionally, since α-decay cluster models with double-folding potentials can be applied to estimate nuclear charge radii [22–24], we tentatively calculated the root-mean-square (RMS) charge radius of the daughter nucleus as an additional test of the DDFP model' s effectiveness.

Theoretical Framework

In cluster models for α decay, the relative motion between the α cluster and daughter nucleus is described as two-body dynamics. The α cluster interacts with the daughter nucleus via the α-nucleus potential, which can be expanded as:

$$V(R) = V_N(R) + V_C(R) + \frac{L(L+1)\hbar^2}{2\mu R^2}$$

In the DDFP framework [25, 26], the nuclear potential V_N and Coulomb potential V_C are constructed using a dynamical double-folding procedure:

$$V_{N,C}(R) = \int \rho_1(r_1)\rho_2[r_2, \rho_1(R)]V_{N,C}(s)dr_1dr_2$$

where r_1 and r_2 are the intrinsic coordinates of the daughter nucleus and α cluster, respectively, and $s = R + r_2 - r_1$ is the vector between interacting nucleons. A notable distinction in the DDFP formalism, compared with conventional double-folding formalism, is the incorporation of the surface medium effect within the dynamical density distribution of the α cluster $\rho_2[r_2, \rho_1(R)]$:

$$\rho_2[r_2, \rho_1(R)] = \rho_{2,s}(R)\exp\{-\beta[\rho_1(R)]r_2^2\}$$

with

$$\beta[\rho_1(R)] = \frac{16\rho_{1,s}}{\rho_1(R)}$$

which satisfies the critical constraints on the intrinsic dynamics of the α cluster from microscopic calculations [12]. The saturation density of the α cluster

$\rho_{2,s}(R)$ is determined by normalizing the density distribution for each R. The medium density is approximated by the local density of the daughter nucleus, described by the two-parameter Fermi (2pF) distribution:

$$\rho_1(r_1) = \frac{\rho_{1,s}}{1 + \exp[(r_1 - R_{1/2})/a]}$$

where a represents the diffuseness parameter and $R_{1/2}$ is the half-density radius. Based on nuclear saturation properties, the half-density radius is usually expressed as $R_{1/2} = r_0 A^{1/3}$ under spherical symmetry with $r_0 = 1.070$ fm. However, studies on nuclear density distributions and surface properties have indicated that the radius parameter r_0 for heavy nuclei is slightly larger than for light nuclei [27, 28]. Accordingly, we fitted the theoretical half-density radius derived from calculations using the SkM* functional in Ref. [28], yielding $r_0 = 1.125$ fm for heavy nuclei with $Z = 58 - 96$. The diffuseness parameter a of each daughter nucleus was determined in subsequent calculations, whereas the saturation density $\rho_{1,s}$ was determined by normalizing Eq. (4).

The effective nucleon-nucleon (NN) interaction V_N is crucial for double-folding potentials because it significantly influences the derived potential' s geometry. Strong repulsive behavior for V_N in regions of large density overlap is essential for simulating the Pauli blocking experienced by the α cluster, which leads to a pocket-type potential [17, 21, 29]. Here, we adopt the density-dependent Migdal NN interaction [21, 30, 31]:

$$V_N(\rho_1, \rho_2, s) = C_0\{F_{in}x(\rho_1, \rho_2) + F_{ex}[1 - x(\rho_1, \rho_2)]\} \times \delta(s)$$

with interaction parameters $C_0 = 300$ MeV fm^3 and $F_{in} = 0.09$ well justified by fitting experimentally measured nuclear properties [27, 30], and parameter $F_{ex} = -3.82$ tuned to reproduce the experimental decay energy of ^{210}Po and the diffuseness parameter of the daughter nucleus ^{206}Pb derived from elastic electron scattering [32]. The interaction strength between touching nucleons is determined by the density-dependent term $x(\rho_1, \rho_2)$:

$$x(\rho_1, \rho_2) = \frac{\rho_{00}(R)}{\rho_{1,s} + \rho_{2,s}(R)}$$

where $\rho_{00}(R) = \rho_1(r_1) + \rho_2(r_2, R)$. The medium effect also influences the NN interaction through the density-dependent term $x(\rho_1, \rho_2)$ because both ρ_2 and ρ_{00} depend on R.

