

Resonances in deformed nuclei: R-matrix theory and oscillator expansion

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Abstract. Single-particle resonances in deformed nuclei are considered using the coupled-channel Schrödinger equation method with the outgoing boundary conditions. Two variants of this method are investigated: the non-adiabatic one (based on the weak-coupling scheme) and the adiabatic one (based on the strong coupling). The R-matrix theory and the Gamow state approach are discussed and compared with each other. It is shown that the widths of very narrow proton resonances can be calculated by combining the harmonic oscillator expansion method with the R-matrix approach.

I INTRODUCTION

The Gamow (resonant) state approach is among the best time-independent methods for discretizing the single-particle continuum. The Schrödinger equation for deformed proton emitters leads to an eigenvalue problem with coupled-channel differential equations. Solving these equations accurately and reliably requires special care. Calculating the parameters of the resonances can be carried out directly by employing the pure outgoing wave boundary condition of a Gamow state or indirectly by using the R-matrix theory of Wigner and Eisenbud.

In order to avoid the cumbersome numerical solution of the coupled-channels eigenvalue problem, the simple harmonic oscillator expansion method, which leads to a matrix eigenvalue problem, can be applied to get the energy of a Gamow state. We show that the combination of the R-matrix theory and the harmonic oscillator expansion method is able to reproduce the widths of very narrow proton resonances.

In Sec. II the coupled-channel equations with and without Coriolis coupling are given. In Sec. III we discuss the different boundary conditions leading to the R-matrix and Gamow formalism. The exact R-matrix calculations are discussed in

Sec. IV. Finally, Sec. V shows an example of the application of the harmonic oscillator expansion method to the proton decay of ^{131}Eu .

II COUPLED EQUATIONS FOR PROTON EMISSION

We describe the scattering of an inert, spin one-half projectile by a nucleus. The Hamiltonian is

$$H = H_0(\xi) + T + \sum_{\lambda} V_{\lambda}(r)(Q_{\lambda}(\xi) \cdot Y_{\lambda}(\hat{r})), \quad (1)$$

where $H_0(\xi)$ is the internal Hamiltonian of the target, ξ denotes the internal coordinates of the target, and T is the kinetic energy of the relative motion. The target-projectile relative coordinate is \vec{r} . The projectile is considered to be inert so it is not necessary to specify its Hamiltonian in Eq. (1). The third term in Eq. (1) is the target-projectile interaction. It is given by an appropriately chosen inner product of tensor operators.

A Non-adiabatic method: weak coupling

In the non-adiabatic method, the wave function of the parent nucleus (i.e., particle emitter) can be written in the weak-coupling form:

$$\Psi^{JM}(\vec{r}, \xi) = \frac{1}{r} \sum_{Ijl} u_{Ijl}(r) \Phi_{Ijl}^{JM}(\hat{r}, \xi) \quad (2)$$

where the channel function is

$$\Phi_{Ijl}^{JM}(\hat{r}, \xi) = \sum_{m,\mu} \langle jmI\mu | JM \rangle \mathcal{Y}_{jlm}(\hat{r}, m_s) \psi_{I,\mu}(\xi). \quad (3)$$

In Eq. (3)

$$\mathcal{Y}_{jlm}(\hat{r}, m_s) = \sum_{m_l, m_s} \langle lm_l \frac{1}{2} m_s | jm \rangle i^l Y_{lm_l}(\hat{r}) \chi_{m_s}, \quad (4)$$

with χ_{m_s} being the spin function of the projectile (in our case: emitted nucleon). The states $\psi_{I,\mu}(\xi)$ are eigenstates of the target (i.e., daughter nucleus) Hamiltonian $H_0(\xi)$:

$$H_0(\xi) \psi_{I,\mu}(\xi) = \epsilon_I \psi_{I,\mu}(\xi). \quad (5)$$

The radial functions $u_{Ijl}^J(r)$ are the solutions of the coupled differential equations

