Exact dynamical approach to spherical ground-state proton emitters

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The proton emission from ground-state spherical nuclei is investigated exactly through the numerical solution of the time-dependent Schrödinger equation for initial single-proton quasistationary states. Contrary to common belief, it is shown that such calculations can be performed for any proton half-life ranging from 10^{-22}–20 s, the longest proton lifetime observed at present. The important and careful choice of the initial metastable state is clarified. Applied to the calculation of the decay width of several ground-state spherical emitters, this method gives comparable results with the distorted wave-Born approximation and therefore justifies its use.

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The search for and study of proton emitters is a very active field in nuclear physics nowadays. The very rich nuclear structure information which can be extracted from this phenomenon at the proton dripline and the new prospects offered by radioactive ion beam facilities contribute to the current wealth of this field.

The decay of a nucleus by emission of one proton is a simple example of a quantum tunneling process. If the nucleus is deformed, the proton feels an anisotropic potential barrier and therefore undergoes a multidimensional tunneling. Ground-state proton emitters are commonly described as single-particle quasistationary states which decay with a rather long but finite lifetime. Theoretical approaches [1–3] have mainly dealt with the determination of the main observable of this phenomenon, i.e., the half-life of the proton decay. These approximate, stationary, schemes have been applied quite successfully to interpret the fast growing amount of experimental data for spherical as well as deformed nuclei. It has also been argued that the observation of the proton decay of a deformed nucleus can bring reliable information about its deformation [4–7].

In spite of these efforts, one still lacks a direct, exact, fully time-dependent approach to encompass the richness of the dynamical tunneling process which lies at the heart of the proton emission. Such a method has in fact been proposed recently to treat α [8] and p decays [9]. It consists of solving numerically the time-dependent Schrödinger equation (TDSE) for initial quasistationary single-particle states. This approach is exact (up to the numerical accuracy), intuitive, and fully dynamic (one follows the wave function in time). Moreover, its multidimensional counterpart is straightforward [10].

The question now is why such a method is not more commonly used. We believe that the answer is built on two main arguments which have been raised against this approach. One is of a numerical nature, the other one has a more physical tone. Until now, it was believed that the numerical accuracy required to localize tiny single-proton quasistationary widths, typically of the order of 10^{-20} MeV, could not be reached within the TDSE scheme, except in going towards highly accurate computer codes which would, therefore, be prohibitively expensive in computer time. The second argument is related to the coexistence of two drastically different characteristic times in the decaying system. Indeed, its lifetime is typically a fraction of a second, many orders of magnitude larger than typical oscillations of the proton wave function inside the metastable well. The critical question of how one can get a stable numerical solution of the Schrödinger equation that describes simultaneously these two different dynamics has been raised recently by Bertulani *et al.* [11], while applying a similar scheme to the study of the bremsstrahlung by a tunneling α particle.

It is the purpose of this paper to show how these two arguments can be overcome, and that the TDSE approach is indeed able to provide reliable results for the half-lives of long-lived metastable proton states. It will also be argued that this method presents many advantages compared to the existing stationary methods to treat more difficult problems (fine structure in proton decay from deformed nuclei [7], proton emission from a deformed parent nucleus to a spherical daughter nucleus [12,13], etc.).

For now, let us briefly describe the TDSE approach (for more details, see [8,10]). As explained above, the idea of this method is to solve numerically the time-dependent Schrödinger equation for initial single-proton quasistationary states. In one-dimension (spherical decaying nucleus), this equation reads

$$i\hbar \frac{\partial}{\partial t}\psi_p(r,t)=\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}+V(r,t)\right]\psi_p(r,t), \qquad (1)$$

where $\psi_p(r,t)$ represents the quasistationary proton state, and $V(r,t)$ is the interaction between the emitted proton and the core daughter nucleus. In this paper, we will assume that this interaction is static, i.e., $\langle V(r,t)\rangle = V(r)$. The initial wave function $\psi_p(r,0)$ is chosen as a quasistationary, or metastable, state. The commonly used method to prepare