The α-decay width was calculated using a two-potential approach (TPA) [33]. Within the TPA framework, the tunneling problem is divided into bound-state and scattering-state problems. The decay width is expressed in terms of the bound-state wave function $\phi(R)$ and the regular scattering wave function $\chi_l(kR)$:

$$\Gamma = \frac{\hbar^2 k}{\mu} \frac{|\phi(\bar{R})[\alpha\chi_l(\bar{R}) + \chi_l'(\bar{R})]|^2}{|\chi_l(\bar{R})|^2 + |Y_l(\bar{R})|^2}$$

Here, $k = \sqrt{2\mu Q_\alpha/\hbar^2}$, $\alpha = \sqrt{2\mu(V(\bar{R}) - Q_\alpha)/\hbar^2}$, and $\bar{R}$ denotes the separation radius selected as the midpoint between the top of the Coulomb barrier and the outer classical turning point. The bound-state wave function $\phi(R)$ was numerically computed by solving the Schrödinger equation within the inner potential defined in TPA [33]. Regarding the scattering term, $\chi_l(R)$ can be approximated using the regular Coulomb wave function $F_l(R)$. The eigenvalue of the bound state was adjusted to match the decay energy Q_α by varying the diffuseness parameter a of the daughter nucleus.

Finally, the decay half-life was calculated using:

$$T_{1/2} = \frac{\hbar \ln 2}{\Gamma P_\alpha}$$

where P_α is the α preformation factor representing the probability of α cluster formation inside the parent nucleus.

To calculate decay half-lives using Eq. (9), the P_α factor is required as theoretical input. Because P_α is strongly correlated with shell structure, a precise description of P_α during shell evolution is crucial for reliable half-life calculations. However, direct evaluation of the exact P_α within a microscopic formalism is challenging due to the complexity of many-body problems. Alternatively, P_α can be estimated phenomenologically from well-established systematics derived from experimental half-lives:

$$P_\alpha^{\exp} = \frac{\hbar \ln 2}{T_{1/2}^{\exp} \Gamma}$$

For instance, a simple formula depending on the valence nucleon number of the α emitter provides a reasonably accurate description of P_α, as demonstrated in previous systematic calculations [34–38]. Figure 2(a) shows the $P_\alpha^{\exp}$ factors extracted from experimental half-lives using Eq. (10) as a function of valence neutron number relative to the nearest neutron magic number N_0. As shown, $P_\alpha^{\exp}$ generally decreases with increasing valence neutron number until the next shell closure, exhibiting a linear correlation with valence neutron number. Based on these systematics, we employed an N-dependent formula for the P_α factor as theoretical input in half-life calculations:

$$P_\alpha = -0.0015(N - N_0) + 0.0692$$

with $N_0 = 82$ for nuclei with $82 < N \leq 126$ and $N_0 = 126$ for nuclei with $N > 126$, as denoted by the red line in Fig. 2(a). This input P_α formula

differs from that used in our previous work, which was based on a Heaviside step function formalism [21]. The previous approach was intended to describe abrupt changes in P_α near shell closure, whereas the present valence-nucleon-dependent formula is more appropriate for describing systematic P_α behavior in both closed-shell and open-shell regions.

Results and Discussion

A. The Pocket-Type DDFP and α-Decay Half-Life Calculations

As mentioned in Sec. I, α-clustering primarily occurs at the surface of heavy nuclei where nucleon density is below the Mott density. This is illustrated by the pocket-type DDFP depicted in Fig. 1. A pocket-like geometry forms in the surface region beyond the critical radius r_c corresponding to the Mott density. This feature enables formation of a quasi-bound state for the α-daughter system, with the α cluster located at the pocket center. Conversely, within the internal region ($R < r_c$), Pauli repulsion suppresses α correlation, preventing α-cluster state formation. Consequently, the strongly repulsive core in the α-nucleus potential effectively inhibits the α cluster, as illustrated by the amplitude of the α-cluster wave function. The first classical turning point is close to the critical radius r_c, marking the boundary of the classically forbidden region where the α-cluster wave function amplitude rapidly reduces. A comparable reduction in α-clustering is expected when medium density surpasses the Mott density; specifically, when the cluster moves into the daughter nucleus interior, crossing the critical radius. Therefore, the positions of the first classical turning point and the critical radius are expected to be close. Our calculations indicate that the average distance between these two positions was 0.085 fm for the 129 α emitters studied, reinforcing the universality of this phenomenon.