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) + \epsilon_I - E \right] u_{Ijl}^J(r) + \sum_{\lambda I'j'\nu'} V_\lambda(r) \mathcal{V}_{Ijl, I'j'\nu'}^J(\lambda) u_{I'j'\nu'}^J(r) = 0, \quad (6)$$

where the coupling matrix element is defined by

$$\begin{aligned} \mathcal{V}_{Ijl, I'j'\nu'}^J(\lambda) &= (4\pi)^{-1/2} (-1)^{J-1/2-I'+j+j'+\frac{1}{2}(l'-l)} \hat{j}_j \hat{j}' \hat{I}' \\ &\times \langle j - \frac{1}{2} j' \frac{1}{2} | \lambda 0 \rangle \langle I' 0 \lambda 0 | I 0 \rangle W(j I j' I'; J \lambda). \end{aligned} \quad (7)$$

The coupling matrix (7) is derived under the assumption of the rigid rotational motion of the daughter nucleus. The detailed form of the form factors and the derivation of (7) can be found in Ref. [1].

B Adiabatic approximation: strong coupling

In the adiabatic approximation, one assumes the complete degeneracy of the rotational states in the daughter nucleus: $\epsilon_I = \epsilon_0 = 0$. Using a Racah identity, one can prove

$$\begin{aligned} \sum_I (-1)^{J+K+j+1/2} \langle j K J - K | I 0 \rangle \mathcal{V}_{Ijl, I'j'\nu'}^J(\lambda) &= \\ \mathcal{V}_{j'l, j'\nu'}^K(\lambda) (-1)^{J+K+j'+1/2} \langle j' K J - K | I' 0 \rangle, \end{aligned} \quad (8)$$

where

$$\mathcal{V}_{j'l, j'\nu'}^K(\lambda) = (-1)^{K+j+j'+1/2} \hat{j}_j \hat{j}' \hat{\lambda}^{-1} \langle j \frac{1}{2} j' - \frac{1}{2} | \lambda 0 \rangle \langle j K j' - K | \lambda 0 \rangle. \quad (9)$$

By introducing the functions

$$g_{jl}^{JK}(r) = \sqrt{2} \sum_I (-1)^{J+K+j+1/2} \langle j K J - K | I 0 \rangle u_{Ijl}^J(r), \quad (10)$$

the set (6) reduces to the following coupled equations:

$$\left[-\frac{\hbar^2}{2\mu} \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right) - E \right] g_{jl}^{JK}(r) + \sum_{\lambda j'\nu'} V_\lambda(r) \mathcal{V}_{j'l, j'\nu'}^K(\lambda) g_{j'l\nu'}^{JK}(r) = 0. \quad (11)$$

Since the coupling potential in (11) is independent of J , from now on this index is dropped from $g_{jl}^{JK}(r)$ in the adiabatic method.

One can easily show that Eq. (11) describes the scattering of the projectile by a deformed potential. The adiabatic single-particle wave function

$$\Psi^K(\vec{r}) = \sum_{jl} g_{jl}^K(r) \mathcal{Y}_{j l K}(\hat{r}, m_s) \quad (12)$$

is equivalent to a deformed Nilsson orbit. The fact that the eigenstates of (11) do not depend on J implies that in the adiabatic limit the rotational band built upon the Nilsson orbital (12) is degenerate (i.e., its moment of inertia is infinite).

III R-MATRIX AND GAMOW THEORY

By specifying the boundary conditions, the coupled differential equations (6) and (11) correspond to an eigenvalue problem. It is always assumed that the solutions are regular at the origin, i.e., $u_{I_{jl}}^J(0) = g_{jl}^K(0) = 0$. In the following, we shall use the shorthand notation $u_c(r)$ either for $u_{I_{jl}}^J(r)$ or for $g_{jl}^K(r)$, and l_c will denote the single-nucleon orbital angular momentum in the channel c .

