

Proton emission from Gamow resonance

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Abstract. We developed two computer codes: CCGAMOW and NONADI for calculating the complex energy eigenvalues and eigenfunctions of deformed Gamow resonances with high accuracy by using the piecewise perturbation method. The code CCGAMOW calculates resonant Nilsson orbitals using the adiabatic approximation in which the energies of the ground and excited rotational states of the daughter nucleus are degenerate. In the code NONADI this approximation is lifted and the rotational degree of freedom of the core and the Coriolis coupling in the parent nucleus are taken into account. The difference between adiabatic and non-adiabatic approaches is found to be non-negligible for the proton emission from the ground state of ¹⁴¹Ho.

I INTRODUCTION

Nuclear states decaying predominantly by proton emission are often described by using single-particle (s.p.) proton states with complex energy eigenvalues, i.e. by Gamow resonances. Gamow states were introduced by Gamow [1] in order to describe α -decay. Since they describe a time-dependent process within a stationary picture, Gamow states are not wave functions in the normal quantum mechanical sense. They have complex energy eigenvalues which correspond to poles of the S -matrix extended to complex energy, \mathcal{E} and wave number, k . Nevertheless, they are extremely useful mathematical tools to describe narrow resonances or long-lived quasistationary states [2].

In this paper we use Gamow states to describe proton emission. We shall focus attention on the mathematical and numerical approaches needed for calculating narrow Gamow resonances in spherically symmetric and axially deformed nuclei.

We compare the adiabatic and non-adiabatic approaches to proton emission from the deformed ^{141}Ho nucleus and demonstrate the importance of the non-adiabatic description.

II DEFINITION OF GAMOW STATES

Let us first consider the simplest case in which the proton moves in a spherically symmetric, finite potential $v(r)$, which is a sum of the central nuclear potential, v_N , the nuclear spin-orbit term, v_{so} , and the Coulomb potential, v_C :

$$v(\mathbf{r}) = v(r) = v_N(r) + v_{so}(r) + v_C(r). \quad (1)$$

The Gamow state, ψ_n , is the eigenvector of the single-particle Hamiltonian $\hat{h} = \hat{t} + v(r)$, where the kinetic energy operator is $\hat{t} = -\frac{\hbar^2}{2\mu}\Delta$ (μ is the reduced mass):

$$\hat{h}\psi_n = \mathcal{E}_n\psi_n. \quad (2)$$

The eigenfunction ψ_n is characterized by the angular momentum quantum numbers (l, j, m) :

$$\psi_n = \psi_{l,j,m}(\mathbf{r}, k) = \frac{u_{l,j}(r, k)}{r} [Y_l(\hat{r})\chi_{1/2}]_{j,m}. \quad (3)$$

Let us abbreviate l and j as a single subscript $i = \{l, j\}$ and introduce the complex wave number, k ($k^2 = \frac{2\mu}{\hbar^2}\mathcal{E}$). We can write the radial equation as

$$u_i''(r, k) = \left[\frac{l(l+1)}{r^2} + V(r) - k^2 \right] u_i(r, k), \quad (4)$$

where $V(r) = \frac{2\mu}{\hbar^2}v(r)$ is the potential in units of k^2 . The Gamow solution should be regular at the origin,

$$u_i(0, k) = 0, \quad (5)$$

and asymptotically, where only v_C is present, it should join to an outgoing Coulomb wave, $O_l = G_l + iF_l$. Therefore, at $r = r_{as}$ (where r_{as} is the asymptotic radius, which is much larger than the range of the average potential) the logarithmic derivative of the solution should be

$$D(r_{as}, k) = u_i'(r_{as}, k)/u_i(r_{as}, k) = O_l'(\eta, kr_{as})/O_l(\eta, kr_{as}), \quad (6)$$

where $\eta = \frac{Ze^2\mu}{\hbar^2 k}$ is the Sommerfeld parameter. The solutions defined by Eqs. (4-6) are either bound states, $\mathcal{E}_n = E_b < 0$, with negative real energies and imaginary wave numbers $k_n = i\gamma_n$ ($\gamma_n > 0$), or Gamow states, $\mathcal{E}_n = E_r - i\frac{\Gamma}{2}$, with a nonzero imaginary part $\Gamma \neq 0$, and $k_n = \kappa_n - i\gamma_n$.