Utilizing this pocket-type DDFP model, we investigated ground-state-to-ground-state α transitions in even-even nuclei ranging from Nd to Cf. To calculate decay half-lives using Eq. (9), the P_α factor is required as theoretical input. Because P_α is strongly correlated with shell structure, a precise description of P_α during shell evolution is crucial for reliable half-life calculations. However, direct evaluation of the exact P_α within a microscopic formalism is challenging due to the complexity of many-body problems. Alternatively, P_α can be estimated phenomenologically from well-established systematics derived from experimental half-lives using Eq. (10). For instance, a simple formula depending on the valence nucleon number of the α emitter provides a reasonably accurate description of P_α, as demonstrated in previous systematic calculations [34–38].

Figure 2(a) shows the $P_\alpha^{\rm exp}$ factors extracted from experimental half-lives using Eq. (10) as a function of valence neutron number with respect to its nearest neutron magic number N_0. As shown, $P_\alpha^{\rm exp}$ generally decreases with increasing valence neutron number until the next shell closure. This dispersion exhibits a linear correlation with valence neutron number. Based on these systematics, we employed an N-dependent formula for the P_α factor as theoretical input in

half-life calculations using Eq. (11), with $N_0 = 82$ for nuclei with $82 < N \leq 126$ and $N_0 = 126$ for nuclei with $N > 126$, as denoted by the red line in Fig. 2(a). This input P_α formula differs from that used in our previous work, which was based on a Heaviside step function formalism [21]. The previous approach was intended to describe abrupt changes in P_α near shell closure, whereas the present valence-nucleon-dependent formula is more appropriate for describing systematic P_α behavior in both closed-shell and open-shell regions.

In Fig. 2(b), the deviations between theoretical and experimental half-lives are plotted (denoted by black circles) on a logarithmic scale as a function of the parent nucleus neutron number. The agreement between theoretical and experimental results was systematically evaluated using the average deviation:

$$\sigma = \frac{1}{N}\sum_{i=1}^{N} |\log_{10} T_{1/2,i}^{\mathrm{theor}} - \log_{10} T_{1/2,i}^{\mathrm{expt}}|$$

We obtained $\sigma = 0.1820$ for the 129 even-even nuclei investigated. This corresponds to an average factor $S = 10^{\sigma} = 1.521$ between theoretical and experimental half-lives, slightly larger than $S = 1.475$ obtained from our previous calculation [21]. Relatively large deviations were observed for isotopes ^{214,216,218}U, as shown in Fig. 2. These deviations primarily arise from limitations of the N-dependent formula for P_α [Eq. (11)], which cannot adequately describe P_α behavior during proton shell evolution [34, 35]. The input P_α for uranium isotopes farther from the proton shell at $Z = 82$ is underestimated compared to the extracted P_α^{exp}, as illustrated in Fig. 2(a). Hence, a more refined P_α considering both neutron and proton shell evolution would likely improve agreement in half-life calculations. Furthermore, large deviations were observed for ^{194}Pb and ^{228}Pu. The deviation in ^{194}Pb likely stems from its extremely small α-branching ratio $[(7.3 \pm 2.9) \times 10^{-6}\%]$ with relatively large uncertainty [39], while the deviation in ^{228}Pu arises primarily from uncertainty in the measured half-life of $1.1^{+2.0}_{-0.5}$ s [40]. Nevertheless, as an extended calculation of our previous study [21], the present results further validate the reliability and accuracy of the pocket-type DDFP in describing α-decay half-lives.