The R-matrix theory, developed by Wigner, Eisenbud [2], and later by Lane and Thomas [3], is intended to give the parameterization of the scattering S-matrix on the real energy axis and subsequently the parameterization of the scattering cross section. The R-matrix boundary condition is

$$a \frac{u_c'(a)}{u_c(a)} = B_c, \quad (13)$$

where the boundary condition parameters, B_c , are arbitrary real numbers. It is assumed that the short-range interaction between the projectile and target can be neglected beyond the (large) channel radius a . The boundary condition (13) defines a discrete complete set of functions $u_c^\lambda(r)$ corresponding to the real eigenvalues E_λ . They are normalized to one inside the channel surface, $\sum_c \int_0^a |u_c(r)|^2 dr = 1$. Written in terms of the real reduced width amplitudes,

$$\gamma_{\lambda c} = \left(\frac{\hbar^2}{2m_c a} \right)^{1/2} u_c^\lambda(a), \quad (14)$$

the R-matrix can be written as

$$R_{cc'} = \sum_\lambda \frac{\gamma_{\lambda c} \gamma_{\lambda c'}}{E_\lambda - E}. \quad (15)$$

(In Eq. (14), m_c is the reduced mass.) The R-matrix is related to the scattering S-matrix in a complicated way [3]. It can be demonstrated that if all the eigenstates are taken into account in Eq. (15), then the calculated S-matrix does not depend on the boundary condition parameters or on the exact choice of the channel radius.

The Gamow (or Siegert) states of Eqs. (6) and (11) are defined by the following boundary condition

$$\frac{u_c'(a)}{u_c(a)} = \frac{k_c O_{l_c}'(k_c a)}{O_{l_c}(k_c a)}, \quad (16)$$

where O_{l_c} is the outgoing wave (e.g., Coulomb function for protons). A solution with complex wave number $k_c = \sqrt{2m_c(E - \epsilon_c)}/\hbar$ leads to a Gamow state with complex energy $E_r - i\Gamma_r/2$. At that energy the scattering S-matrix has a pole [4] in the complex energy plane. Lane and Thomas in Ref. [3] call that pole of the S-matrix a “radioactive state”. The real-energy states defined by the R-matrix theory of Wigner and Eisenbud should not be confused with the Gamow states.

The advantage of the Gamow state is that the particle-decay half-life can be readily obtained from the width Γ_r , $T_{1/2} = \hbar \ln 2 / \Gamma_r$. Since the R-matrix theory gives the scattering S-matrix only on the real energy axis, further considerations are needed to determine the parameters of a resonance if the R-matrix boundary condition is selected for the solution of the coupled equations. Assuming that in a given energy region only one term $\lambda = \lambda_0$ dominates in Eq. (15), Thomas showed [5] how to obtain the Gamow resonance energy E_r and its width Γ_r within the R-matrix theory. Specifically, if the R-matrix boundary condition parameters are set so that

$$B_c = S_{l_c}(E_\lambda), \quad (17)$$

the complex-energy pole of the S-matrix, \mathcal{E} , satisfies the equation

$$E_{\lambda_0} - \mathcal{E} + (\mathcal{E} - E_{\lambda_0})\dot{\Delta}_{\lambda_0}(E_{\lambda_0}) - \frac{1}{2}i\Gamma_{\lambda_0}(E_{\lambda_0}) = 0, \quad (18)$$

where

$$\frac{1}{2}\Gamma_\lambda(E) \equiv \sum_c P_{l_c}(E)\gamma_{\lambda c}^2 \quad (19)$$

and

$$\dot{\Delta}_\lambda(E_\lambda) \equiv -\sum_c \dot{S}_{l_c}(E_\lambda)\gamma_{\lambda c}^2. \quad (20)$$

The functions $P_{l_c}(E)$ and $S_{l_c}(E)$ are referred to as the penetration and shift functions, respectively. (They are expressed by the Coulomb F_{l_c} and G_{l_c} functions, see, e.g., Ref. [3].) The dot in Eqs. (18) and (20) denotes the derivative with respect to energy. Assuming that (20) is negligible, one obtains $E_r = E_\lambda$ and the resonance width is given by the frequently quoted expression $\Gamma_r = \Gamma_\lambda(E_\lambda)$.

