Localisation and alpha radioactivity

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Relativistic energy density functional approaches are known to well describe nuclear states which involve alpha clusters. Here, the alpha preformation probability is analysed through the behavior of the spatial localization of nucleonic states calculated with an axially deformed RHB approach over the nuclear chart. The systematic occurrence of more localised valence states, having a n=1 radial quantum number, allows to pinpoint nuclei in agreement with experimentally known alpha emitters. The cases of 212Po and 104Te are investigated, showing the concomitant roles of the pseudospin symmetry and the presence of n=1 states on the alpha preformation probability. A phenomenological law relating this probability to the radial quantum number of the valence states is also derived, allowing to describe the impact of shell effects on this probability over isotopic and isotonic chains. Finally the behavior of the alpha preformation factor is also analysed on several isotopic chains.

I. INTRODUCTION

The description of alpha radioactivity is a long standing problem. Since about one century, a large variety of models have been devoted to this task, such as semi-classical approaches, or microscopic ones [1]. However several open questions remain, such as is a positive Q-value a sufficient condition for alpha emission? The identification of all alpha emitters nuclei may not be achieved yet, as proven by the discovery of alpha-emission of 208Bi in 2003 [2], or the remaining question of the possible alpha radioactivity of 208Pb [3]. One of the first successful model is the well-known Geiger-Nuttall law [4] and its description involving tunneling effect by Gamow [5] and the class of WKB models [1]. In these approaches, the alpha emission probability is decomposed into the product of an alpha preformation one with the Coulomb barrier tunneling one, taking into account the frequency of impact of the alpha particle on the barrier.

The tunneling effect probability depends on the Q-value. However the alpha preformation probability itself has been less studied, often being approximated to 1. In addition, some points remain to be clarified as first discussed by Buck and collaborators [6], such as the difference of behavior of the alpha emission probability for N smaller or larger than 126, respectively. This was first analysed by introducing a global quantum number in an alpha plus core description of the system, namely the Wildermuth condition [7,8]. It points towards the possible role of quantum numbers in alpha radioactivity, and it could be relevant to further provide a description of this effect at the nucleonic scale, involving nucleon quantum numbers. Relating this effect to nuclear structure, and studying the possible impact of the alpha preformation probability would also be of interest.

The study of the discrepancy between an accurate phenomenological law (i.e. an enhanced Geiger-Nuttall law) [9] assuming an alpha preformation probability of 1 and the experimental alpha emission probability, also brought relevant questions: the observed patterns compared to experiment are imaging the preformation probability. For instance the N=126 shell effect has an impact on this probability, but not the Z=82 one. Considering a large variety of alpha emitters, a variation up to a factor 30 of the preformation probability can be inferred [9]. More recently, the alpha emission probability was deduced from the alpha emission lifetime measurement in the 104Te nucleus [10,11], showing a larger emission probability than in 212Po, which remains to be fully explained.

Nuclear structure properties could therefore help to better understand the alpha preformation probability. Indeed light nuclei are known to exhibit alpha cluster states. They are of course not alpha emitters (except for 8Be) because of their negative Q-value. However the occurrence of alpha cluster states and the alpha preformation probability in heavier nuclei shall be closely related. A recent work has for example showed how to describe alpha emission in 104Te and alpha cluster states in 20Ne on the same ground, using and alpha+core approach [12]. 212Po alpha decay was also described with a significant alpha+core contribution [13]. Hence a description of alpha emission at the fully nucleonic level could be also interesting.