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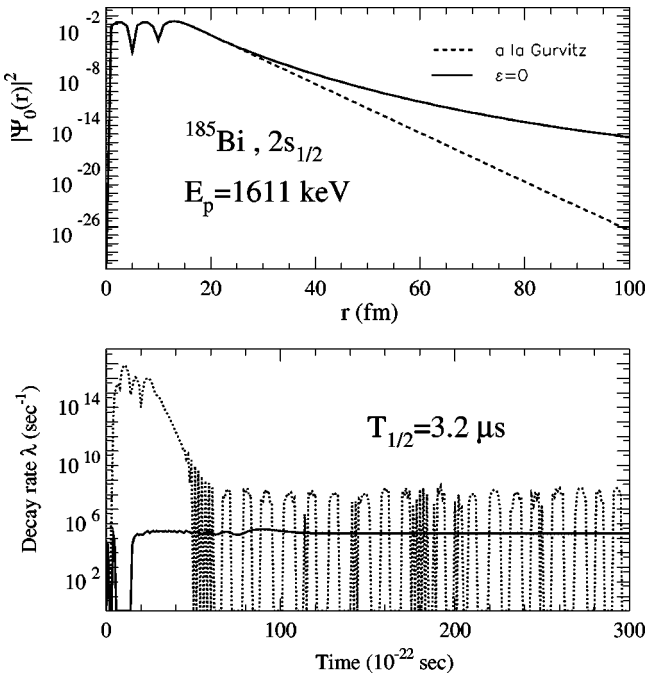

FIG. 1. Importance of the choice of the initial quasistationary state for its half-life calculation. Note the removal of the ''bump'' in the early stage of the decay between the two $\lambda(t)$ curves.

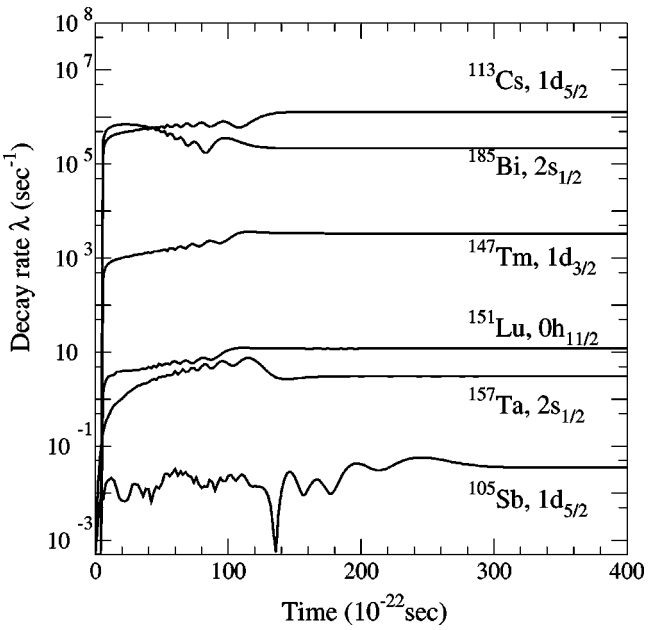

FIG. 2. Time evolution of the decay rates for several observed ground-state proton emitters.

such a state is the Gurvitz and Kalbermann procedure [14], i.e., a quasistationary state is defined as an eigenstate of a modified Hamiltonian

$$[\mathcal{H}(r)+\epsilon(r)]\psi_{qs}(r)=E_{qs}\psi_{qs}(r). \tag{2}$$

In the original Gurvitz procedure, the modification of the potential reads

$$\epsilon(r)=\begin{cases} V_B-V(r) & \text{if } r\geqslant r_B \\ 0 \quad \text{elsewhere,} \end{cases} \tag{3}$$

where r_B denotes the position of the top of the barrier, and $V_B=V(r_B)$. This form of $\epsilon(r)$ implies that only the tail of the wave function is significantly perturbed. We solved the *stationary* Schrödinger equation for the Hamiltonian $(\mathcal{H}+\epsilon)(r)$, discretized on a spatial grid characterized by an $r_{\max}$ ranging from 30 to 100 fm, and a typical mesh ranging from 0.1 to 0.5 fm. The resulting, quasistationary, wave function is then introduced as the initial wave function in Eq. (1). This TDSE is integrated using a time propagator method called MSD2 [15], which is simply the predictor-corrector ''leap-frog'' method [16] without the correction step (this step is only necessary for nonlinear potentials). The integration has been performed on a discretized space-time, with a typical mesh $(\Delta r,\Delta t)=(0.5\text{ fm},\ 10^{-25}\text{ s})$, and $r_{\max}=2000$ fm, $T_{\max}=4\times10^{-20}$ s. Typical computation times on a CRAY J90[1] are of the order of a few minutes for a one-dimensional calculation.

