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The Bound-State Solution of Wave Equations for Real or Complex Eigenvalues

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ABSTRACT

A simple but efficient computational procedure is given for calculating bound state solutions of wave equations, valid even for absorptive interactions and corresponding complex eigenvalues. The method also applies to eigenvalues in nonlinear form. The integration is deliberately made in the direction of instabilities, but this does not spoil the accuracy.

During an investigation of the interaction of π-mesons with nuclei we have met the following problem:

Negative π-mesons interact with the electrostatic potential $Z\alpha/r$ outside the nucleus, and because of this attractive potential they can form bound states ("mesic atoms"). Both the eigenvalues and wave functions for the unperturbed problem (Klein–Gordon equation with an external Coulomb field) are well known. In addition to this interaction the pion has short-range interactions in a region of nuclear dimensions. These interactions have a double origin: (*1*) the strong interaction and the *absorption* of the pion by the nucleus, (*2*) the deviation of the Coulomb field from $Z\alpha/r$ inside the nuclear region due to smeared out charges. The result of these interactions is to change the eigenvalue of the bound state and, due to the absorption, to transform the eigenvalue from a real one to a complex one (level broadening). Our problem is to calculate this complex eigenvalue to high precision under various hypotheses for the detailed interaction.

To tackle this problem we have developed a simple, unusual, but general method which has not been previously used to our knowledge. The method can be applied generally to bound-state problems of the wave equation type (Schroedinger,

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Klein-Gordon) whether the interaction is described by potentials, by boundary conditions or otherwise.

We now describe the essence of the method in a simplified case. Consider an equation of the type

$$\frac{d^2u}{dr^2} + (k_0^2 + q(r))u = 0, \tag{1}$$

with the (complex) eigenvalue k_0.

The interaction $q(r)$ [in general complex and also including the centrifugal potential $l(l+1)/r^2$] is assumed for the moment to go to zero faster than $1/r$ at infinity. The regular and irregular solutions $U_k^{(1)}(r)$ and $U_k^{(2)}(r)$ for arbitrary k then behave as decreasing and increasing exponentials for large r:

$$U_k^{(1)}(r) \to e^{-kr}; \qquad U_k^{(2)}(r) \to e^{+kr}. \tag{2}$$

The bound-state solution behaves like r^{l+1} at the origin and goes exponentially to zero at infinity for $k = k_0$. Our method of solution is as follows: impose the correct behavior, $u_k(r) = Ar^{l+1}$, at the origin with an arbitrary constant A for a trial value of k. Integrate outwards to large r by standard procedures. The wave function is then

$$\begin{aligned} u_k(r) &= B(k)\left[U_k^{(1)}(r) + \left(\frac{k-k_0}{k_0}\right) C(k)\, U_k^{(2)}(r)\right] \\ &\xrightarrow[r\to\infty]{} B(k)\left[e^{-kr} + \left(\frac{k-k_0}{k_0}\right) C(k)\, e^{+kr}\right]. \end{aligned} \tag{3}$$

The function $C(k)$ vanishes for all the remaining eigenvalues, but like $B(k)$, it is nearly constant in region of the order of the eigenvalue spacing around k_0. We will therefore treat both as constants here. For large values of r the irregular component of $u_k(r)$ rapidly becomes exponentially dominant when k is not an eigenvalue. It is therefore extremely tempting to seek a procedure which systematically makes $u_k(r)$ small for large r. Equivalently, and more suitably in the case of a complex k, one searches for a minimum in $|u_k(r)|^2$ for a fixed and large $r = r_0$,

$$\begin{aligned} |u_k(r_0)|^2 \approx |B|^2 \Big\{ & e^{-2\mathrm{Re}(kr_0)} + \mathcal{O}\left[\frac{(k-k_0)}{k_0} C\right] \\ & + |C|^2 \left|\frac{k-k_0}{k_0}\right|^2 e^{2\mathrm{Re}(kr_0)} \Big\}. \end{aligned} \tag{4}$$

While such a procedure is possible in principle, and has an intrinsic relative precision in eigenvalue of $\mathcal{O}(e^{-2\mathrm{Re}(k_0 r_0)})$, the minimization procedure is extremely

inefficient, with a very small region of convergence. The reason is that the irregular function depends exponentially on $\mathrm{Re}(kr_0)$. Therefore the zero which results from $|k - k_0|^2$ occurs as an extremely narrow, deep minimum superimposed on an exponential variation (see Fig. 1).

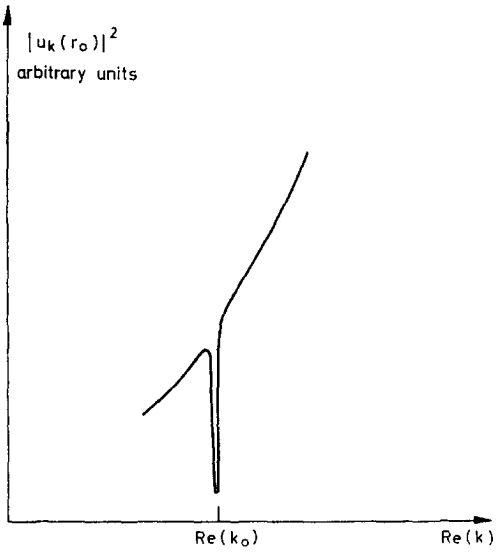

FIG. 1. The absolute square of the wavefunction, $|u_k(r_0)|^2$, has a narrow minimum for correct eigenvalue superposed on a rapid exponential variation for large r_0.