In a previous work, we showed that the so-called localisation parameter, at the nucleonic scale, was driving the occurrence of cluster states [14]: the radial quantum number n is the key quantity impacting spatial localisation of nucleons and hence cluster occurrence in nuclei. Therefore nuclei with spatially localised valence states should appear throughout the nuclear chart as favoured alpha emitters, providing a universal and simple approach: a first link with alpha radioactivity was explored in this work. In the present work we propose to investigate links between alpha cluster formation in nuclei and the alpha preformation probability, considering them on the same ground. In section II we refine the prediction of alpha emitters on the nuclear chart by
calculating the spatial dispersion of valence states with a fully microscopic relativistic Hartree-Bogoliubov approach: the relativistic EDF class of model have proven to be a relevant tool to analyse cluster occurrence in nuclei on a general ground [15–20], as well as to provide a sound comparison with measured excited spectrum of cluster states such as in Ne isotopes [21] and for the $^{12}$C Hoyle state [22]. In section III the role of localisation is analysed with the comparison of the alpha preformation probability in $^{104}$Te and $^{212}$Po. Section IV provides a study of the alpha preformation factor both on phenomenological ground and deduced from the microscopic approach.

II. ALPHA EMITTERS OVER THE NUCLEAR CHART

In order to predict the general behavior of alpha emitting nuclei over the nuclear chart, microscopic energy density functional calculations are performed. Namely, the fully self-consistent relativistic Hartree-Bogoliubov (RHB) approach is used with the DD-ME2 functional for axially symmetric nuclei [23]. Such an approach has proven to be successful to describe on the same ground a large variety of phenomena in nuclei [24] and the occurrence of cluster states [15–22]. The pairing interaction used in the RHB calculation is separable in momentum space and driven by the bell-shape pairing gap in symmetric nuclear matter [24].

A first analysis of the occurrence of cluster states can be investigated from the spatial localisation of the nucleonic degree of freedom, through the localisation parameter, defined as [14–16]:

$$\alpha_{loc} = \frac{2\Delta r}{r_0}$$  \hspace{1cm} (1)

where $\Delta r = \sqrt{r^2} > - < r^2 >$ is the typical spatial dispersion of the nucleonic wave function and $r_0 \simeq 1.25$ fm the typical inter-nucleon distance determined by nuclear saturation density ($\rho \approx 0.16 \text{ fm}^{-3}$).

In order to better understand the role of the spatial dispersion, it has been shown that the dispersion of a given single-particle state is to a good approximation only driven by the radial quantum number $n$ and not the orbital one [14]:

$$\alpha_{loc} \simeq \sqrt{\frac{2n-1}{(2mV_0r_0^2)^{1/4}}} A^{1/6}$$  \hspace{1cm} (2)

where $V_0$ is the depth of the confining potential of the considered nucleus composed of $A$ nucleons of mass $m$. Microscopic calculations of the dispersion, using Eq. (1) does show that the smallest dispersion pattern appears for single particle states with $n=1$ [14], independently from the orbital quantum number. This key point opens the possibility to pinpoint nuclei having spatially localised valence nucleons (namely $n=1$ valence states) throughout the nuclear chart: localisation should facilitate the preformation of an alpha particle in view of its emission.

In order to generalise this approach, taking into account pairing and deformation effects, the spatial dispersion is microscopically calculated on the whole nuclear chart of even-even nuclei in the axially-symmetric RHB framework as the average one of valence states (weighted by their occupation probability), taken until a particle number (either neutrons or protons) of 2 is reached. The resulting mean dispersion allows then to pinpoint nuclei having small spatial dispersion by using the following criteria:

$$\langle \Delta r \rangle \cdot A^{-1/6} < 0.7 \text{ fm}$$  \hspace{1cm} (3)

where the 0.7 fm value is the condition to have a small dispersion of the state (i.e. a $n=1$ state) in a given nuclei taking into account the dependency on $A$, as calculated from Eqs. (1) and (2) (see also the discussion of Figs. 1 and 2 in Ref. [14]).

In order to investigate if spatially localised valence states increase the alpha preformation probability, either the neutron or proton dispersion is calculated with the RHB approach (depending on the closest lower $N$ or $Z$ magic number) and the condition (3) is applied, as well as $Q_\alpha > 0$ which is a necessary condition for alpha radioactivity. Fig. 1 displays such even-even nuclei, compared to the experimentally known alpha emitters. The $Q_\alpha > 0$ condition is taken from experimentally measured masses. The present approach allows to recover a large majority of experimentally known alpha-emitting nuclei. The overall behavior over the nuclear chart is well described, showing that the $n=1$ localisation condition is relevant for alpha-particle emission.

