Spherical-box approach for resonances in presence of Coulomb interaction postprint

Authors: Shan-Gui Zhou, Jie Meng, En-Guang Zhao

Date: 2017-08-22T00:00:00+00:00

Abstract

The spherical-box approach is extended to calculate the resonance parameters and the real part of the wave function for single particle resonances in a potential containing the long-range Coulomb interaction. A model potential is taken to demonstrate the ability and accuracy of this approach. The calculated resonance parameters are compared with available results from other methods. It is shown that in the presence of the Coulomb interaction, the spherical-box approach works well for not so broad resonances. In particular, for very narrow resonances, the present method gives resonance parameters in a very high precision.

Full Text

Preamble

Spherical-box approach for resonances in presence of Coulomb interaction

Shan-Gui Zhou[1,2,3], Jie Meng[4,5,1,2,3] and En-Guang Zhao[1,2,3,4]

[1]Key Laboratory of Frontiers in Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China
[2]Kavli Institute for Theoretical Physics China at the Chinese Academy of Sciences, Beijing 100190, China
[3]Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou 730000, China
[4]School of Physics, Peking University, Beijing 100871, China
[5]Department of Physics, University of Stellenbosch, Stellenbosch, South Africa

E-mail: sgzhou@itp.ac.cn

Abstract. The spherical-box approach is extended to calculate the resonance parameters and the real part of the wave function for single-particle resonances in potentials containing long-range Coulomb interactions. A model potential

is employed to demonstrate the capability and accuracy of this approach. The calculated resonance parameters are compared with available results from other methods. It is shown that in the presence of Coulomb interaction, the spherical-box approach works well for resonances that are not too broad. In particular, for very narrow resonances, the present method yields resonance parameters with very high precision.

PACS numbers: 02.60.Lj, 31.10.+z, 32.70.Jz
(Some figures in this article are in colour only in the electronic version)

---

1. INTRODUCTION

The investigation of continuum and resonant states constitutes an important subject in quantum physics. For the theoretical determination of resonance parameters (energy and width), several bound-state-like methods have been developed, including the complex scaling method (CSM) [1–9], the complex absorbing potential (CAP) method [10, 11], the analytical continuation in the coupling constant (ACCC) approach [12–20], and the real stabilization method (RSM) [21–30]. These approaches complement methods based on connecting unbound states (including resonances and antibound or virtual states) to poles of the S-matrix.

In the real stabilization method, the Schrödinger equation (or the Dirac equation in relativistic models) for the system is solved within a finite-sized basis [21] or box [24], thereby imposing a bound-state problem. The RSM is founded on the principle that the energy of a "resonant" state remains "stable" against variations in the basis or box size. Considerable effort has been devoted to calculating resonance parameters more efficiently with the RSM [24–30]. One particularly effective implementation is the "spherical-box approach" [24], where the energy and width of resonances in finite-range potentials are determined from the variation of discrete positive energies with the box radius. The spherical-box approach for short-range potentials has been rigorously validated [31], and in recent work [30], single-neutron resonances in atomic nuclei were investigated by combining the RSM with the relativistic mean-field model [32, 33].

In many atomic, molecular, and nuclear processes, long-range Coulomb interactions play crucial roles. Therefore, it is necessary to extend the spherical-box approach to resonances in the presence of long-range forces and to verify its validity and accuracy. In the present work, we generalize the spherical-box approach to incorporate the influence of the Coulomb force.

The paper is organized as follows. Section 2 presents the formalism of the spherical-box approach for resonances with Coulomb interaction. Section 3 provides numerical details, results for a model potential, and discussion. Finally, Section 4 summarizes our work.

---

2. FORMALISM

We consider a central field problem. The radial Schrödinger equation reads (in atomic units):

$$\left[-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_0(r) + V_C(r)\right]\Psi_k(r) = E\Psi_k(r),$$

where $V_0(r)$ is a finite-range potential and $E = k^2/2$. Under box boundary conditions, the continuum becomes discretized, reducing the problem to a bound-state formulation. When the box size is sufficiently large, the energies of any bound states become independent of the box dimension. In the continuum region, certain states remain stable against box-size variations—that is, their energies remain nearly constant as the box radius changes. These stable states correspond to resonances. It should be noted that the spherical-box approach is fundamentally different from the "variable phase approach," where the potential is truncated beyond a distance $\bar{r}$ and one must solve a series of scattering problems for different $\bar{r}$ values [34].