In addition to ground-state-to-ground-state α decay discussed above, testing the proposed model' s performance in estimating α-decay half-lives between excited states would be valuable. For instance, we calculated the half-life of the favored α transition from the first isomeric state of ^{193}Po ($I^\pi = 13/2^+$) to that of ^{189}Pb ($I^\pi = 13/2^+$). The theoretical result is $T_{1/2}^{\mathrm{theor}} = 9.53 \times 10^{-2}$ s with P_α estimated using Eq. (11). This value is in close agreement with previous theoretical studies [41, 42]. Our result is smaller than the experimentally measured half-life $T_{1/2}^{\mathrm{expt}} = 2.47 \times 10^{-1}$ s by a factor of 2.6, which is acceptable particularly considering that P_α for odd-A nuclei are usually smaller than for even-even nuclei due to Pauli blocking from the unpaired nucleon [42, 43].

B. Nuclear Charge Radii Estimated by the Pocket-Type DDFP Model

Within the double-folding framework, the daughter nucleus density distribution is involved in constructing the α-nucleus potential. Consequently, deducing the nuclear charge radius of the daughter nucleus from its density distribution is feasible once the α-nucleus potential is determined using experimental decay data. For instance, in Refs. [22, 23], charge radii of daughter nuclei were determined using both experimental half-lives and decay energies within the generalized density-dependent cluster model (GDDCM). In an extension of this work, Ref. [24] improved the GDDCM (labeled GDDCM*) by considering neutron skin structure, differences between proton and neutron density distributions, and a more refined α preformation factor. This modification provides a better description of charge radii. To a certain extent, the accuracy of deduced charge radii serves as an additional test of the model' s effectiveness in describing α-nucleus interactions.

As described in Sec. II, the diffuseness parameter a in the daughter nucleus density distribution is determined by ensuring that the pocket-type DDFP, within the TPA framework, can support a bound state with its eigenvalue matching the experimental α-decay energy. Therefore, the pocket potential embodies both α-decay dynamics and information from the decay energy, linked to the density distribution and surface diffuseness property a of the daughter nucleus through a double-folding procedure. Once a is determined, we obtain not only the α-nucleus potential for half-life calculations but also the daughter nucleus density distribution. The RMS charge radius of the daughter nucleus can then be calculated as:

$$R_{\rm ch} \equiv \langle r^2 \rangle^{1/2} = \left[\frac{\int \rho_1(r) r^4 dr}{\int \rho_1(r) r^2 dr} \right]^{1/2}$$

This strategy is notably simpler than previous cluster models, which require experimental decay energy, half-life, and α preformation factor as separate inputs, because it employs only one set of parameters ($R_{1/2}$ and a). The $N = 126$ shell effect from the decay energy is incorporated into parameters shared by both proton and neutron density distributions [21], resulting in magnification of the shell effect for proton distributions and thereby impacting charge radii. Therefore, separate treatment of proton and neutron density profiles considering neutron skin structure is expected to reduce this discrepancy and provide a more accurate description of both charge radii and α-decay half-lives [48, 49].

The charge radii from the pocket-type DDFP and previous GDDCMs can be quantitatively compared [22, 24]. Table 1 lists the standard deviations $\sigma_{\rm ch}$ of nuclear charge radii for these models compared with experimental data from [44, 45]. Notably, although DDFP relies solely on experimental decay energy and reduces one free parameter by avoiding empirical P_α input, it yields a more accurate description of charge radii. Specifically, the standard deviation is reduced

by 67.3% compared to GDDCM and by 53.3% compared to GDDCM*. This significant improvement underscores the importance of α-clustering features in the α-decay mechanism, particularly the medium effect and strong Pauli repulsion, which make the pocket-type DDFP a more realistic description of the involved α-nucleus interaction.

Having determined the charge radii, it is instructive to investigate the correlation between daughter nucleus charge radii and pocket positions r_p of the α-nucleus potentials (see Fig. 1 for ^{212}Po). As seen in Fig. 5, the pocket position is linearly correlated with the daughter nucleus charge radius with a correlation coefficient of 0.9885. This finding was expected because both quantities relate to the spatial extent of the daughter nucleus density distribution. The pocket position corresponds to the region where the α cluster is most likely to form, located at the nuclear surface with nucleon density below 1/5 of saturation density. If the daughter nucleus has a broader density distribution, the pocket position shifts away from the core region, yielding a larger charge radius. Therefore, the correlation between these quantities embodies the α-clustering feature of the pocket-type potential.