IV EXACT R-MATRIX CALCULATIONS

The phrase ‘‘exact R-matrix calculation’’ means that the coupled differential equations are solved numerically. The solution with the R-matrix boundary condition is generated by a modified version of the code CCGAMOW [6] which is based on the piecewise perturbation technique.

Since we are interested in describing decaying systems, our main objective is to calculate the position and width of Gamow states. Hence the result of the R-matrix calculation will be compared with the calculation using the Gamow state boundary condition; the latter will be referred to as the exact one. The Gamow states are generated by the code CCGAMOW using extended precision. All calculations based on the R-matrix theory are done in double precision. It is not necessary to use extended precision in R-matrix theory but it is unavoidable to apply extended

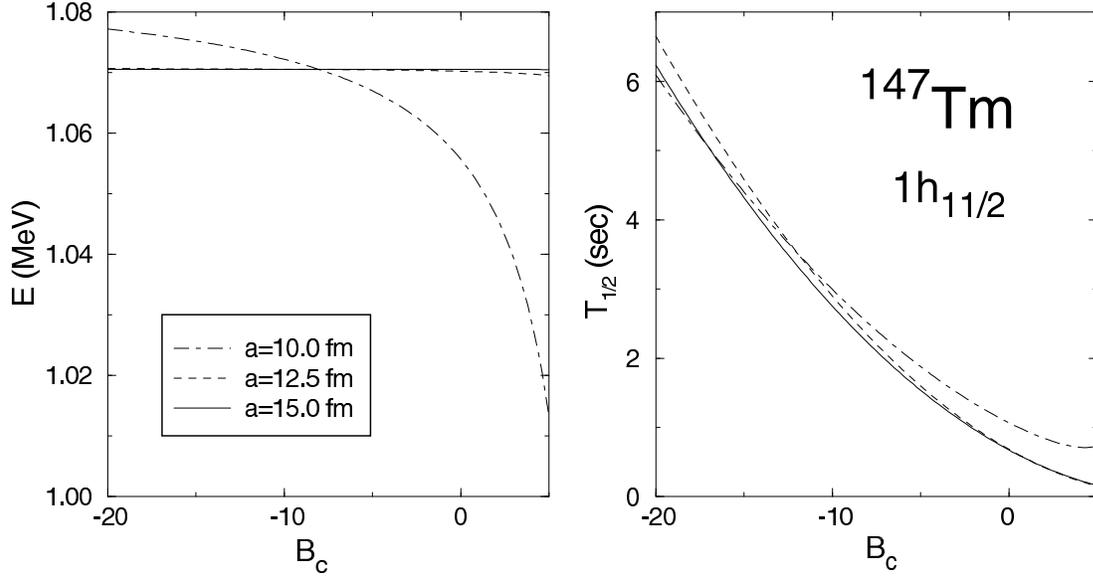


FIGURE 1. Energy and half-life of the spherical $1h_{11/2}$ proton orbit in ^{147}Tm calculated in the R-matrix theory as a function of the boundary condition parameter B_c for different values for the channel radius.

precision in Gamow state calculations if the width of the resonance is very small ($\Gamma_r < 10^{-16}$ MeV).

Consider first a narrow spherical proton emitter, e.g., the $1h_{11/2}$ orbit of ^{147}Tm discussed in Ref. [8]. The R-matrix calculations have been performed for three different values of the channel radius. Figure 1 shows the calculated eigenvalue and the half-life as functions of the boundary condition parameter. The eigenvalue is quite stable if the channel radius is large and it is very close to the exact position of the resonance (1.70562 MeV). The calculated width however varies greatly. In this form, the R-matrix theory is unable to give a reliable prediction for the resonance's half-life.

