Exact calculation of proton decay rates from excited states in spherical nuclei

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An *exact* approach for the determination of proton-decay widths in spherical nuclei is presented. It consists of solving numerically the one-dimensional time-dependent Schrödinger equation for initial proton quasistationary states obtained in the framework of a single-particle model. From the time dependence of the metastable state one can infer the dynamics of the decay and calculate the lifetime. The validity of this approach is demonstrated and quantitative comparisons with existing approximate, stationary methods are reviewed. Finally, the advantages and perspectives of this new method are discussed. [S0556-2813(99)04111-4]

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I. INTRODUCTION

Since the first observation of proton radioactivity from an isomeric state in ^{53}Co in 1970 [1], much experimental [2–4] and theoretical [5–9] effort has been devoted to the study of this rare decay phenomenon. It has been stressed that proton emission from ground states of exotic nuclei limits the range of possible isospin values on the proton-rich side of the valley of stability. Moreover, the single-particle character of the resonances in nuclei far from stability can provide valuable nuclear structure information that complements other experimental measurements [3].

From the theoretical perspective it is believed that the calculation of proton-decay rates can be done through a straightforward application of the α-decay theory albeit with the simplification that there is no need to calculate the preformation factor. The physical picture is that of a single proton tunneling through the average, spherical Coulomb, and centrifugal barrier created by its interaction with the (core) daughter nucleus. Historically, the lifetime for this process was calculated using a time-independent approach, e.g., the WKB approximation. In addition to the intrinsic limitations imposed by this simple picture, unavoidable errors are expected because of the approximations involved in the usual stationary approaches.

In this paper the proton-decay rate is calculated via an alternate method, namely, through the numerical solution of the time-dependent Schrödinger equation (TDSE) for prepared initial quasistationary proton states. The purpose of this paper is to demonstrate the validity of this new method and to use it to estimate the ''errors'' of the usual stationary approaches. A simple model of spherical proton decay is introduced in Sec. II. We then compare several methods to compute the decay width Γ_p in Sec. III: the two most commonly used stationary approaches [WKB and distorted wave Born approximation (DWBA)] and our new time-dependent method. Finally, Sec. IV gathers results obtained with the TDSE approach and compares them with WKB and DWBA results. A summary and discussion end this paper.

Although this paper is concerned with the presentation of this new method applied to the simple model mentioned above, it will be argued that it can be extended, unlike most of the approximate schemes, to encompass much more difficult problems (deformed interacting potential [10], dynamical deformation of the nuclear surface during proton emission [11], etc.).

II. PROTON DECAY: A SIMPLE MODEL

Following the literature [8], the interaction between the proton and the rest of the nucleus is described by a single-particle spherical potential as

$$V(r)=V_n(r)+V_c(r)+\frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}. \tag{1}$$

The nuclear term $V_n(r)$ is given by the sum of a Woods-Saxon part and a related Thomas spin-orbit term

$$V_n(r)=-V_0 f_0(r)+V_{so}(\vec{\sigma}\cdot\vec{l})\lambda_\pi^2\frac{1}{r}\frac{d}{dr}f_{so}(r), \tag{2}$$

with

$$f_i(r)=\frac{1}{1+\exp[(r-R_i)/a_i]}. \tag{3}$$

The quantity V_c is the usual Coulomb potential that describes the interaction of a pointlike proton with a uniformly charged spherical nucleus of radius R_c. The parameters used in our calculations have been taken from [12] and are gathered in Table I. However, the depth V_0 of the nuclear Woods-Saxon potential has not been taken from [12] but rather adjusted according to our needs as explained in Sec. III C.

TABLE I. Single-particle potential parameters.

$R_0=1.17\times A^{1/3}$ fm	$a_0=a_{so}=0.75$ fm	$R_c=1.21\times A^{1/3}$ fm
$R_{so}=1.01\times A^{1/3}$ fm	$V_{so}=6.2$ MeV	$\lambda_\pi^2\simeq 2.0$ fm^2

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III. ESCAPE RATE

In this section, we summarize two widely used stationary approaches to compute the proton-decay width, namely, the WKB and DWBA approximations. In a third part, we will introduce our numerical method dedicated to the same problem.