[1]All the computations presented here have been performed on the CRAY J90 computers at NERSC, Berkeley.

Following the wave function in time, one has access to the probability $P_{\text{tun}}(r_B,t)=\int_{r_B}^{\infty}|\psi(r,t)|^2dr$ that the proton has tunneled at time *t*. From this quantity, the decay rate can easily be computed

$$\lambda(t)=\frac{1}{1-P_{\text{tun}}(r_B,t)}\frac{dP_{\text{tun}}(t,r_B)}{dt}. \tag{4}$$

As shown in [8], the ''asymptotic,'' constant value of this quantity does not depend on the arbitrary value r_B (in the following calculations, the border has been chosen to be the classical outer turning point). Moreover, it has been demonstrated that the choice of the modification $\epsilon(r)$ does not modify the results obtained for physical quantities at large times. This point is indeed crucial to the validity of the TDSE scheme.

In Refs [8–10] we have shown the feasibility of such calculations for high-lying initial quasistationary states, prepared *à la* Gurvitz. Studying deep sub-barrier decaying states brings new difficulties. Besides common numerical accuracy details, one has to pay attention to another unexpected problem: the introduction of a constant potential at the top of the barrier (Gurvitz procedure) shifts the energy spectrum of the resulting state toward its higher components. These high-energy components leave the well first, during the nonexponential stage of the decay. Two dramatic numerical consequences arise: first, the tunneling probability P_{tun} quickly increases toward unity, drowning any subsequent slow decay into the round-off errors of the machine. Second, these high-energy components reach the boundary of the discretized spatial grid very quickly, get reflected, and finally go back, unphysically, into the metastable well. A first look at this problem would suggest to either use larger spatial grids or use an absorbing imaginary wall. Unfortunately, the first so-

TABLE I. Half-lives of known ground-state proton emitters. DWBA, WKB, and WKB1 estimates are from [1], while TDSE gathers results from the current approach. Q is the laboratory proton energy corrected for electron screening and recoil of the daughter nucleus.

Nucleus	Q (keV)	Orbit	DWBA	WKB	WKB1	TDSE
$^{105}_{51}$Sb	491	$1d_{5/2}$	20 s	24 s	19 s	(19.6±0.1) s
$^{113}_{55}$Cs	977	$1d_{5/2}$	540 ns	640 ns	510 ns	(534±0.1) ns
$^{147}_{69}$Tm	1132	$1d_{3/2}$	210 μs	260 μs	210 μs	(206.80±0.05) μs
$^{151}_{71}$Lu	1255	$0h_{11/2}$	60 ms	90 ms	63 ms	(58.4±0.1) ms
$^{157}_{73}$Ta	947	$2s_{1/2}$	220 ms	170 ms	210 ms	(227±2) ms
$^{185}_{83}$Bi	1611	$2s_{1/2}$	3.2 μs	2.5 μs	3.1 μs	(3.17±0.01) μs

lution implies a big cost in computation time, while the second destroys the unitarity of the wave function.

Another solution consists of modifying the procedure of the preparation of the initial state in order to create a state closer to the so-called Gamow state, i.e., an eigenstate of the full Hamiltonian with outgoing boundary conditions. Such a state is characterized by a complex eigenvalue, in which the imaginary part is proportional to its decay width (see, for example, [17]). A word of caution is required at this stage. As stated above, the ''asymptotic'' value of the decay rate of a quasistationary state does not depend on its initial formation. Nevertheless, the *numerical* observation of such a value, constrained by space-time meshes, dimensions of the spatial grid, etc., can be strongly hindered by the procedure of Gurvitz if one looks at very low-lying energy states. This effect is illustrated in Fig. 1 where we have represented two differently prepared initial states, along with their decay rates calculated according to Eq. (4).