Fortunately, the “natural boundary condition” assumption of Eq. (17) turns out to work well. In the iterative R-matrix technique, first we take a boundary condition parameter, calculate the eigenvalue E_λ , and check whether the condition (17) is satisfied or not. If this condition is violated, the boundary condition parameter is modified and the whole procedure is repeated until the correct solution is found. The result of this type of calculation is shown in Fig. 2. Here the half-life is shown as a function of the channel radius. At each channel radius, the optimal boundary condition is determined and then the half-life is calculated. The exact result is reproduced extremely well. Note the difference of the scales on Fig. 1 and Fig. 2. The small deviation between the Gamow and R-matrix results is probably related

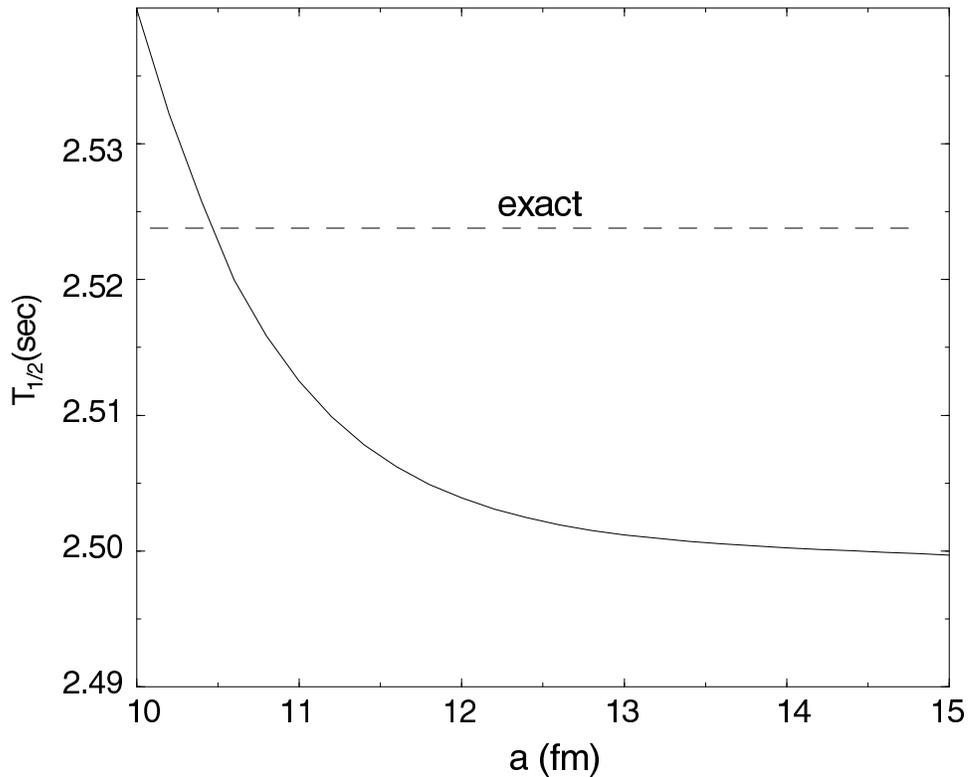


FIGURE 2. Half-life of the spherical $1h_{11/2}$ orbit in ^{147}Tm calculated in the R-matrix theory as a function of the channel radius using the “natural boundary condition”.

to the fact that only the one-channel R-matrix expression is used. The iterative R-matrix technique, “the natural boundary condition” method, can be applied also in the case of a deformed mean field. In the many-channel case the accuracy of the iterative R-matrix approach is similar to the one-channel calculation.

V OSCILLATOR EXPANSION

The eigenfunctions of an axially deformed average nuclear field, the Nilsson orbits, can be expanded in a complete set of functions. In this way one can avoid the numerical solution of the eigenvalue problem of coupled differential equations. The wave function (12) may be approximated [7] by

$$\Psi^K(\vec{r}) \approx \sum_{n_\rho, n_z, m_s} C(K, n_\rho, n_z, m_s) |n_\rho, n_z, K, m_s\rangle, \quad (21)$$

where $|n_\rho, n_z, K, m_s\rangle$ is the eigenfunction of the axially deformed harmonic oscillator in the cylindrical basis. The coefficients $C(K, n_\rho, n_z, m_s)$ are determined by