A. WKB approximation

In this semiclassical approximation, the width of a low-lying metastable state is given by

$$\Gamma_{\mathrm{WKB}}=\mathcal{N}\frac{\hbar^2}{4\mu}\exp\left[-2\int_{r_1}^{r_2}k(r)dr\right], \tag{4}$$

where

$$\hbar k(r)=\sqrt{2\mu|E_0-V(r)|} \tag{5}$$

is the classical momentum of the emitted particle. The normalization factor is

$$\mathcal{N}^{-1}=\int_{r_0}^{r_1}dr\,\frac{1}{k(r)}\cos^2\left[\int_{r_0}^{r}k(r')dr'-\pi/4\right], \tag{6}$$

where (r_0,r_1,r_2) are the classical turning points ordered by increasing distance from the origin.

Very often, the $\cos^2$ term in this last equation is approximated by its average value of $\frac{1}{2}$; then,

$$\mathcal{N}^{-1}=\frac{1}{2}\int_{r_0}^{r_1}\frac{dr}{k(r)}. \tag{7}$$

Following [8], we will denote this approximation as WKB1 to differentiate it from the WKB approximation given by Eq. (6).

B. Distorted wave Born approximation

The calculation of the proton-decay width can also be carried out through the distorted wave Born approximation used in direct reaction theory [13]. In this case, the proton decay is treated as a resonance, the proton being trapped in the target nucleus for a certain length of time.[1] The heart of this approach relies on the transition amplitude $T(A+1,Z+1\rightarrow A,Z)$ which is related to the proton-decay width by

$$\Gamma=2\pi|T(A+1,Z+1\rightarrow A,Z)|^2. \tag{8}$$

In the DWBA, this transition amplitude reads

$$T(A+1,Z+1\rightarrow A,Z)=\langle\chi_{Ap},\phi_A\phi_p|V_{Ap}|\phi_{A+1}\rangle, \tag{9}$$

where χ_{Ap} represents the relative motion of the proton with respect to the daughter nucleus, ϕ_A and ϕ_p represent the intrinsic wave functions of the daughter nucleus and proton, and ϕ_{A+1} represents the quasistationary state of the parent nucleus. Of course, V_{Ap} represents the interaction between the proton and daughter nucleus, represented by the simplified one-body potential of Eq. (1).

Assuming that the proton is in its ground state and considering the daughter nucleus as an inert core, one can show that the decay width is given by

$$\Gamma_{\mathrm{DWBA}}=\frac{4\mu}{\hbar^2k}\left|\int_0^\infty dr\,F_l(r)(V_N+\delta V_c)\phi_{nlj}(r)\right|^2. \tag{10}$$

$F_l(r)$ is the regular Coulomb wave function and $\phi_{nlj}(r)$ is the radial wave function representing the quasistationary proton state. $\delta V_c=V_c-(Ze^2)/r$ is the correction from a point-like charge distribution. In our work, $\phi_{nlj}(r)$ has been obtained within the two-potential approach (TPA) developed by Gurvitz and Kalbermann [14]. This method will be presented and discussed in the next section.[2]

C. Numerical approach

Within the same simple model of a quasibound state leaking by the tunneling effect through a one-body potential, the most straightforward (and intuitive) way to compute the decay rate (or decay width) of this state is to perform a numerical integration of the time-dependent Schrödinger equation describing this process. This method has already been applied to α decay [15] and nuclear fission [16].

The TDSE describing the interaction between the proton and the spherical daughter nucleus has the form

$$i\hbar\frac{\partial}{\partial t}\psi_p(r,t)=\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r)\right]\psi_p(r,t), \tag{11}$$

in which $\psi_p(r,t)$ represents the quasistationary proton state and $V(r)$ the interacting potential described in Eq. (1).