In the spherical-box approach, the resonance energy is determined by a stability condition. The width can be evaluated from the stability behavior of positive-energy states [24]. When r is large enough that the finite-range potential $V_0(r)$ vanishes, the wavefunction $\Psi_k(r)$ satisfies the asymptotic form:

$$\Psi_k(r) \sim \sin\left(kr - \gamma\ln(2kr) + \eta_l\right),$$

where η_l is the phase shift and $\gamma = Z/k$ arises from the long-range Coulomb interaction. The box boundary condition $\Psi_k(R) = 0$ yields:

$$kR - \gamma\ln(2kR) + \eta_l = n\pi.$$

Thus, the derivative of the phase shift with respect to box size is:

$$\frac{\partial\eta_l}{\partial R} = -k + \frac{\gamma}{R}.$$

Around an isolated resonance, the energy E and phase shift $\eta_l(E)$ satisfy:

$$\eta_l(E) = \eta_{l,\mathrm{pot}}(E) + \tan^{-1}\left(\frac{\Gamma/2}{E_r - E}\right),$$

where E_r is the resonance energy and Γ is the width. Under the assumption that the potential scattering phase shift $\eta_{l,\mathrm{pot}}(E)$ varies slowly with box size (i.e., $\partial\eta_{l,\mathrm{pot}}/\partial R \approx 0$), we derive the width formula:

$$\Gamma = \frac{2k_r}{\left|\frac{\partial^2 E}{\partial R^2}\right|_{R=\bar{R}}} \left[1 + \left(\frac{\gamma}{k_r \bar{R}}\right)^2\right]^{-1},$$

where $k_r = \sqrt{2E_r}$ and $\bar{R}$ is the box size at the stable point. Note that this formula reduces to equation (8) in [24] when the Coulomb interaction is absent ($Z = 0$).

---

3. A MODEL PROBLEM

To test the capability and accuracy of the spherical-box approach for resonances in potentials with long-range interactions, we solve a model problem and compare our results with predictions from other methods. We employ the potential:

$$V(r) = V_0 r^2 e^{-r} + \frac{Z}{r},$$

which has been extensively studied for $Z = 0$ and/or $Z = 1$ [35, 24, 26, 36, 37]. In the present work, we take $V_0 = 7.5$.

3.1. Numerical procedure

The Schrödinger equation (1) with potential (8) is solved under box boundary conditions using the shooting method [38, Chapter 18] with a fourth-order Runge-Kutta algorithm. For $Z = 0$, the energy calculated from the shooting method converges as the step size decreases, achieving a relative error within 10^{-8} with step size $\delta r = 0.001$. For $Z = 1$, a step size of $\delta r = 0.0001$ yields relative accuracy comparable to literature values. In the following, we present results for potential (8) with $Z = 1$ using $\delta r = 0.0001$ to achieve high precision.

3.2. Resonance parameters

We first present results for s-states. Figure 1 [Figure 1: see original paper] shows the potential $V(r)$ from equation (8) and the energies of s-states versus box size. Examination of the figure reveals two resonances with energies near 1.8 and 4.0 atomic units, respectively. The former is very narrow, as indicated by sharp avoided crossings, while the latter lies above the barrier and is very broad.

Table 1 lists the resonance parameters for the narrow resonance evaluated at different stable regions. For comparison, results from complex-scaling methods are also included [36, 37]. As $\bar{R}$ increases, the resonance energy converges rapidly to a stable value. For this narrow resonance, the spherical-box approach yields extremely precise energy and width comparable to the exact values in [37]. Seven-significant-digit accuracy for the energy is achieved at the third avoided crossing with $\bar{R} = 8.7509$, and four-significant-digit accuracy for the width at

the ninth avoided crossing with $\bar{R} = 18.5633$. These high precisions are very encouraging, suggesting that the spherical-box approach can be reliably applied to narrow resonances with computational effort far less than that required for complex calculations.

Table 2 presents parameters for the second s-wave resonance, which is quite broad. When $\bar{R} > 13.3808$, no stable region satisfying the condition $\partial^{2E}/\partial R^2 = 0$ can be found within our numerical accuracy. At the last observed avoided crossing, the resonance energy deviates from the exact value by 8% and the width by 15% [37]. This provides a guide for estimating the accuracy of the spherical-box approach for broad resonances.

