

From bound states to resonances: analytic continuation of the wave function

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Abstract

Single-particle resonance parameters and wave functions in spherical and deformed nuclei are determined through analytic continuation in the potential strength. In this method, the analyticity of the eigenvalues and eigenfunctions of the Schrödinger equation with respect to the coupling strength is exploited to analytically continue the bound-state solutions into the positive-energy region by means of Padé approximants of the second kind. The method is here applied to single-particle wave functions of the ^{154}Sm and ^{131}Eu nuclei. A comparison of the results with the direct solution of the Schrödinger equation shows that the method can be confidently applied also in coupled-channel situations requiring high numerical accuracy.

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In recent years there has been an increasing experimental activity [1] on nuclei far from the stability line. These nuclear systems are usually unbound or weakly bound, and often exhibit resonances with a pronounced single-particle character, since the Fermi level is close to or even immersed in the continuum. This phenomenology has prompted people to look for more and more efficient methods for the description of unbound states, which could compete with the techniques presently available for the discrete part of nuclear spectra. A possible approach, which proved to be rather successful, exploits the fact that resonances can be described by wave functions with purely outgoing behavior and complex eigenvalues $E_R - i\Gamma/2$ (Gamow states) [2]. One is then confronted with the solution of a complex eigenvalue problem for a non-Hermitian Hamiltonian. Even if Gamow states are characterized by the at first sight unpleasant feature of an exponentially growing oscillatory behavior at large distances, they can be however normalized by a suitable generalization of the quantum-mechanical inner product. This can be achieved in several, essentially equivalent ways, either introducing convergence factors in the integrals expressing their norm [3,4], or by analytic continuation from the upper half of the k -plane to the resonance poles [5,6]. These recipes can be implemented by solving the Schrödinger equation along a deformed contour in the complex r -plane [4], which amounts to an analytic continuation $\mathbf{r} \rightarrow \exp(i\theta)\mathbf{r}$ in configuration space. This is very convenient under a computational point of view, resonance states being transformed into square-integrable wave functions, while leaving untouched the corresponding poles of the S-matrix in the energy plane. If this is done for a value of r so large that the effective nucleon-core interaction can be neglected (exterior complex scaling), one has the advantage that the potential itself remains unchanged in the contour deformation. Complex-coordinate rotation methods have found interesting applications both in nuclear [7] and in atomic [8] physics.

Recently, unbound states in exotic nuclei have been studied by means of Analytic Continuation in the Coupling Constant (ACCC) [9,10]. This method, proposed already several years ago by Kukulín and co-workers [11,12], starts from the intuitive expectation that, for an attractive potential, a resonance state will become a bound state as the coupling strength is increased. Under a mathematical point of view, one can prove that the wave number $k = \sqrt{2\mu E}/\hbar$ is an analytic function of the strength λ , with the same restrictions on the potential which guarantee the analyticity of the Jost function [12,13]. Here and in the following μ denotes the reduced mass of the nucleon-core system. Near the value λ_0 for which $k(\lambda_0) = 0$ (*i.e.* near the scattering threshold), one has [12,13]

$$k(\lambda) \sim i\sqrt{\lambda - \lambda_0} \quad , \quad k(\lambda) \sim i(\lambda - \lambda_0), \quad (1)$$

for $l \neq 0$, and for $l = 0$, respectively. These properties suggest the analytic continuation of k in the complex λ -plane from the bound-state region into the resonance region through the employment of Padé approximants of the second kind [12]

$$k \simeq k^{(N,M)}(x) = i \frac{c_0 + c_1 x + c_2 x^2 + \cdots + c_M x^M}{1 + d_1 x + d_2 x^2 + \cdots + d_N x^N}, \quad (2)$$

where $x \equiv \sqrt{\lambda - \lambda_0}$. In practice, the following procedure can be followed to find the resonance parameters for an interaction V , when $l \neq 0$. One endows V with a strength parameter λ , $V \rightarrow \lambda V$, and solves the bound-state problem for λV in correspondence to $N + M + 1$

different values λ_i of the coupling strength. Given the threshold value λ_0 , the $N + M + 1$ coefficients in the Padé approximant (2) can be determined by equating $k^{(N,M)}(x_i)$ to the actual values k_i of the wave number. The approximant can then be used to estimate the resonance wave number k_r , and hence the resonance position and width, in correspondence to the “physical” value $\lambda = 1$ of the potential strength. This procedure can be easily modified if the potential V supports an s -wave resonance, in which case the corresponding pole leaves the negative imaginary axis at $k(\bar{\lambda}_0) = -i\bar{\chi}_0$ [9,10,12]. The method has been applied with some success to unbound states in ${}^5\text{He}$ and ${}^5\text{Li}$, as well as in three-cluster nuclei [9,10]. An extrapolation procedure similar the one described above can be used in the complex k -plane to analytically continue the bound-state wave function $\psi_l^{(B)}(kr)$ into the scattering region for any value of the radial variable r .