The asymptotic behavior of these solutions is determined by k_n ; at a very large distance the outgoing solution (for $\eta = 0$) is proportional to $e^{ik_n r}$. The resonance is called a decaying Gamow resonance if $\Gamma > 0$ or a capturing resonance if $\Gamma < 0$. For a real potential v , the pair of resonances lies symmetrically with respect to the imaginary k -axis; hence decaying Gamow states have $k_d = \kappa_n - i\gamma_n$ and capturing ones have $k_c = -\kappa_n - i\gamma_n$, with $\kappa_n > 0$ and $\gamma_n > 0$. The radial wave function of the capturing Gamow state is the complex conjugate of that of the decaying one, $u_c(r) = u_d(r)^*$. Both u_c and u_d oscillate with increasing amplitude as a function of r .

Berggren proposed a new completeness relation, which includes Gamow states [3], by generalizing the scalar product. He introduced a bilinear basis set and a regularization procedure (*Reg*). With this generalization, the norm is

$$\langle u_c | u_d \rangle = \text{Reg} \int_0^\infty u_d^2(r) dr = 1. \quad (7)$$

A convenient method for regularization is to rotate r to the first quadrant of the complex r -plane beyond a certain distance r_{max} . This is often referred to as the exterior complex scaling method.

The total width of the Gamow resonance with complex energy \mathcal{E}_d is given by

$$\Gamma = -\frac{1}{2} \text{Im}(\mathcal{E}_d). \quad (8)$$

The half-life of the state is $T_{1/2} = \hbar \ln 2 / \Gamma$.

III NUMERICAL CALCULATION OF SPHERICAL GAMOW STATES

For realistic potentials, the radial equation has to be solved by means of numerical integration. In Ref. [4] the code GAMOW was introduced, which uses the Fox-Goodwin method for solving the radial equation. A more powerful method, the piecewise perturbation, is used for the same purpose in Ref. [5] (code ANTI). The main features are similar in the two codes. The total r domain of Eq. (4) consists of a real r domain, $[0, r_{max}]$, and a complex ray $I_3 = [r_{max}, r_{as}]$, where r_{as} is complex. The real domain is further divided into two intervals, $I_1 = [0, r_{min}]$ and $I_2 = [r_{min}, r_{max}]$. For some approximate value of k_n , one finds the “left” solution of Eq. (4), $u^L(r, k)$, that satisfies the boundary condition at the origin, and it is calculated by integrating numerically from $r = 0$ to r_m . The “right” solution of Eq. (4), $u^R(r, k_n)$, satisfies the asymptotic boundary condition at $r = r_{as}$; the numerical integration proceeds on I_3 inward from the point r_{as} to the real axis at r_{max} ; and then continues along the real r -axis in region I_2 until reaching the matching point, r_m . The complex eigenvalue, k_n , can be found by finding the zero of the transcendental function

$$\Phi(k) = D^L(r_m, k) - D^R(r_m, k) = 0, \quad (9)$$

where the logarithmic derivatives of u_L and u_R at the matching distance are

$$D^L(r_m, k) = \frac{u'_L(r_m, k)}{u_L(r_m, k)}, \quad D^R(r_m, k) = \frac{u'_R(r_m, k)}{u_R(r_m, k)}. \quad (10)$$