The integration of TDSE has been achieved through a space and time discretization and with the use of a time propagator method called MSD2 [17]. Obviously, we are dealing with an initial-value problem, hence requiring knowledge of the state at time $t=0$. As mentioned above, the initial state is obtained through the scheme of Gurvitz and Kalbermann [14]; i.e., we define a quasistationary state ψ_{qs} as an eigenstate of a modified Hamiltonian

$$[H(r)+\epsilon(r)]\psi_{\mathrm{qs}}=E_{\mathrm{qs}}\psi_{\mathrm{qs}}. \tag{12}$$

[1]It has been argued in Ref. [13] that this two-step process can still be seen as a ''direct reaction'' since it does not imply the formation of an equilibrated compound nucleus.

[2]To be totally rigorous, $\phi_{nlj}(r)$ should be obtained by joining continuously the quasistationary ''TPA'' wave function with the irregular Coulomb wave function $G_l(r)$ describing the behavior of the proton as $r\rightarrow\infty$. Nevertheless, it has been shown in Ref. [8] that the contribution of the integrand in Eq. (10) to the decay width Γ is mainly due to the region around the nuclear surface, allowing us to safely neglect the influence of $G_l(r)$ on the lifetime of not-very-high-lying quasistationary states.

In most of our calculations, the modification $\epsilon(r)$ has been defined by

$$\epsilon(r)=\begin{cases} V_B - V(r) & \text{if } r \geqslant r_B \\ 0 & \text{elsewhere}, \end{cases} \tag{13}$$

where r_B denotes the position of the top of the barrier, and $V_B = V(r_B)$. We will see that the arbitrary choice of the modification $\epsilon(r)$ does not influence the computation of the decay width.

Following the proton wave function in time, one can compute the following quantities.

(i) The *tunneling probability* defined by

$$P_{\text{tun}}(t,r_B)=\int_{r_B}^{\infty} dr |\psi(r,t)|^2, \tag{14}$$

which represents the probability that the proton is outside the nuclear surface (i.e., has been emitted) by the time *t*.

(ii) The *decay rate* which is related to the tunneling probability through

$$\lambda(t,r_B)=\frac{1}{1-\rho(t,r_B)}\frac{d\rho(t,r_B)}{dt}. \tag{15}$$

This quantity can then be directly compared to the stationary values λ_{WKB} and λ_{DWBA} related to the decay width by the simple expression

$$\Gamma = \hbar\lambda.$$

IV. RESULTS

We have computed proton-decay widths for hypothetical excited states in the (spherical) ^{109}I nucleus, and then compared the values obtained with the usual stationary ones.

A. Quasistationary proton states

Before going further, we mention here the main difficulty of our numerical approach. For very-low-lying states (low energy+large potential barrier), the tunneling rates can be very small (very narrow decay widths), making difficult their numerical computation. In order to avoid this problem but without losing any interest in this approach, we will consider here only proton-excited states for which the computation of their decay rates is made easier. Nevertheless, it is worth noting that this concession is not too harmful: first, within this method, one can still study (time dependently) processes like βp, $\beta 2p$, etc., for which semiclassical methods are not well suited; second, one can still study the ''errors'' of these latter approaches through a wide range of energies and angular momenta; finally, numerical improvements of our method have indeed proved that one can reach experimentally observable ground-state proton emitters [18].

High-energy levels can easily be obtained by varying the depth V_0 of the nuclear Woods-Saxon potential. In Fig. 1, such an hypothetical quasistationary proton state in ^{109}I, with angular momentum $l_p=2$, has been represented, along with the total interacting potential $V_{pA}(r)$ of depth $V_0 = 51$ MeV.