In addition to α-decay models, theoretical approaches based on mean-field models have proven very effective in describing nuclear structural properties, including nuclear charge radii [46, 50–57]. For instance, the deformed relativistic Hartree–Bogoliubov method accurately reproduced charge radii of 369 even-even nuclei with $Z = 8 - 96$, achieving a standard deviation $\sigma_{\rm ch} = 0.032$ fm [46], significantly more accurate than results presented in Table 1. This higher accuracy is expected because mean-field models typically have more fitting parameters than α-decay models. For instance, the present calculation uses only three free parameters (r_0, a, and F_{ex}) to achieve reasonable descriptions of both α-decay half-life and nuclear charge radius. The calculation was simpler and the accuracy acceptable as a comparative reference. Specifically, the present pocket-type DDFP approach offers a more accessible means of calculation, provided experimental decay energy data are available.

The diffuseness parameters determined using the double-folding procedure are shown in Fig. 3. The diffuseness parameters of daughter nuclei generally fluctuate around the average value $\bar{a} = 0.545$ fm. A clear shell effect is observed around $A = 208$, corresponding to a neutron number approaching the $N = 126$ shell closure.

In Fig. 4, we present calculated charge radii of daughter nuclei with $Z = 58-96$ and corresponding experimental values from Refs. [44, 45]. The empirical relationship between charge radius and mass number is indicated by the gray line for reference:

$$R_{\rm ch} = (r_1 + r_2 A^{-2/3} + r_3 A^{-4/3}) \times A^{1/3}$$

with parameters $r_1 = 0.9071(13)$ fm, $r_2 = 1.105(25)$ fm, and $r_3 = -0.548(34)$ fm

[44]. As shown, our results align with experimental data trends as well as those indicated by the empirical formula. The standard deviation of the discrepancy between theoretical and experimental values is evaluated as:

$$\sigma_{\rm ch} = \left[\frac{1}{84}\sum_{i=1}^{84}(R_{{\rm ch},i}^{\rm theor} - R_{{\rm ch},i}^{\rm expt})^2\right]^{1/2}$$

yielding $\sigma_{\rm ch} = 0.0420$ fm, comparable to empirical results (13). However, a notable discrepancy is observed at $A = 208 - 214$, where calculated radii indicate an abrupt decrease, whereas corresponding experimental radii vary more smoothly. This abrupt variation is related to the $N = 126$ shell effect, which significantly affects the daughter nucleus neutron density distribution [46]. The resulting variation in neutron distribution, in turn, affects the proton distribution, reflected in a less pronounced kink appearing in experimental charge radii variation at the neutron magic number (see Fig. 1 in Ref. [47] and Fig. 3 in Ref. [44]). However, the present DDFP formalism does not treat proton and neutron distributions separately.

Summary

This study employed the pocket-type dynamical double-folding α-nucleus potential (DDFP) to calculate α-decay half-lives for 129 even-even nuclei with $Z = 60 - 98$. Experimental half-lives were accurately reproduced with an average discrepancy factor of 1.521, demonstrating DDFP' s precision in describing α decay. Moreover, determination of the DDFP enabled estimation of nuclear charge radii from daughter nucleus density distributions. As an improvement over previous cluster models, DDFP achieves more accurate charge radius description with fewer parameters and relies solely on experimental α-decay energies. The standard deviation between theoretical and experimental charge radii for 84 even-even nuclei with $Z = 58-96$ is 0.0420 fm, representing a 53.3% reduction relative to previous calculations [24], although it remains larger than some microscopic calculations based on mean-field theories. Notably, the present model provides an approach for estimating nuclear charge radius from α-decay data, provided experimental decay energy is available. DDFP accuracy can be further improved by refining daughter nucleus density distributions, such as including differences between proton and neutron density distributions and considering nuclear deformations. Overall, strong agreement between theoretical and experimental charge radii serves as further validation of DDFP accuracy for α-decay calculations.

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Note: Figure translations are in progress. See original paper for figures.