In this paper we study the application of this technique to single-particle resonances in deformed nuclei, a situation quite common in the drip-line region. The numerical evaluation of resonance (Gamow) states for nonspherical nuclei is a major challenge, which has been only recently solved [14]. Bound-state wave functions, on the other hand, can be calculated nowadays through very efficient and quick algorithms [15]. Here, we shall enquire whether the solution of the coupled-channel bound-state problem, obtained for a set of values of the coupling strength λ , can be analytically continued into the unbound region. We shall consider the Padé extrapolation both for the resonance parameters and for the wave function. The latter case is particularly interesting for proton decay, since one has to deal with lifetimes $\tau \geq 1\mu s$, which implies resonance widths $\Gamma = \hbar/\tau$ smaller than 10^{-16} MeV. Such small widths are difficult to obtain with enough accuracy starting directly from the energy eigenvalue, and can be best estimated from the wave-function behavior [16,17].

To test the validity of the ACCC method in the present case, we have solved exactly the problem both for bound-state energies and in the continuum, and we have compared the results with the outcome of the Padé extrapolation obtained starting from the bound-state region, for different, decreasing values of the coupling strength. The radial Schrödinger equation with outgoing-wave boundary conditions has been solved in the standard way, namely starting from the origin and from the outer region, and matching the logarithmic derivative of these functions at some radius R . For real, negative energies one gets normalized wave functions, with the proper exponentially decreasing tail, in correspondence to the energy eigenvalues of the bound system; in the scattering case, on the other hand, one gets purely outgoing states for complex eigenvalues $E_R - i\Gamma/2$ [2]. The normalization of our unbound wave functions agrees with the Zel’dovich [3] or Gyarmati-Vertse [4] prescriptions for Gamow states.

As a first step, let us consider single-particle resonances in spherical nuclei. In Fig. 1 we report the results of our calculations for the $f_{5/2}$ neutron state in the nucleus ${}^{154}\text{Sm}$. The neutron is assumed to move in a spherical Saxon-Woods potential, supporting a bound state for $\lambda = 1$. Fig. 1(a) exhibits the real and imaginary part of the energy E , as a function of the decreasing strength parameter λ . The full dots represent the outcome of the numerical solution of the Schrödinger equation, whereas the crosses correspond to the bound-state energies used for the Padé extrapolation into the scattering region, the extrapolated results being given by the full lines. As it can be seen, the neutron is bound for λ decreasing from 1 down to $\lambda_0 \simeq 0.84$, where the neutron state becomes unbound and the energy acquires a non-vanishing imaginary part. With a (7,7) approximant of the form (2), the agreement

between the exact and the extrapolated results is quite good both for $Re(E)$ and $Im(E)$ in the whole considered region of the strength–parameter values. In Figs. 1(b) and 1(c) we show the calculated (full dots) and extrapolated values of the real and imaginary part of $r\psi_{lj}(r)$ at $r = 7$ fm and $r = 15$ fm, respectively. The results are plotted as functions of the real part $Re(E)$ of the corresponding eigenvalue. As in Fig. 1(a), the crosses denote the bound–state points used as input to the extrapolation procedure. Note that at $r \sim 7$ fm the neutron is feeling the strongest effect from the nuclear potential, and the wave function is attaining its largest value; for $r \sim 15$ fm, on the other hand, one is far away enough from the nuclear core, to have an indication of the quality of the extrapolation in reproducing the tail of the wave function. This is crucial in order to obtain an accurate evaluation of the resonance width. Indeed, in the spherical case the partial width for the decay to the channel lj can be related to the value of the wave function $\psi_{lj}(r)$ at $r = R$ by [16]

$$\Gamma_{lj} = \frac{\hbar^2 k}{\mu} \frac{R^2 |\psi_{lj}(R)|^2}{|G_l(R) + iF_l(R)|^2}, \quad (3)$$

where F_l and G_l represent the free regular and irregular radial wave functions, respectively. If R is large enough to be outside of the range of the potential, Eq. 3 provides a width which is actually independent from the value of R , as it should be [16]. These considerations can be extended to the coupled–channel case [17]. As Figs. 1(b) and 1(c) clearly exhibit, the results of the (7,7) extrapolation agree very well with the numerical calculation both in the inner and in the tail region. In particular, the non–trivial behavior of the real part of the inner wave function in the threshold region is accurately reproduced by the extrapolation, an indication that the Padé analytic continuation performs well in transferring the information from the bound–state into the scattering region. Similarly, the steep increase of the wave–function tail when going to positive energies is successfully reproduced by the Padé approximation. We have also considered the behavior of the Padé extrapolation for lower–rank approximants, and verified that the analytic continuation still compares well with the exact results when a (4,4) Padé approximant is employed.