The root finding can be done by means of the Newton-Raphson technique. Note that in order to get the contribution of the asymptotic region to the norm in Eq. (7), r must be complex in region I_3 . The corresponding rotation angle (which for large values of r_{as} coincides with $\arg(r)$) should satisfy the condition

$$\pi - \arg(k) > \arg(r) > -\arg(k) \quad (11)$$

so that the magnitude of the solution converges to zero as $r_{as} \rightarrow \infty$ along the complex ray. The contribution to the norm beyond r_{as} is neglected, and at r_{as} we use the asymptotic series of the outgoing Coulomb function O_l (and its derivatives)

$$O_l(\eta, \rho) = \exp \left[i \left(\rho - \eta \ln 2\rho - l \frac{\pi}{2} + \sigma_l \right) \right] \left\{ 1 + \sum_{n \geq 1} \prod_{j=1}^n \frac{(i\eta + l + j)(i\eta - l + j - 1)}{j(2i\rho)} \right\} \quad (12)$$

with $\rho = kr_{as}$. We use the convergence acceleration procedures of Wynn [6] and Levin [7] to speed the convergence of the summation.

For the known proton emitters, the width Γ is so small that extremely high numerical accuracy is required for \mathcal{E}_d . The width can also be calculated from the outgoing probability current [9]

$$\Gamma(r) = i \frac{\hbar^2}{2\mu} \frac{u_d^*(r, k_n) u_d(r, k_n) - u'_d(r, k_n) u_d^*(r, k_n)}{\int_0^r |u_d(x, k_n)|^2 dx}, \quad (13)$$

which, by construction, does not depend on r . If we use extended precision arithmetic, the width calculated using Eq. (13) is indeed r -independent, and it agrees well with the value obtained from Eq. (8). Another way to estimate the width is to use the R-matrix expression of Thomas [10],

$$\Gamma = \frac{\hbar^2 \kappa_n}{\mu} \frac{\mathcal{R}e(u_d(a, k_n))^2}{|O_l(\mathcal{R}e(\eta), \kappa_n r_{as})|^2}, \quad (14)$$

where we approximate the (real) R-matrix resonant wave function with the real part of the normalized Gamow resonance. This approximation works fairly well for the narrow Gamow resonances corresponding to the known proton emitters [11]. For large values of r_{as} , expression (14) is generally within 5% of the values calculated from Eqs. (8) and (13).

IV GAMOW STATES IN THE DEFORMED POTENTIAL

A Adiabatic approach

The generalization of the s.p. Hamiltonian to an axially symmetric, deformed potential, $v(\mathbf{r})=v(r, \theta)$, leads to a system of n coupled, differential equations. In the *intrinsic* frame of reference, defined by the principal axis of the deformed average potential, the proton moves in an orbit with good quantum numbers π (parity) and Ω (projection of the total s.p. angular momentum \mathbf{j} onto the symmetry axis). The s.p. wave function can be expanded in spherical partial waves

$$\psi^{\Omega, \pi}(\mathbf{r}, k) = \sum_{l, j}^{l_{max}, j_{max}} \frac{u_{l, j}(r, k)}{r} [Y_l(\hat{r}) \chi_{1/2}]_{j, \Omega} ; \quad (15)$$

in which the radial wave functions are the solutions of a set of coupled differential equations

$$u_i''(r, k) = \sum_{i'} \left[\frac{l_i(l_i + 1)}{r^2} \delta_{i, i'} + V_{i, i'}(r) - k^2 \delta_{i, i'} \right] u_{i'}(r, k) . \quad (16)$$

Here $i = 1, 2, \dots, n$ runs over all partial waves which can be coupled to the given Ω and π , and $V_{i, i'}(r) = \langle l j \Omega | V(\mathbf{r}) | l' j' \Omega \rangle$ are the matrix elements of the deformed potential. The system of coupled equations can be written in matrix form as

$$\mathbf{u}''(r, k) = \left(\frac{\underline{L}}{r^2} + \underline{V}(r) - k^2 \underline{1} \right) \mathbf{u}(r, k), \quad (17)$$

where the underlined quantities denote $n \times n$ matrices. In Eq. (17) \underline{V} is the potential matrix, \underline{L} is the diagonal matrix $l_i(l_i + 1)\delta_{ij}$, $\underline{1}$ is the identity matrix, and