A third s-wave resonance was predicted at 4.66 by the complex method [37], with a width of 5.34. Figure 1 shows no hint of this resonance, indicating that such broad resonances lie beyond the capability of the spherical-box approach. For very broad resonances, the assumption that the potential scattering phase shift $\eta_{l,\mathrm{pot}}(E)$ in equation (6) varies slowly with box size may not hold, which could explain why the method performs poorly for broad resonances.

Figure 2 [Figure 2: see original paper] shows p-state energies as a function of box size, along with the effective potential $V_{\mathrm{eff}}(r) = V(r) + l(l+1)/2r^2$. Only one resonance is found near the barrier, with energy around 3.8. This state is broader than the first but narrower than the second s-wave resonance. Table 3 lists the parameters for this resonance. Both energy and width converge well with increasing $\bar{R}$. At the sixth stable point with $\bar{R} = 9.6945$, the relative deviation of the energy from the converged value (obtained from the last avoided crossing near 19.8229) is less than 0.1%, and that of the width is less than 1%.

Figure 3 [Figure 3: see original paper] shows the energy plot for d-states. The effective potential has almost no pocket, yet slightly stable regions can still be identified in the energy curves. Indeed, we find stable points satisfying $\partial^{2E}/\partial R^2 = 0$ at the first six avoided crossings for the d-state. The resonance parameters are listed in Table 4 . At $\bar{R} = 9.3164$, the relative deviation of the resonance energy is within 3% and that of the width is about 8% compared with values at the previous stable point $\bar{R} = 8.1438$. Similar to the second s-wave resonance, no further stable behavior is found for $\bar{R} > 9.3164$. No higher partial-wave resonances are observed in the present study.

3.3. Wave functions of the resonances

Since the Schrödinger equation (1) is solved within a spherical box, we obtain only the real part of the wavefunction for each resonant state. Figure 4 [Figure 4: see original paper] shows the wavefunctions for the resonances identified in this work. The wavefunction behavior correlates with the resonance width. For the very narrow first s-wave resonance, the wavefunction is almost completely localized within the range of the finite-range potential $V_0(r) = 7.5r^{2e^{-r}}$. In contrast, for the broad s-wave resonance, the radial wavefunction inside the potential barrier is strongly suppressed and exhibits pronounced oscillations in the

asymptotic region. The p-wave resonance wavefunction still shows localization, though less prominent than the first s-wave state. The d-wave resonance wavefunction resembles that of the second s-wave state (note the different scales in the upper and lower panels), except that it vanishes at the origin.

The real stabilization method is based on the principle that a resonance is more or less localized, making its energy only weakly dependent on the spherical-box size, as demonstrated in [24, 30] and the present work. Figure 5 [Figure 5: see original paper] illustrates the convergence of the real radial wavefunction with respect to box size for the p-wave resonance. To clearly show the asymptotic behavior, the wavefunction $\Psi(r)$ is multiplied by the radial coordinate r. As $\bar{R}$ increases, more nodes appear while the wavefunction inside the potential barrier decreases only slightly, confirming that the wavefunction of a narrow resonance is largely unaffected by box-size variations due to its localization property.

---

4. SUMMARY

The spherical-box approach, an effective implementation of real stabilization methods for single-particle resonances, has been extended to cases where long-range forces such as the Coulomb interaction are present. The formalism is presented and numerically implemented for this extended approach.

Using model potential (8) as a test case, we have demonstrated the capability and precision of the method. In the presence of Coulomb interaction, the spherical-box approach remains effective for narrow resonances, yielding resonance parameters with high precision for very narrow states. The energy and width converge reasonably quickly with increasing box size. Within the spherical-box framework, the real wavefunctions of these resonances are obtained, with the localization behavior of the radial wavefunction consistent with the resonance width. The convergence of the radial wavefunction with box size further shows that the wavefunction of a narrow resonance is "stable" against box-size variations.

ACKNOWLEDGMENTS

We thank Professor Shun-Jin Wang for helpful discussions. This work was partly supported by the National Natural Science Foundation (10705014, 10775004, and 10875157), the Major State Basic Research Development Program of China (2007CB815000), and the Knowledge Innovation Project of CAS (KJCX3-SYW-N02). The computations were supported by the Supercomputing Center, CNIC, CAS.