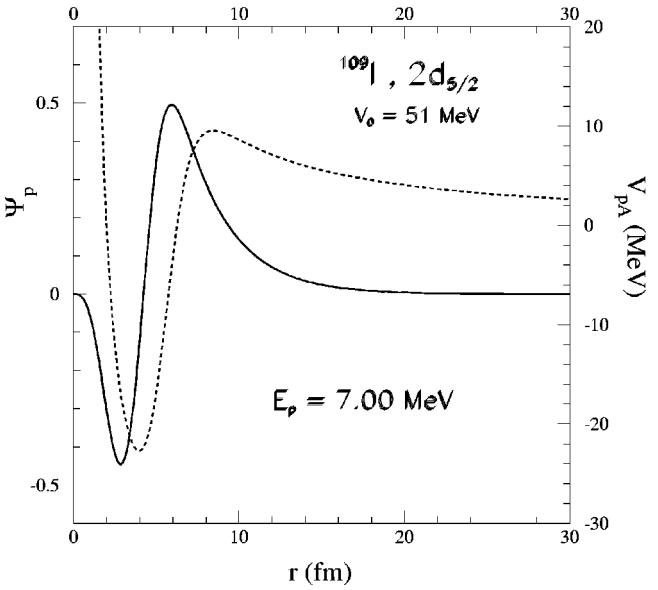

FIG. 1. The wave function of a quasistationary proton state in ^{109}I (solid line) and potential $V_{pA}(r)$ (dashed line).

B. Time evolution

Performing the numerical integration of the TDSE for this particular state allows us to follow ψ in time. The square root of this wave function in the vicinity of the potential well is represented at four times in Fig. 2. At the observed times, it is interesting to note that the shape of the wave function inside the potential well is retained. This is related to the onset of exponential decay [19].

As observed earlier [15], the time behavior of the decay rate $\lambda(t)$ (see Fig. 3) can be split into two distinct stages: an initial one during which the decay rate strongly varies (i.e., there are deviations from an exponential decay) and corresponding to the ''acclimation'' of the quasistationary state to its new environment at time $t=0$, and a second stage during which the decay is exponential. From the ''asymptotic'' value of the decay rate, $\lambda(\infty)$, it is possible to infer a decay width through the simple relation

$$\Gamma_{\text{TDSE}} = \hbar\lambda(\infty) \tag{16}$$

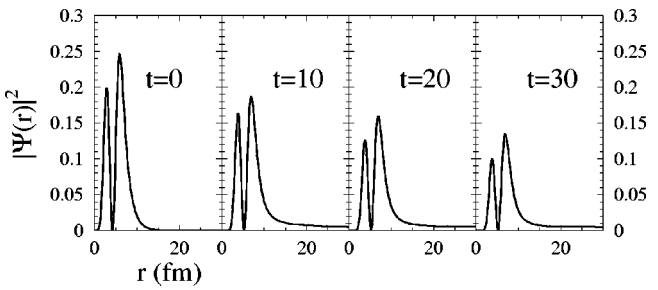

FIG. 2. Time evolution of the quasistationary state from Fig. 1. Times are in 10^{-22} sec.

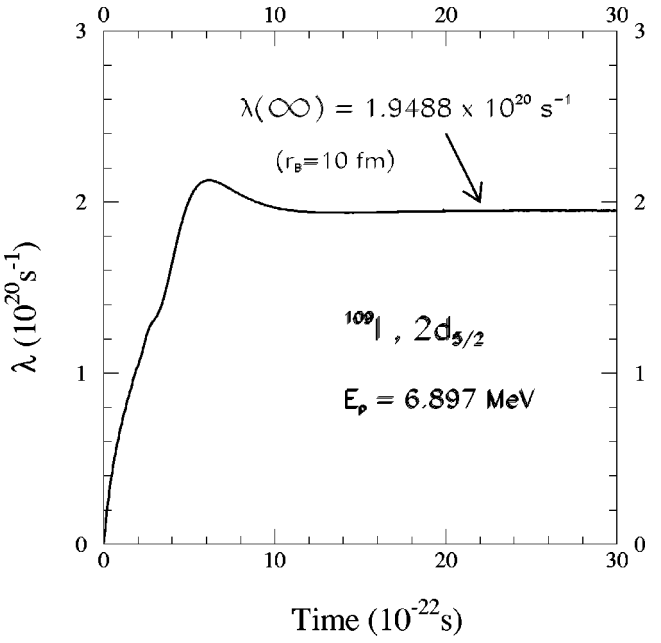

FIG. 3. Time-dependent decay rate $\lambda(t)$ obtained with the initial quasistationary state of Fig. 1.

and compare it to the values obtained using the usual stationary approaches.