$$\mathbf{u}(r, k) \equiv [u_1(r, k), u_2(r, k), \dots, u_n(r, k)]^T \quad (18)$$

is an n dimensional column vector. This eigenvalue problem is solved with boundary conditions given by Eqs. (5) and (6). First, the radial wave functions are regular at the origin, $u_i(0, k)=0$. At large values of r ($r > r_{as}$), all the off-diagonal coupling terms vanish and (17) reduces to a decoupled set of n differential equations. Therefore, an adiabatic Gamow state should satisfy Eq. (6) in every channel ($i = 1, \dots, n$) with the same value of k .

The problem of determining complex eigenvalues and eigenfunctions can be reduced to a set of initial value problems for the system of coupled equations (17). As in the spherically symmetric case, one calculates “left” and “right” solutions which are then matched at r_m .

For solving the initial value problems with high accuracy, a package of subroutines based on the piecewise perturbation methods are used (see Ch. 3 of Ref. [12] and

Ref. [5]). This package is aimed at solving initial value problems for systems of ordinary differential equations of the form

$$\mathbf{u}''(r, k) = \left(\frac{L}{r^2} + \frac{S(r)}{r} + P(r) - k^2 E \right) \mathbf{u}(r, k), \quad a < r < b, \quad (19)$$

along a straight-line segment $s = [a, b]$ in the complex plane. The matrices $S(r)$ and $P(r)$ are symmetric and their elements are complex functions of (complex) r . Furthermore, it is assumed that each matrix element is well approximated by a polynomial of second degree inside any reasonably large subinterval of the segment.

The package consists of two sets of subroutines. One set is designed for the vicinity of the origin $r \in [0, r_{min}] = I_1$, where the centrifugal term has the largest importance. It produces the regular solution inside the I_1 -interval by a perturbative technique in which the centrifugal term is taken as the reference potential and the sum of the other three terms is taken as a perturbation. The other set of routines is designed for the remaining part of the r -domain, i.e., for I_2 and I_3 . Here the integration is performed on a lattice of non-equidistant mesh-points which is determined by the variation of the potential and the accuracy required. On each subinterval, matrix elements of the sum of the three potentials are first approximated by their average values. The deviations from the second degree polynomial are considered to be perturbations which are then taken up to the second order. In both regions, the respective packages produce the vector \mathbf{u} and its derivatives. A detailed description of this package will be given elsewhere [13].

The code which calculates the Gamow states in a deformed potential using the adiabatic approximation is called CCGAMOW. Besides the energy eigenvalue and the normalized wave function, it computes the partial widths using the current expression [9],

$$\Gamma_i(r) = i \frac{\hbar^2}{2\mu} \frac{u_i^{t*}(r, k_n) u_i(r, k_n) - u_i'(r, k_n) u_i^{t*}(r, k_n)}{\sum_{i'}^n \int_0^r |u_{i'}(r', k_n)|^2 dr'}, \quad (20)$$

where the sum of the partial widths,

$$\Gamma(r) = \sum_i^n \Gamma_i(r), \quad (21)$$

gives the total decay width as a function of r . A serious check of our calculation is that for large r -values the condition $\mathcal{I}m(\mathcal{E}) = -1/2 \Gamma(r)$ is satisfied if we use extended precision arithmetic. (In principle, $\Gamma(r)$ should be independent of r at any r .) The partial widths of Eq. (20) are in reasonably good agreement with those calculated by using the Thomas formula of Eq. (14) at large values of r_{as} . (This R-matrix expression was used recently in Refs. [14,15] dealing with deformed proton emitters.)

In our calculations, we assume that the spin-orbit term v_{so} is spherical; i.e., it does not contribute to the off-diagonal couplings of Eq. (17). As discussed by

Nilsson [17], the impact of the deformed component of the spin-orbit term, δv_{so} , on the Nilsson orbitals is weak. In addition, there is some arbitrariness in defining the average spin-orbit interaction, and the influence of δv_{so} on the final result is well below this uncertainty.