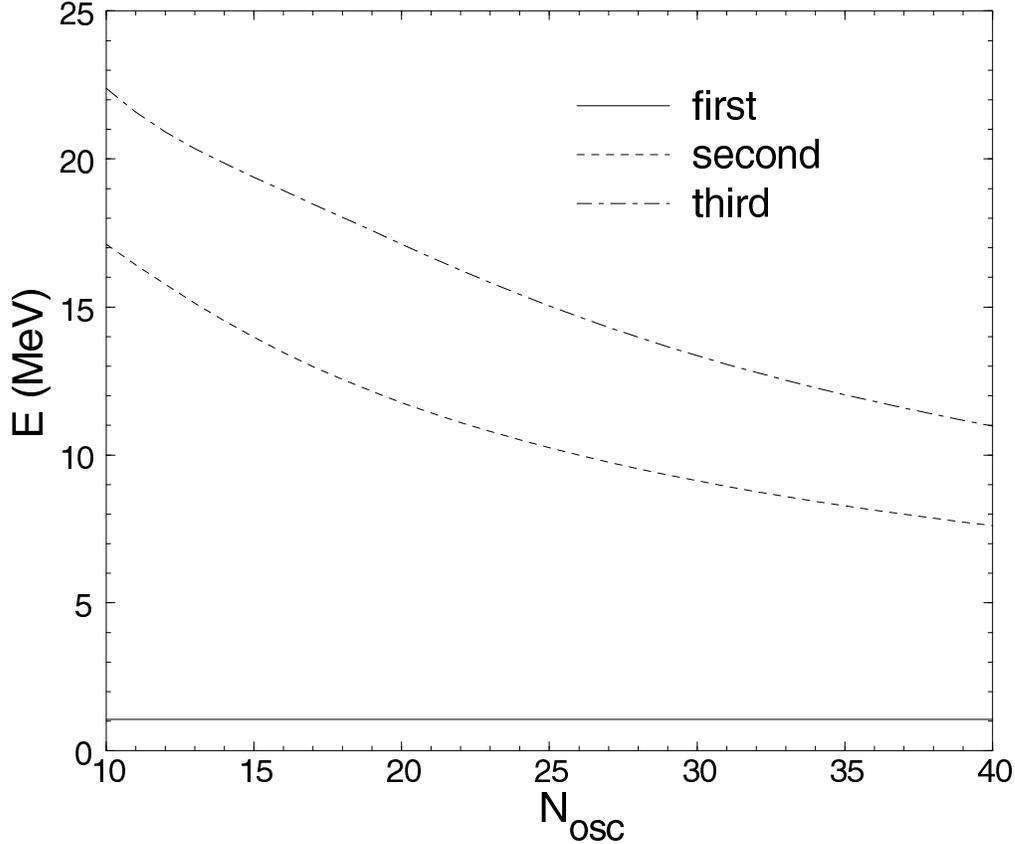


FIGURE 3. The energies of the three lowest spherical proton $h_{11/2}$ orbitals of ^{147}Tm in the spherical Woods-Saxon model as a function of the size of harmonic oscillator basis N_{osc} . The length parameter of the spherical basis is 2 fm.

matrix diagonalization using the code SWBETA [7]. After the the eigenvalue problem of the Hamiltonian matrix has been solved, the wave function (21) can be transformed into a similar form as in Eq. (12) with

$$g_{jl}^K(r) \approx \sum_n A(K, n, j, l) R_{nl}(r), \quad (22)$$

where $R_{nl}(r)$ is the radial function of the spherical harmonic oscillator. (We carried out the transformation from cylindrical variables ρ, z, ψ to polar variables r, Θ, ϕ because it is easier to formulate the R-matrix theory in these variables.)