C. Validity of the TDSE approach

Our goal here is to show the validity of such an approach in allowing the several *arbitrarily chosen* parameters to vary freely. First of all, is the ''asymptotic'' decay rate $\lambda(\infty)$ sensitive to the choice of the potential modification in the Gurvitz procedure? To answer this question, we have considered three different modifications of the ''true'' potential $V(r)$, namely,

$$\epsilon(r)=\begin{cases} V_B+(r-r_B)\tan(\theta)-V(r) & \text{if } r\geqslant r_B \\ 0 \quad \text{elsewhere}, \end{cases} \tag{17}$$

with $\theta=0°$ (modification used previously), $\theta=80°$, and without any modification. In this last case, the quasistationary state is obtained through a numerical integration of the *stationary* Schrödinger equation on a discretized space r:0 $\rightarrow$30 fm, while the numerical integration of the TDSE is performed on a much larger grid, let us say r:0$\rightarrow$400 fm. This fact along with the unavoidable numerical errors, make the *eigenstate* a true quasistationary state for our problem.

The three different wave functions corresponding to the ''same'' quasistationary state are represented in Fig. 4.

Note that for the ''unmodified'' potential, the proton wave function exhibits nonvanishing values outside the well, which are due to the presence of an artificial infinite potential wall at the end of the numerical discretized grid ($r_{\max}$ =30 fm). Obviously, this state is not really suited to our problem since the wave function is not initially confined inside the well. Nevertheless, we will see that even in this ''dramatic'' situation, our numerical approach still gives a reliable value for the half-life of the state.

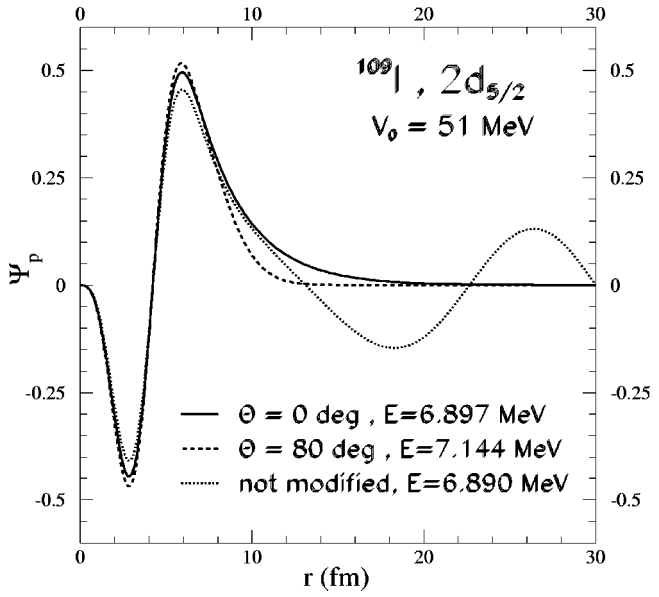

FIG. 4. Three ''different'' wave functions representing the ''same'' initial quasistationary state.

The time-dependent decay rates $\lambda(t)$ obtained considering the three initial wave functions represented in Fig. 4 are plotted in Fig. 5. One can clearly see that the first transition stage strongly depends on the way of constructing the quasistationary state. On the other hand, the following (exponential) stage is independent of the particular choice made for the modification of the initial potential, though noisy oscillations appear on the third curve but without modifying the ''mean asymptotic'' value $\lambda(\infty)$. This result confirms the hypothesis suggested by Goldberger and Watson [20] that the long time behavior of a metastable state is independent of its particular formation.