Several nuclei on Fig. 1 are however predicted as alpha emitters but have not been experimentally tagged so. This could of course be due to a limitation of the general description of alpha radioactivity into steps initially assuming its localisation and preformation. Another reason could be that a majority of these nuclei are beta-unstable, and it may be experimentally difficult to look for alpha-emission when the partial beta-decay half life is several orders of magnitude smaller than the possible alpha one. Hence these nuclei could be also considered as possible predictions for alpha emitters which may have not been detected yet. For instance it could be interesting to experimentally look for nuclei which are predicted both beta and alpha emitters around the $^{142}$Gd region. Finally a last reason could be the role of more elaborate deformations than the axially symmetric one, such as triaxiality and/or octupole deformations. However the present approach does not aim to provide a fully detailed prediction of all the alpha emitters over the nuclear chart, but rather to show how the spatial localisation of valence states increases alpha preformation probability.
Although the quantitative role of the $Q_\alpha$ value on alpha radioactivity is rather well described through the tunnel barrier and Gamow like models, its qualitative role remains to be fully understood: is $Q_\alpha > 0$ a necessary or a sufficient condition for alpha radioactivity? As stated above, open questions remain about possible additional alpha emitting nuclei which are experimentally looked for. In order to evaluate the impact of the $Q_\alpha > 0$ condition, Figure 2 displays nuclei having a small spatial localisation from the RHB calculations, as discussed above, removing the $Q_\alpha > 0$ condition. It should be reminded that the $Q_\alpha > 0$ condition is taken from the available measured masses. The comparison between Figs. 1 and 2 first shows that a few more nuclei for experimentally known masses appear: one of the largest change occurs for exotic nuclei for which there is no available experimental masses yet. For these very exotic nuclei, detecting alpha disintegration may be challenging because of the large branching ratio to other decay modes such as beta emission.

Another difference between Fig. 1 and Fig. 2 deals with intermediate mass nuclei, above $N,Z=50$: this is due to the frequent occurrence of $n=1$ states in these nuclei, compared to heavier one. Hence the hindrance of alpha emission for these nuclei is largely due to the $Q_\alpha > 0$ condition, whereas for heavier nuclei, both this condition and the delocalisation effect contribute to the hindrance of alpha emission. For instance several nuclei in the Pb isotopic chain and below are not predicted to be alpha emitters, in agreement with the data. This is explained, in the present approach, by the presence of for instance the $3p_{1/2}$ state, having a large spatial extension due to its $n=3$ value. On the contrary, Sn isotopes can have a large alpha preformation probability due to the presence of $n=1$ states in these lighter nuclei. However most of them have a negative $Q_\alpha$ value, and hence cannot be detected as alpha emitters. These effects shall be discussed in more details into the next section, with the comparison of the $^{104}$Te and $^{212}$Po cases.

### III. ROLE OF LOCALISATION

In order to investigate more precisely the role of spatial localisation on alpha preformation and emission probability, two benchmark cases are compared: $^{212}$Po and $^{104}$Te. The former is a well-known alpha emitter whereas the latter has recently been evidenced as an alpha emitting nuclei [10, 11]. Indeed, the deduced alpha preformation probability has been found larger than in $^{212}$Po. Moreover the alpha lifetime of $^{104}$Te has also been recently described by an alpha+core approach [12], showing the relevance of connecting alpha cluster approaches to alpha emission.

Figure 3 displays the single-particle spectrum of $^{212}$Po obtained with the RHB calculations. Because of the pairing effect, the occupation probability of each state is indicated. For the valence neutrons states, not only $n=1$ states are involved, but also the $2g_{9/2}$ state, which increases the spatial dispersion because it is $n=2$ [14]. The contribution to the spatial localisation is detailed on the bottom of the figure, displaying the partial densities obtained from RHB calculations. The $1i_{11/2}$ state, although of large $\ell$ value, is much more localised than both the $2g_{9/2}$ and $3p_{1/2}$ states, in agreement with our main point on spatial localisation (namely $n$ dependence but $\ell$ independence). It should be noted that the vicinity of the $2g_{9/2}$ state with the $1i_{11/2}$ one is due to the pseudo-spin symmetry (PSS) [25], which plays an impor-


**FIG. 3: Spectrum and partial densities predicted for $^{212}$Po with the RHB calculations**

tant role to describe the behavior of nuclei in this region of the nuclear chart [20].