Similar calculations have been done for a proton state in the ^{154}Sm nucleus, with the proton moving in a $h_{9/2}$ state. In this case, when solving the Schrödinger equation, the inner wave function has to be matched to the radial Coulomb wave function $r\psi_{lj}^{out}(r) = N_{lj}[G_l^{(C)}(r) + iF_l^{(C)}(r)]$, where $G_l^{(C)}$ and $F_l^{(C)}$ are the usual regular and irregular Coulomb functions and N_{lj} is a normalization factor. The outcome of the calculations is reported in Fig. 2. As for the neutron case, Fig. 2(a) displays the real part of the energy eigenvalue for decreasing λ , whereas Figs. 2(b) and 2(c) refer to the real part of $r\psi_{lj}(r)$ at $r = 5$ fm and $r = 15$ fm, respectively, the symbols having the same meaning as in Fig. 1. The imaginary parts of both the energy and the wave function remain vanishingly small in passing from the bound–state into the scattering region, so that they are not even reported in the figures. The proton state becomes unbound at $\lambda \sim 1$, with $Re(E)$ scaling linearly with the strength parameter. Similarly, the wave function exhibits a smooth behavior when the scattering threshold is crossed. It is not surprising, therefore, that a low–rank (4,4) Padé approximant can provide an extremely good reproduction of the exact results. Note that, because of the Coulomb barrier, the proton wave function in the exterior region is much smaller than in the neutron case.

The ACCC method has been finally tested for proton resonances in deformed nuclei. As

is well-known, such a calculation is much more challenging than in the spherical case, since it requires the solution of a coupled-channel problem to determine the intrinsic, single-particle wave functions [14,16,17]. In Fig. 3 (left panel) we report the real part of the energy of the $3/2+$ state in ^{131}Eu as a function of λ . Improved experimental data have been recently given for this highly deformed proton emitter, leading to the identification of a fine structure splitting in the radioactive decay from the ground state [18]. The process can be successfully described in the framework of a model where the proton is emitted from a deformed single-particle Nilsson level [17,19]. The energy of the $3/2+$ state turns out to be a linear function of λ , much as in the spherical situation, the imaginary part remaining always very close to zero. The relevant wave-function components at $r = 15$ fm are given in the right panel of Fig. 3. For the proton decay of the ^{131}Eu nucleus from the $K = 3/2+$ state they are the $d3/2$ and $d5/2$ components of the $3/2+$ Nilsson orbital (higher- l partial waves giving a negligible contribution to the decay width [19]). The former determines the ^{131}Eu proton decay to the ^{130}Sm ground state, while the latter is by far the dominant term in the decay to the 2^+ excited state of the daughter nucleus [17,19]. The bound-state solution has been analytically continued into the scattering region by means of a simple (3,3) Padé approximant. One can see that the extrapolation reproduces the outcome of the numerical solution extremely well both for the energy and for the wave-function components. Note that, in passing from the bound-state into the positive-energy region the imaginary part of the wave functions is again so small, that it is not given in the figure.

In summary, we have applied a Padé extrapolation to determine the resonance parameters and wave function for single-particle resonances in nuclei, starting from bound-state calculations. This has been obtained by varying the coupling strength so as to analytically continue the bound-state energy eigenvalue and wave function into the positive-energy region. The method has been applied to the single-particle decay of both spherical and deformed nuclei, which entails the solution of a single- or a coupled-channel problem, respectively. A comparison of the extrapolated results with the outcome of the direct solution of the Schrödinger equation with the proper boundary conditions shows that the ACCC method can be confidently applied to these situations, where high numerical accuracy is required in order to have a meaningful comparison with the experimental data.

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FIGURES

FIG. 1. Energy eigenvalue and wave function for the neutron $f5/2$ state in the ^{154}Sm nucleus. In (b) and (c) the wave function has been multiplied by the radius r , and evaluated at $r = 7$ fm and $r = 15$ fm, respectively. Full dots represent the results obtained from the numerical solution of the Schrödinger equation, whereas crosses are the input values used for the analytic continuation. Full curves are the outcome of the Padé extrapolation.

FIG. 2. As in Fig. 1 for the real part of the energy and of the quantity $r\psi_{lj}(r)$ referring to the proton $h9/2$ state in the ^{154}Sm nucleus. In (b) and (c) the wave function is evaluated at $r = 5$ fm and $r = 15$ fm, respectively.

FIG. 3. As in Fig. 2 for the proton $3/2+$ state in the deformed nucleus ^{131}Eu . The dominant wave-function components $r\psi_{lj}(r)$ are evaluated at $r = 15$ fm.