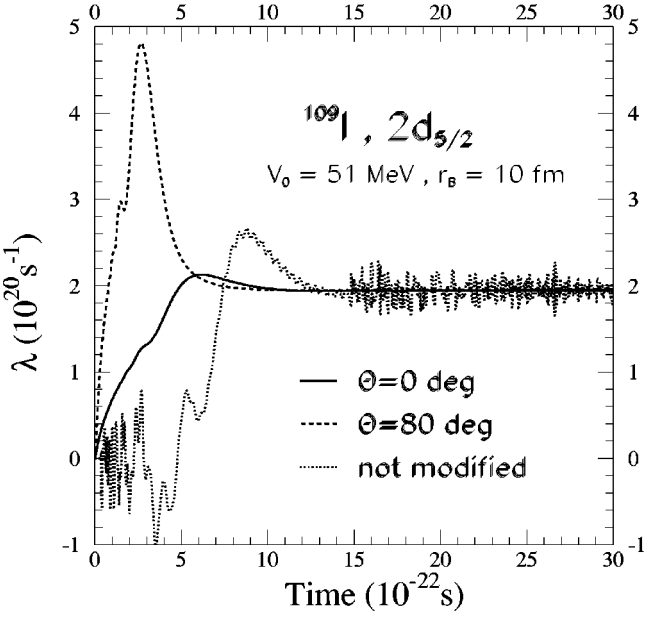

FIG. 5. Time-dependent decay rates corresponding to the three ''different'' initial states represented in Fig. 4.

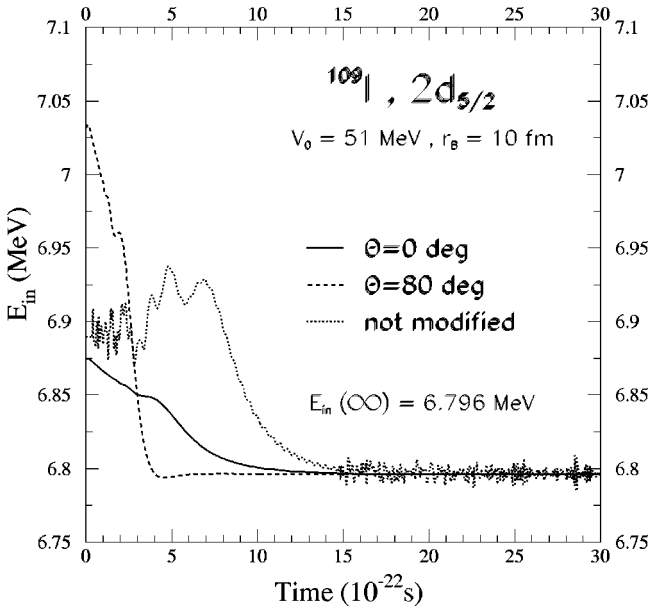

FIG. 6. ''Internal'' energy of the quasistationary states of Fig. 4.

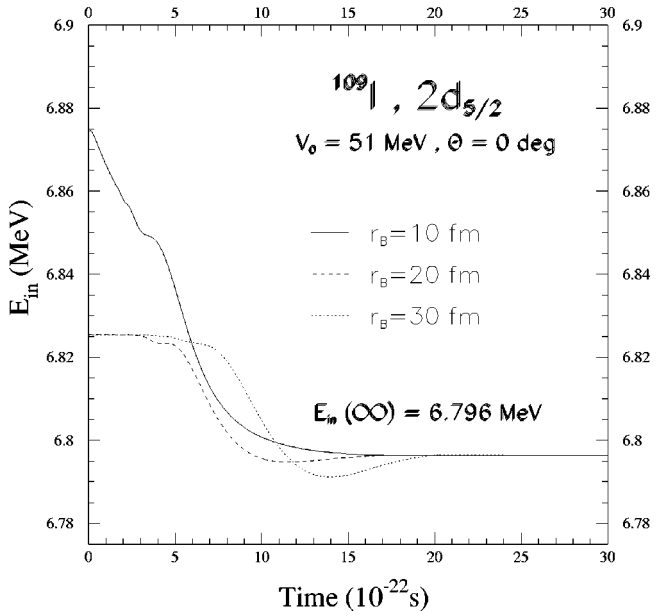

FIG. 7. Dependence of $E_{\rm in}$ on the ridge parameter r_B.