It was recognized long ago that by using the harmonic oscillator expansion (or any expansion in a square integrable basis) not only can the bound states be determined, but also the positions of narrow resonances. If M basis functions are used in the expansion, then M eigenvalues are obtained from the matrix diagonalization. When the size of the basis is increased, the eigenvalues of all the positive energy solutions

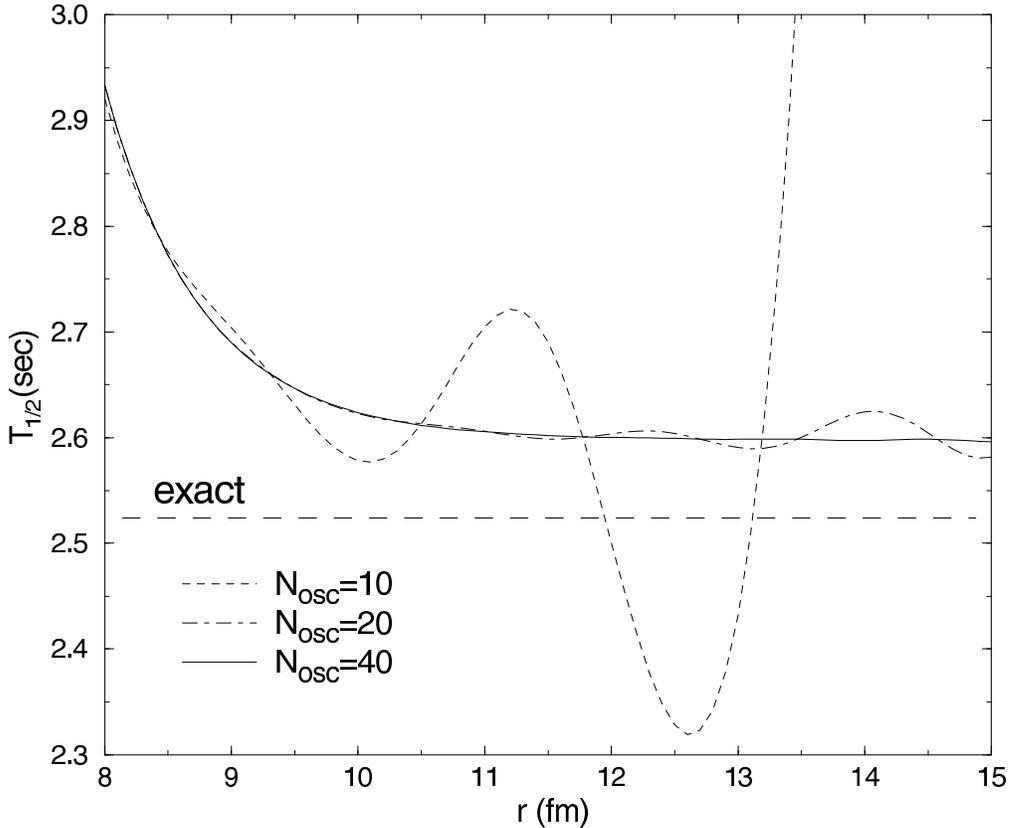


FIGURE 4. Half-life of the spherical $1h_{11/2}$ orbit of ^{147}Tm as a function of the channel radius calculated in the R-matrix theory based on the harmonic oscillator expansion. Three different basis sizes are used in the calculation.

tend toward zero. The sign of a resonance is that specific positive energy solutions are relatively stable with respect to increasing the size of the basis. This is shown in Fig. 3 for the three lowest spherical $h_{11/2}$ proton orbits of ^{147}Tm . The lowest $h_{11/2}$ state obtained from the diagonalization is a good approximation to the resonance; its energy is very stable with respect to the size of the oscillator basis used, at least in the range of N_{osc} considered. (In the calculations we take all the deformed oscillator states with principal quantum number $N \leq N_{\text{osc}}$.) The higher-lying states cannot be represented by the expansion procedure; they correspond to the high-energy $h_{11/2}$ continuum.

Thus the position of the resonance can be found, but how can its width be determined? Several proposals exist in the literature. They are dubbed “ L^2 stabilization methods” (since only square integrable functions are used in the expansion). Here we combine the oscillator expansion method and the R-matrix formalism.