The decay rate corresponding to the ''Gurvitz state'' does not reveal any ''asymptotic'' stationary behavior, while its partner corresponding to a $\epsilon=0$ state shows a clean and accurate constant value. Note also that the ''bump'' observed in the early stage of the decay (which goes up to 10 orders of magnitude higher than the asymptotic stationary rate) and which is due to the high-energy components of the metastable state, is not present on the solid curve. The initial wave function corresponding to this latter decay rate has been obtained by solving the stationary Schrödinger equation with $\epsilon(r)=0$. Nevertheless, the boundary condition $\psi(r=r_{\max})=0$ where $r_{\max}$ corresponds to the end of the spatial grid used in the initial stationary problem, still implies that the resulting state is not an eigenstate of the hamiltonian $\mathcal{H}$ on the full spatial grid used in TDSE ($r \gg r_{\max}$). The value of $r_{\max}$ is chosen such that only the far tail of the wave function is modified (for which $|\psi(r)|^2 \leqslant 10^{-20}$). This procedure then enables us to calculate accurately the decay width of any quasistationary low-energy state.

From the observation of the same figure, one can also dismiss the second argument raised against the TDSE approach. Indeed, the initial *transient time* during which the decay does not follow the usual exponential law is much shorter than the half-life of the decaying state. These deviations from the exponential law are predicted by quantum mechanics, and have actually been observed recently in atomic physics [18]. The initial delay of the onset of the exponential decay law does depend slightly on the quasistationary state studied, namely on the value of the outer turning point (which can be as much as 110 fm for some ground-state proton emitters). Nevertheless, it is clear that one does not need to calculate until $T_{\max}=T_{1/2}$ to infer the decay rate λ, hence the half-life $T_{1/2}=0.693\lambda^{-1}$ of the decaying state. This last point renders TDSE calculations accessible to current common computers. In the case of a time-dependent interaction, though, one should in practice push the calculations until the potential reaches a stationary regime (see [13]).

Finally, we would like to emphasize that this initial *transient* time during which the decay deviates from an exponential law is physical and is a signature of the early formation process of the compound nucleus and consequently of the quasistationary state. Our calculations confirm the hypothesis of Goldberger and Watson [19] that the long-time behavior of a metastable state does not depend on its initial formation process. In addition, our time-dependent calculations enable the study of this nonexponential decaying stage and to relate it to the physics of the metastable state formation.

Returning, let us now apply the TDSE scheme to the computation of the decay widths of known spherical ground-state proton emitters.[2] In order to determine the half-lives of these states, nuclear structure effects need to be included through the use of the so-called spectroscopic factors. These quantities can be evaluated within the independent-quasiparticle approximation (BCS) [1]. In the present work, we are mainly interested in providing exact results for the barrier penetration part of the process. Hence, we did not include such structural effects and constrained ourselves to compare our results to the ones obtained within more traditional approaches. Figure 2 shows the time evolution of several decay rates of known proton emitters, the half-lives of which are spread over several orders of magnitude. The half-lives inferred through this approach are gathered in Table I along with results taken from [1], using the distorded wave-Born approximation (DWBA) formalism and the usual semiclassical estimates WKB-WKB1 (see [1] for details). Our exact calculations demonstrate that DWBA results are accurate and can be considered as a reference for the calculation of ex-

[2]The form and the parameters of the interacting potential have been taken from [1]. The set WS1 of parameters has been used (see [1]).

perimental spectroscopic factors. Note that the numerical accuracy obtained in TDSE depends mainly on the space-time mesh $(\Delta r, \Delta t)$ used for the integration of the Schrödinger equation. The present accuracy could indeed be improved, requiring a necessary trade-off with larger computation times.

In conclusion, we have shown that solving the time-dependent Schrödinger equation for initial ''good'' quasistationary states is a reliable and very powerful method to study particle emission from nuclei. It is exact, intuitive, and fully dynamic. It can be applied to any energy state. It can also be extended to any space dimension, and can treat complex phenomena for which the interacting potential is time dependent. For the special case of stationary, one-dimensional interacting potentials (spherical nuclei), we have shown that the distorted wave-Born approximation provides accurate results for the half-lives of the ground-state proton emitters observed at present. Nevertheless, this latter approach, unlike TDSE, is applicable only to time-independent problems.

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