As noted above, from this unambiguous ''asymptotic'' value $\lambda(\infty)$ one can easily calculate the lifetime of the state, which in turn can be compared to semiclassical estimations. Nevertheless, because the form of the potential was different in each of the three cases, one has to pay attention that the three ''different'' states do not have the same energy when introduced in the TDSE, as shown in Fig. 4. But this energy is an important ingredient in stationary recipes. This question is actually solved in looking at the energy of the state truncated (and renormalized) inside the potential well. This ''internal'' energy is given by

$$E_{\rm in}(r_B,t)=\int_0^{r_B}\psi^*(r,t)H(r)\psi(r,t)dr \Big/ \int_0^{r_B}\psi^*(r,t)\psi(r,t)dr \qquad (18)$$

and is represented in Fig. 6 for the three wave functions considered. Like the decay rate time behavior, this quantity shows two clearly distinguished stages. The first one which again depends on the formation of the state and the second one which is common to all three wave functions. This ''asymptotic'' internal energy $E_{\rm in}(\infty)$ corresponds to the experimental proton energy Q_p corrected from electron screening and recoil energies, and is the one that should be used in the stationary approaches. Finally, Fig. 7 shows that the quantity $E_{\rm in}(r_B,\infty)$ does not depend on the particular value of the arbitrary ridge r_B.[3] Only the tunneling probability $P_{\rm tun}(t,r_B)$ is actually affected by the chosen value r_B. The decay rate $\lambda(\infty)$, and so the lifetime of the state, is independent of this particular value.

A last question remains: how can one determine *a priori* the energy $E_{\rm in}(\infty)$ of the quasistationary state without having to solve the TDSE? This question can be answered in the following way: Figure 8 displays the difference between the initial energy $E_{\rm in}(t=0)$ and the ''asymptotic'' one $E_{\rm in}(\infty)$. This difference clearly decreases with decreasing the energy of the metastable state. Hence, for ground-state proton energies (of the order of 1 MeV), $E_{\rm in}(\infty)=E_{\rm in}(t=0)$.

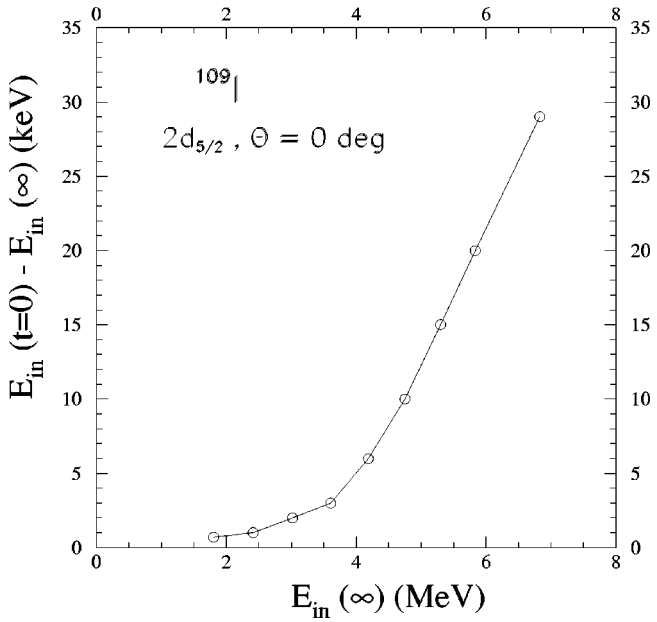

FIG. 8. Initial minus ''asymptotic'' internal energies for different quasistationary states obtained in varying the potential depth V_0.

[3]Of course, an infinite value for r_B would imply an infinite time to reach the value $E_{\rm in}(\infty)$.

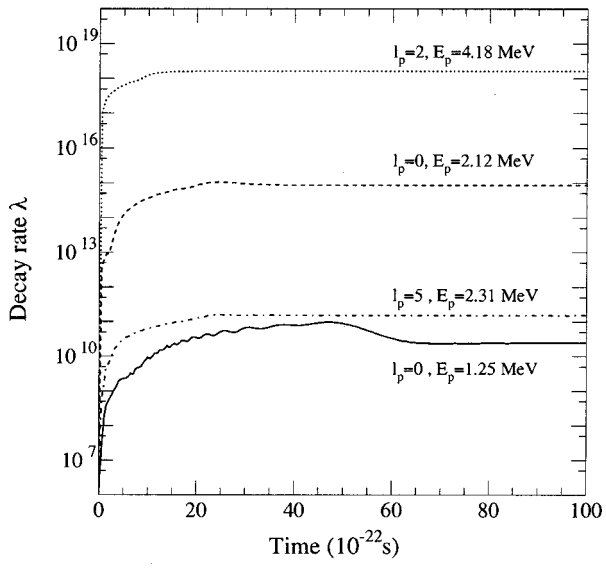

FIG. 9. Time evolution of the decay rate λ for several proton states. The lowest state studied lies at 1.25 MeV, with zero angular momentum. The corresponding half-life is $T_{1/2}=(2.8\pm0.1)\times10^{-11}$ sec.