B Non-adiabatic approach

The deformed Gamow state can be associated with a deformed, resonant Nilsson orbital in a finite potential. Since it describes the s.p. motion in the intrinsic frame, it breaks angular momentum conservation. In order to restore rotational invariance, one can adopt the strategy of the particle-plus-rotor model and couple the intrinsic, deformed state to the deformed core. This is the strong-coupling scheme of Ref. [16].

Another strategy, adopted in this work, is the weak-coupling approach in which the wave function of the parent nucleus is obtained by coupling the spherical single-proton wave functions to the deformed states of the daughter nucleus. In this scheme the intrinsic wave function is not introduced, and the parent state preserves the total angular momentum J , its projection M , and the parity π . The Hamiltonian of the deformed core-plus-particle system can be written in the laboratory frame as

$$\hat{H} = \hat{H}_0(\xi) + \hat{t} + \sum_{\lambda} v_{\lambda}(r)(Q_{\lambda}(\xi) \cdot Y_{\lambda}(\hat{r})), \quad (22)$$

where $\hat{H}_0(\xi)$ is the internal Hamiltonian of the core (daughter nucleus), with internal coordinates ξ . The eigenstates $\psi_{I,\mu}(\xi)$ of $\hat{H}_0(\xi)$ are that of the symmetric top, and the corresponding eigenvalues, ϵ_I , can be either taken from experiment or modeled according to the rotational expression $\epsilon_I = \kappa I(I + 1)$. In Eq. (22) \hat{t} is the kinetic energy of the particle and the third term is a multipole expansion of the core-particle interaction. (A similar Hamiltonian was introduced in Ref. [18] to describe alpha emission from deformed nuclei.)

The parent wave function,

$$\Psi^{JM}(\mathbf{r}, \xi) = \sum_{Ijl} \frac{u_{Ijl}(r)}{r} \Phi_{Ijl}^{JM}(\hat{r}, \xi), \quad (23)$$

is composed of the radial function and the channel function,

$$\Phi_{Ijl}^{JM}(\hat{r}, \xi) = \sum_{m,\mu} \langle jmI\mu | JM \rangle \mathcal{Y}_{jlm}(\hat{r}, m_s) \psi_{I,\mu}(\xi), \quad (24)$$

in which $\mathcal{Y}_{jlm}(\hat{r}, m_s)$ is the spin-angular part of the single-proton wave function. The radial functions, $u_{Ijl}^J(r)$, are the solutions of the coupled, differential equations

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) + \epsilon_I - E \right] u_{Ijl}^J(r) + \sum_{\lambda I'j'l'} v_\lambda(r) \mathcal{V}_{Ijl, I'j'l'}^J(\lambda) u_{I'j'l'}^J(r) = 0, \quad (25)$$

where the matrix element $\mathcal{V}_{Ijl, I'j'l'}^J(\lambda)$ corresponds to the rotational coupling (for details, see Refs. [19–21]) and the channels are characterized by quantum numbers $i = \{Ijl\}$. In order to solve the system of coupled equations (25), the program CCGAMOW had to be extended. Since the resulting coupled-channel code, NONADI, does not employ the adiabatic approximation, the k values in the different Ijl channels,

$$k_I^2 = \frac{2\mu}{\hbar^2}(E - \epsilon_I), \quad (26)$$

and the Sommerfeld parameter, $\eta_I = \frac{Ze^2\mu}{\hbar^2 k_I}$, both depend on the excitation energy ϵ_I . Consequently, the boundary condition at large distance, Eq. (6), has to be modified as:

$$D_i(r_{as}, k_I) = u'_i(r_{as})/u_i(r_{as}) = O'_l(\eta_I, k_I r_{as})/O_l(\eta_I, k_I r_{as}). \quad (27)$$

The eigenvector of Eq. (25), with proper boundary conditions, represents the Gamow states in the laboratory system of reference. The normalization of the solution is done exactly in the same way as in CCGAMOW. The method of solution also follows the adiabatic case, but the degeneracy in I is lifted. For more details, see Refs. [22,23].