In the R-matrix theory, the coupled equations are solved with the boundary

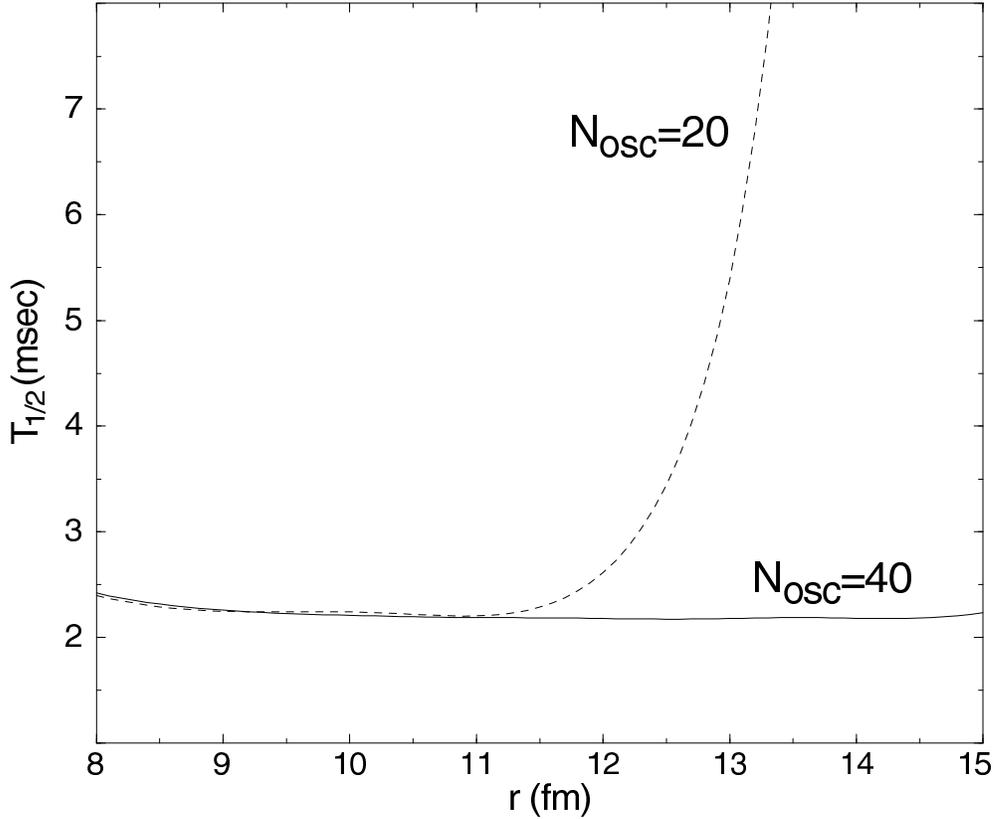


FIGURE 5. Half-life of the $K^\pi = 3/2^+$ deformed Nilsson resonance resonance in ^{131}Eu calculated in the R-matrix theory based on the harmonic oscillator expansion as a function of the channel radius. Two different basis sizes are used in the calculation.

conditions given in advance. This cannot be achieved in the framework presented here, but the procedure can be reversed: Starting from the approximate solution (22), the corresponding boundary condition parameter can be derived at each r , and then the machinery of the R-matrix theory can be applied. It is to be noted, however, that although the boundary condition is independent of the wave function normalization, the reduced width amplitude depends critically on it. Thus, at each r the approximate solution (22) must be normalized to one inside the channel surface.

Figure 4 shows the half-life of the lowest spherical $h_{11/2}$ orbit of ^{147}Tm as a function of the channel radius using three different basis sizes. A perfect stabilization of the result is obtained at large N_{osc} . The quality of the oscillator-expansion method is similar to that of the R-matrix result discussed in Fig. 2. The deformed nucleus ^{131}Eu with deformation $\beta_2=0.32$ is considered in Fig. 5. The Nilsson orbit is characterized by the quantum numbers $K^\pi = 5/2^+$. The calculations use the

Becchetti-Greenlees potential parameters, with the depth of the potential adjusted to the position of the resonance at 0.950 MeV. The calculations are carried out using $N_{\text{osc}}=20$ and 40 oscillator quanta. Again, at large N_{osc} the result is very stable. In summary, the results presented in Figs. 4 and 5 show that the harmonic oscillator expansion can be successfully used for the determination of widths of very narrow resonances if the size of the basis is large enough.

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