In the case of the protons, the valence state of $^{212}$Po is almost only made of the $1h_{9/2}$ state. It is also more localised than states with larger \( n \), as seen on the partial densities. Table I summarizes the respective dispersions calculated for the valence states of $^{212}$Po, showing the decisive role of the \( n \) quantum number: a \( n > 1 \) value drastically increases the dispersion by about a factor 2 or more. In summary, spatial localisation analysis shows that $^{212}$Po shall have non-negligible alpha preformation probability, leading to alpha emission. However this effect is decreased due to the presence of \( n = 2 \, 3 \) states in the valence region. This has two roots: i) being a heavy nucleus, \( n > 1 \) states are likely to contribute to the single particle spectrum ii) PSS imposes the vicinity of a \( n = 2 \) state close to the \( 1i_{11/2} \) neutron valence state. It is therefore expected that in lighter nuclei such as $^{104}$Te, the blurring of the spatial localisation disappears because of the absence of \( n > 1 \) states. The dispersion is also expected to be smaller because of its \( A \) dependence (see Eq. 2).

| $^{212}$Po | 2g9/2 | 1i11/2 | 3p1/2 | 1h9/2 | 3s1/2 | 2d3/2 |
|---|---|---|---|---|---|---|
| \( \Delta r \) (fm) | 1.95 | 1.17 | 2.40 | 1.08 | 2.45 | 1.91 |

TABLE I: Spatial dispersion of neutron (left part) and proton (right part) single-particle states of $^{212}$Po calculated with the RHB approach

$^{104}$Te is therefore a specifically interesting nucleus to study alpha preformation probability. It belongs to the lightest region where \( Q_\alpha \) remains positive. Moreover this \( N = Z \) nucleus would also correspond in a simple picture to an alpha particle on top of a doubly magic core. However, this nucleus is close to the proton drip-line, making its description delicate. In the present approach, the axially deformed RHB calculation finds its ground state with a small deformation (\( \beta_2 = 0.14 \)) with a proton valence state at a slightly positive energy, by 140 keV. This could be due to a limitation of the model to describe nuclei close to the drip-line. However due to the Coulomb barrier, the static description of this proton quasi-bound state could still be considered as valid, our main goal being to focus on the spatial localisation of the wave functions and not to study the particle emission process itself. We also wish to consider a global approach such as the relativistic EDF one rather than using more dedicated models to accurately describe a given set of nuclei. Finally, it should be noted that the output of the RHB calculations also shows a collapse of the pairing effect, indicating the role of $^{100}$Sn and alpha as clusters in $^{104}$Te.

Fig 4 shows that only \( n = 1 \) states are involved as valence states, namely the $1g_{7/2}$ state both for neutrons and protons. This is due to the fact that, compared to $^{212}$Po, $^{104}$Te is closer from the lightest nuclei, where clusters states can be found. The corresponding partial densities, as well as the one of the $1g_{9/2}$ located below, are spatially localised, although the $1g_{7/2}$ state shows more extension than the $1g_{9/2}$. In addition $^{104}$Te being a lighter nucleus than $^{212}$Po, the dispersion of the \( n = 1 \) state is also smaller: for instance the $1g_{9/2}$ one is 0.98 fm, to be compared with the values for \( n = 1 \) in Table I. It should be noted that the dispersion of the $1g_{7/2}$ state is about 1.5 fm, which is larger, probably due to the difficulty to describe such a nucleus close to the drip-line, involving quasi-bound states: the dispersion of the $1g_{9/2}$ state is more representative of the typical spatial dispersion at work in this nuclei. Under this assumption, the neutron valence states of $^{212}$Po have a spatial dispersion in average, about 40 % larger than the $1g_{9/2}$ of $^{104}$Te.