V RESULTS

We have analyzed proton emission from deformed nuclei using both adiabatic (CCGAMOW) and non-adiabatic (NONADI) approaches. Results of the analysis are presented elsewhere [22,23]. Here we only present an illustration that illuminates the differences between the adiabatic and non-adiabatic methods. For our example, we consider proton emission from the ground state of ^{141}Ho , which according to the adiabatic calculations of Refs. [14,15,24,25] is the $7/2^-$ [523] deformed Nilsson orbit. The parameters of the s.p. potential are those of Chepurnov [26] save the strength, V_0 , which has been fixed by the Q -value of the proton decay to ensure the correct barrier penetrability. We assume that the proton emission feeds the members of the ground state rotational band in ^{140}Dy having a constant moment of inertia. The excitation energy of the 2^+ state is unknown; hence, it has been taken as $\epsilon_2 = 0.16$ MeV based on systematics. As one can see in Table 1, the parent wave function is dominated by the $h_{11/2}$ spherical proton component. On the other hand, the partial width to the 0^+ ground state, Γ_0 , is primarily determined by the $f_{7/2}$ component in the wave function. Though the total summed weights, $|c_{lj}|^2$, of

TABLE 1. Weights $|c_{Nj}|^2$ of the main configurations in the ground state $J^\pi = 7/2^-$ wave function in ^{141}Ho ($\beta_2=0.27, \beta_4=-0.06$) calculated in non-adiabatic and adiabatic approaches. The results of the adiabatic calculations are shown in the third and fourth columns where the $7/2^-$ [523] deformed Nilsson (resonant) orbit is calculated both by CCGAMOW and by NONADI (with $\epsilon_I = 0$).

channel $I l j$	NONADI	NONADI	CCGAMOW
	$\epsilon_2 = 0.16 \text{ MeV}$ $ c_{Nj} ^2$	$\epsilon_2 = 0.0$ $ c_{Nj} ^2$	$ c_{ij} ^2$
2 5 11/2	0.028	0.074	
4 5 11/2	0.289	0.462	
6 5 11/2	0.377	0.260	
8 5 11/2	0.115	0.020	
$\sum_I c_{Nj} ^2$	0.809	0.816	0.817
0 3 7/2	0.011	0.027	
2 3 7/2	0.046	0.063	
4 3 7/2	0.046	0.017	
6 3 7/2	0.018	0.001	
$\sum_I c_{Nj} ^2$	0.121	0.108	0.108

the different partial waves in the parent wave function are influenced very little by the removal of the degeneracy of the daughter states, their distribution among the members of the rotational band, $|c_{Nj}|^2$, are changed considerably due to Coriolis coupling. The removal of the degeneracy reduces the ground-state component in the wave function (0.011) by a factor of 2.5 with respect to the adiabatic case (0.027). This in turn reduces $\Gamma_0^{NA} = 2.6 \times 10^{-20}$ MeV to one-third of the adiabatic value of $\Gamma_0^A = 8.3 \times 10^{-20}$ MeV. In the adiabatic approach, the total width was approximated by $\Gamma^A = \Gamma_0^A + \Gamma_2^A = 8.6 \times 10^{-20}$ MeV. (Γ_2^A was estimated by repeating the adiabatic calculation at the modified Q -value corresponding to the transition to 2^+ state. This gives $\Gamma_2^A = 2.3 \times 10^{-21}$ MeV.) The total width of $\Gamma^{NA} = 2.8 \times 10^{-20}$ MeV turned out to be only one-third of the adiabatic value. This example shows that the effect of the Coriolis coupling might be important in certain cases and, in general, cannot be neglected.

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