REFERENCES

[1] Kato K 2006 J. Phys: Conf. Ser. 49 73–78
[2] Kruppa A T, Lovas R G and Gyarmati B 1988 Phys. Rev. C 37 383–389
[3] Reinhardt W P 1982 Annu. Rev. Phys. Chem. 33 223–255
[4] Ho Y K 1983 Phys. Rep. 99 1–68
[5] Moiseyev N 1998 Phys. Rep. 302 212–293
[6] Gyarmati B and Kruppa A T 1986 Phys. Rev. C 34 95–102
[7] Kruppa A T, Heenen P H, Flocard H and Liotta R J 1997 Phys. Rev. Lett. 79 2217–2220
[8] Moiseyev N and Cederbaum L S 2005 Phys. Rev. A 72 033605–8
[9] Arai K 2006 Phys. Rev. C 74 064311–7
[10] Riss U V and Meyer H D 1993 J. Phys. B: At. Mol. Opt. Phys. 26 4503–4535 ISSN 0953-4075
[11] Mueller I B, Santra R and Cederbaum L S 2003 Int. J. Quantum Chem. 94 75–92
[12] Kukulin V I and Krasnopol' sky V M 1977 J. Phys. A: Math. Gen. 10 L33–L37
[13] Kukulin V I, Krasnopol' sky V M and Miselkhi M 1979 Sov. J. Nucl. Phys. 29 421
[14] Kukulin V I, Krasnopol' sky V M and Hor´acek J 1989 Theory of Resonances: Principles and Applications (Kluwer Academic, Dordrecht)
[15] Tanaka N, Suzuki Y and Varga K 1997 Phys. Rev. C 56 562–565
[16] Tanaka N, Suzuki Y, Varga K and Lovas R G 1999 Phys. Rev. C 59 1391–1399
[17] Yang S C, Meng J and Zhou S G 2001 Chin. Phys. Lett. 18 196–198
[18] Cattapan G and Maglione E 2000 Phys. Rev. C 61 067301–4
[19] Zhang S S, Meng J, Zhou S G and Hillhouse G C 2004 Phys. Rev. C 70 034308–8
[20] Guo J Y, Wang R D and Fang X Z 2005 Phys. Rev. C 72 054319–8
[21] Hazi A U and Taylor H S 1970 Phys. Rev. A 1 1109–1120
[22] Fels M F and Hazi A U 1971 Phys. Rev. A 4 662–674
[23] Fels M F and Hazi A U 1972 Phys. Rev. A 5 1236–1249
[24] Maier C H, Cederbaum L S and Domcke W 1980 J. Phys. B: At. Mol. Phys. 13 L119–L124
[25] Taylor H S and Hazi A U 1976 Phys. Rev. A 14 2071–2074
[26] Mandelshtam V A, Ravuri T R and Taylor H S 1993 Phys. Rev. Lett. 70 1932–1935
[27] Mandelshtam V A, Taylor H S, Ryaboy V and Moiseyev N 1994 Phys. Rev. A 50 2764–2766
[28] Kruppa A T and Arai K 1999 Phys. Rev. A 59 3556–3561
[29] Adamson S, Kharlampidi D and Dementiev A 2008 J. Chem. Phys. 128 024101
[30] Zhang L, Zhou S G, Meng J and Zhao E G 2008 Phys. Rev. C 77 014312–6
[31] Hagedorn G A and Meller B 2000 J. Math. Phys. 41 103–117
[32] Vretenar D, Afanasjev A, Lalazissis G and Ring P 2005 Phys. Rep. 409

101–259
[33] Meng J, Toki H, Zhou S, Zhang S, Long W and Geng L 2006 Prog. Part. Nucl. Phys. 57 470–563
[34] Calogero F 1967 Variable Phase Approach to Potential Scattering (New York: Academic Press)
[35] Isaacson A D, McCurdy C W and Miller W H 1978 Chem. Phys. 34 311–317
[36] Yamani H A and Abdelmonem M S 1995 J. Phys. A: Math. Gen. 28 2709
[37] Sofianos S A and Rakityansky S A 1997 J. Phys. A: Math. Gen. 30 3725
[38] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 2007 Numerical Recipes: The Art of Scientific Computing 3rd ed (Cambridge University Press)

Note: Figure translations are in progress. See original paper for figures.