It should be noted that the lowest neutron Kramers states originating from the $2d_{5/2}$ state in $^{104}$Te are located at -11.2 MeV, showing that the degeneracy raising between PSS partner states [21] is much larger than in $^{212}$Po. This is due to the effect of deformation in $^{104}$Te, overcoming the one of the PSS.

**IV. STUDY OF THE PREFORMATION FACTOR**

A. Phenomenological alpha preformation model

Due to the complexity of the properties of the alpha emission [1], phenomenological models are often used to describe it, as illustrated by the successful Geiger-Nuttall law [1]. Following this spirit, it could be useful to provide as an alternative way, a phenomenological relation between the alpha preformation probability and the spatial localisation, over the nuclear chart.

The microscopic RHB calculations of the spatial dispersion of the valence states of $^{212}$Po (see Table I) and $^{104}$Te allows to calculate their average value, leading to
the following relation, as discussed in the previous section:

\[ <\Delta r(212\text{Po})> \simeq 1.4 <\Delta r(104\text{Te})> \]  

(4)

Inspired by the form of the Geiger-Nuttall law, our ansatz for the alpha preformation probability \( P \) is a power law as a function of the localisation parameter:

\[ P = 10^{-BA_{\text{loc}}+C} \]  

(5)

where \( B \) and \( C \) are constants to be determined. In a recent experiment [10], the alpha preformation probability in \( ^{104}\text{Te} \) was deduced to be at least 3 times larger than in \( ^{212}\text{Po} \). We therefore take \( P(^{104}\text{Te})=1 \) and \( P(^{212}\text{Po})=0.1 \) to mimic this effect. This allows to determine \( B \) and \( C \), namely with Eq. (2):

\[ \text{Log} \sqrt{P} = 1 - \left( \frac{A}{100} \right)^{1/6} \sqrt{2n-1} \]  

(6)

Since the above dependence on \( A \) is rather weak over the nuclear chart, this law can be approximated by

\[ \text{Log} \sqrt{P} \simeq 1 - \sqrt{2n-1} \]  

(7)

where \( n \) is the radial quantum number of the valence state of the considered nucleus. In the case of pairing effect, \( n \) can be taken as the average of the \( n \) values of the valence states weighted by their occupation probabilities. The alpha preformation probability calculated with Eq. (7) is reduced by a factor 20-30 when the valence state switches from a \( n=1 \) to a \( n=2 \) state. This result is in agreement with the typical observed variation of the estimation of the preformation of the alpha probability extracted from the data (see e.g. Fig. 4 of Ref. [9]).

The present description also allows for a more detailed discussion. The \( N=126 \) shell effect is phenomenologically known to impact the alpha preformation probability [9]. In the present analysis, the strong increase of the preformation probability starting from \( N=128 \) comes from the filling of the \( 1i_{13/2} \) state (although partially, i.e. together with the \( 2g_{9/2} \) state, as seen on Fig. 1) whereas the regular decrease of the preformation probability before \( N=128 \) is related to the progressive filling from \( n=1 \) state \( (1i_{13/2}) \) to \( n=2,3 \) states such as \( 2s_{1/2}, 3p_{3/2} \) and \( 3p_{1/2} \).

Another question raised was the non observance of any \( Z=82 \) shell effect on the preformation probability [9]. The present interpretation based on the role of \( n=1 \) localised valence states provides a clear explanation: looking to the experimental alpha emitters (Fig. 1), an isotopic chain of alpha emitters nuclei through \( N=126 \) involves many nuclei which are moreover close to the stability line (i.e. just above \( ^{208}\text{Po} \)). Hence the filling of the \( n=1 \) state beyond \( N=126 \) happens in a similar way for the various isotopic chains, from \( Z=84 \) (Po) to \( Z=92 \) (U). On the contrary, following an isotonic chain of alpha emitters nuclei through \( Z=82 \) involves much fewer nuclei, due in part to the proton drip-line: more intense nuclear structure effects are expected, and the occurrence of the \( n=1 \) state just above \( Z=82 \) is expected to be much less systematic.