To remedy this situation we simply divide out the irregular solution by forming the ratio $v(k)$:

$$v(k) = \frac{|u_k(r_0)|^2}{|U_k^{(2)}(r_0)|^2} \approx \frac{|u_k(r_0)|^2}{\exp[2\mathrm{Re}(kr_0)]} \approx \left|\frac{k - k_0}{k_0}\right|^2 |BC|^2. \tag{5}$$

We have here neglected terms which may affect the eigenvalue to $\mathcal{O}(e^{-2k_0r_0})$. The resulting function $v(k)$ is now approximately a quadratic function of $\mathrm{Re}(k - k_0)$ and $\mathrm{Im}(k - k_0)$. The minimum is clearly defined, with a large region of convergence as illustrated in Fig. 2. An iteration procedure based on the minimization of $v(k)$ converges quadratically to the intrinsic precision of the method. Excellent wave functions are obtained as follows: the function $|u_k(r)|^2$ has a minimum at $r = r_{\min}$ after which it grows exponentially for large r. The wave function $u_k(r)$ is very accurate for the approximate eigenvalue k for $r < r_{\min}$ and should be put equal to zero or exponentially decreasing for $r > r_{\min}$.

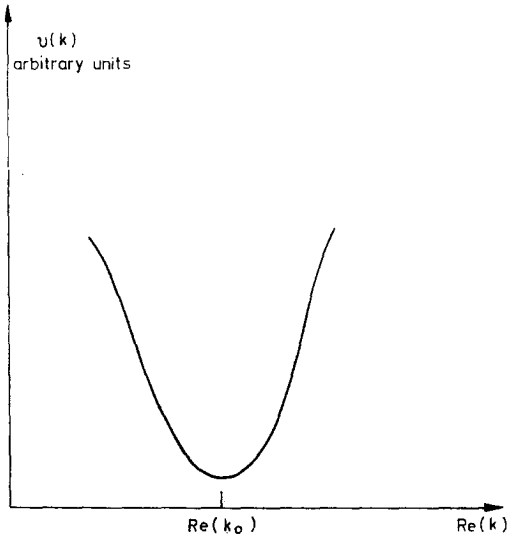

FIG. 2. Division of $|u_k(r_0)|^2$ by the exponential factor gives a broad minimum with rapid convergence of iteration procedures.

As practical test of the usefulness and accuracy of our method (method I), we first compare its results for the Klein-Gordon equation with those of a variational method with integration from both ends inwards (method II) [1] as well as with the exact solution in the case of the purely real Coulomb potential (point nucleus). We used a smeared charge distribution to avoid the technical but unessential problem of the r^{-1} dependence of the potential at the origin. The Coulomb binding energy of the $3d$ orbit in ^{16}O is exactly

$$E_{0,3d} = -26.1857_3 \text{ keV}$$

The finite size effect does not affect the eigenvalue for this orbit to this precision. The numerical methods give

$$E_{3d}^{(0)} = -26.1857_2 \text{ keV} \qquad \text{(method I)},$$

$$E_{3d}^{(0)} = -26.1857_3 \text{ keV} \qquad \text{(method II)}.$$

Thus the method works excellently for a real interaction.

As the next step the pion energy and width in the $1s$ Bohr level of ^{16}O are calculated in the presence of a complex strong interaction potential [2]. Of course the variational method had to be generalized to include complex interactions and

complex eigenvalues, but this is rather straightforward. We required iteration to stop when the relative difference of iterated eigenvalues was less than 10^{-6}.

In the case of method I, the wavefunction $u_k(r)$ and the ratio $v(k)$ were obtained from outwards integration from the origin using Numerov's formula [3] for step-by-step integration in the complex plane[2].

The iterated eigenvalue was then obtained from a complex parabola fitted to $v(k)$ of Eq. (5) using three neighboring values of k. The fixed value of the radial parameter r_0 was chosen so large that the correct wavefunction was less than 10^{-4} of its maximal value. Starting from the eigenvalue in the absence of strong interactions both methods needed four iterations to give the values

$$E_{1s} = (-219.6493_4 - i1.1322_0)\ \text{keV} \qquad \text{from method I,}$$
$$E_{1s} = (-219.6493_6 - i1.1322_0)\ \text{keV} \qquad \text{from method II.}$$

The corresponding energy for a smeared charge but without the strong interaction potential is

$$E_{1s}^{(0)} = -233.3905_6\ \text{keV}.$$

It is thus clear that both numerical methods give identical results. The wavefunctions agree very closely. The real and imaginary parts of the wavefunctions agree to better than $1 : 10^5$ for pion densities larger than $4 \cdot 10^{-6}$ of the maximal density. For a density of $5 \cdot 10^{-7}$ the agreement is still $1 : 10^3$. In other words, the wave functions agree everywhere to better than $1 : 10^5$ of the maximal value. Since the methods differ so widely, this may be regarded as further proof of their accuracy. Also for other cases ($2s$, $2p$, $3d$ levels) we got similar good results with an even smaller number of iterations. Due to the necessity of calculating wavefunctions for three values of k for each iteration our method is, disregarding possible refinements, about three times slower than the method II. This is however compensated by its greater generality and simplicity, in particular since both methods converge rapidly. For example, our method makes it possible to apply closely similar programs to bound state and continuum problems, which is now being exploited.

It should finally be remarked that our application has been to the Klein–Gordon equation, which in principle is nonlinear in the energy eigenvalue. In our case the nonlinearity is very slight and of little importance, but our method should work equally well when the nonlinearity is strong.

[2] Note that contrary to usual recommendations the integration is done deliberately in the direction of the instability. In our case this is completely innocent since our method makes explicit use of the same exponential growth to obtain the eigenvalue from the admixture of the irregular solution. Although the effect of an error is cumulative in the wave function, its relative effect on the eigenvalue therefore stays constant so that it can be made arbitrarily small.

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