D. Comparison with stationary approaches

We have repeated the same time-dependent calculations for several hypothetical initial quasistationary states in order to map the two-dimensional space (E_p, l_p) and to compare the lifetimes obtained with the usual WKB and DWBA computations.

In Fig. 9 the time evolution of the decay rates for several relatively low-lying states is represented. For the lowest state at $E_p=1.25$ MeV, the decay rate reaches an asymptotic behavior much later because its outer turning point lies much further ($r_{\text{out}}\simeq60$ fm).

Finally, Fig. 10 gathers the comparison between the usual WKB and DWBA half-life estimates and our numerical approach.

All the used approximations provide us with the correct order of magnitude of the lifetime of the hypothetical proton metastable states studied. Nevertheless, the WKB lifetimes can overestimate (or underestimate) the numerical (exact) ones by more than 50%. These errors appear also to be strongly influenced by the angular momentum l_p. Interestingly, the somewhat less sophisticated WKB1 approximation reduces the computed errors. Finally, the DWBA scheme seems very well suited to this kind of analysis since, for all low-lying states, errors are contained within less than 5–10 %. The discrepancies observed between the TDSE and DWBA for higher energy levels might be due to the fact that we did not treat correctly in our DWBA calculations the connection between the quasistationary state inside the well and the irregular Coulomb function $G_l(r)$ at larger distances r.

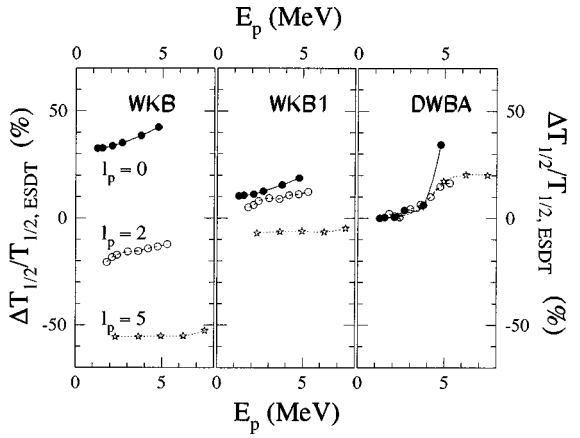

FIG. 10. Comparisons between the lifetimes obtained thanks to the TDSE numerical solution and the ones computed within the stationary approaches WKB and DWBA.

V. SUMMARY AND DISCUSSION

In summary, the one-dimensional time-dependent Schrödinger equation has been solved numerically for initial proton quasistationary states in spherical nuclei. Following the proton metastable wave function $\psi_p(r,t)$ in time, one has access to the proton decay width Γ_{TDSE}. We have demonstrated the validity of this exact approach and compared its results to the ones from widely used stationary methods, namely, WKB and DWBA, for a large range of energies and angular momenta.

Although providing the correct order of magnitude for the proton lifetimes studied, the WKB approach can give rise to errors as high as 50%. Contrarily, the DWBA scheme is found to be reliable through a large range of proton energies and angular momenta. In addition to proton lifetimes, the full dynamics of the decay is made accessible thanks to our numerical approach, hence allowing the study of more complicated problems. One of them is doubtlessly the phenomenon of proton emission from a parent-deformed nucleus, leading to a spherical daughter one [11]. As mentioned in this paper, the current numerical limitation of our code constrains us to study only proton-excited states. Nevertheless, we believe that this drawback will be overcome in the near future and that the TDSE scheme is the right approach to treat all problems encountered in p, n, and α decays of nuclei in their ground states.

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