B. Evaluation of the alpha preformation factor

In order to substantiate the above findings, it could be useful to consider a complementary approach to evaluate the alpha preformation factor. A relevant way is to consider the following formula for the alpha emission half-life:

\[ \text{Log}_{10} T_{1/2}^{\text{Pheno}}(s) = \frac{9.54(Z-2)^{0.6}}{\sqrt{Q_\alpha}} - 51.37 \]  

(8)

where \( Q_\alpha \) is in MeV. In [9] it has been shown that Eq. (3) both accurately describes the experimental data and compares well to theoretical WKB approximation inferring a preformation probability \( P=1 \). Therefore discrepancy of the data with respect to this formula shall be first driven by the behavior of the alpha preformation factor. More precisely the ratio \( T_{1/2}^{\text{Pheno}}/T_{1/2}^{\text{Exp}} = W_{\text{Exp}}/W_{\text{Pheno}} \), where \( W \) is the total \( \alpha \) emission probability, shall give an evaluation of the alpha preformation factor, as discussed in [9].

Fig. 5 displays this ratio for \( Z \geq 82 \) nuclei, where the experimental data is known, which shall scales the alpha preformation factor (see e.g. Fig. 4 of [9]). Only even-even nuclei are displayed but we have also done a systematic calculation showing that almost all the nuclei with the smallest preformation factor are odd ones, in agreement with the hindrance effect of the alpha preformation, known to occur in such nuclei [28, 29]. The present quantity is therefore a good probe for the alpha preformation
factor in nuclei. Fig. first shows that there is a sharp increase of this ratio for \( N \geq 128 \), showing an important shell effect. Nuclei which are predicted as localised ones (see section II for the criteria), both for the protons and neutrons valences wave functions, from the microscopic RHB calculation are displayed in red. They correspond to most of nuclei having the largest alpha preformation factor, especially around the \( N=128 \) shell closure. This shows a clear correlation between localisation and alpha preformation probability and gives quantitative grounds to the present analysis of the role of localisation on the alpha preformation factor.

![Diagram](image.png)

**Fig. 5:** Ratio of the phenomenological to experimental alpha emission half-life for \( Z=84,86,88 \) even-even nuclei. Those predicted with a small dispersion (see text) are displayed in red.

### V. CONCLUSION

The alpha preformation probability has been analysed through the behavior of the spatial localization of nucleonic states. The systematically more localised \( n=1 \) states, independently of the orbital angular momentum value, allow to pinpoint nuclei which are more likely to have a large preformation probability over the nuclear chart. In order to compare with experimentally known alpha emitters, axially deformed RHB calculations have been performed over the nuclear chart to provide microscopic spatial dispersions. The systematic occurrence of more localised valence states (which does have \( n=1 \)) shows a pattern which is in agreement with experimentally known alpha emitters. The investigation of the single-particle spectra of \( {}^{212} \)Po and \( {}^{104} \)Te allows to understand in more details why the alpha preformation probability is larger in the latter than in the former. This is partly due to the PSS symmetry at work in \( {}^{212} \)Po, involving a \( n=2 \) state, and to the fact that being a lighter nucleus, \( {}^{104} \)Te involves almost only \( n=1 \) states, each of them also having a bit smaller dispersion due to the mass effect on the localisation parameter. A phenomenological law relating the preformation probability to the radial quantum number of the valence states has been extracted, allowing to describe the impact of shell effects on this probability. Finally, a phenomenological evaluation of the alpha preformation factor shows that the present microscopic criteria for localised state explains the enhancement of the alpha preformation factor, especially after shell closure. All these results show the relevance of relativistic approaches, not only to describe cluster states in nuclei, but also to grasp the main properties of alpha radioactivity.

The present approach does not aim to be very accurate, especially in the difficult domain of alpha radioactivity, where various orders of magnitudes are at stake. Effects of more advanced deformations could be studied, such as the role of triaxiality and/or octupolar deformations. The description of \( {}^{104} \)Te could also be improved with a more dedicated model, suited for nuclei close to the drip line.

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