

Wigner scattering theory for systems held together by Coulombic forces[★]

Jean-Patrick Connerade^{1,2,a}

¹ Quantum Optics and Laser Science Group, Department of Physics, Imperial College, London SW7 2BW, UK

² European Academy EASAL, 60 Rue Monsieur le Prince, 75006 Paris, France

Received 5 March 2020

Published online 9 June 2020

© The Author(s) 2020. This article is published with open access at [Springerlink.com](https://www.springerlink.com)

Abstract. The relevance of Wigner Scattering theory and in particular of its \mathbf{K} -matrix formulation is stressed for all systems held together by Coulombic forces including not only atoms and molecules but also clusters. Originally developed and formulated for nuclear scattering, Wigner's theory is extremely general, with application in many branches of physics. Atomic Physics often makes use of an apparently separate formalism (MQDT) which is in fact a specialisation of Wigner's theory. The advantage of the \mathbf{K} -matrix is that analytic expressions can be given for interactions between resonances in terms of a meromorphic pole structure in the special case of asymptotically Coulombic potentials. By using the \mathbf{K} -matrix, a number of novel effects (q -reversals, vanishing radiative and particle widths, vanishing fluctuations, etc.) are understood as general phenomena.

1 Introduction

Spectral structures observed for atoms, molecules, and clusters are usually analysed or simulated by using a numerical approach. In atomic physics, for example, a highly successful approach is multichannel quantum defect theory (MQDT) [1]. Simulations by MQDT are capable of reproducing very precisely the observed phenomena. MQDT is not a separate theory for atomic and molecular physics but represents a special case of Wigner scattering theory [2]. What specific simulations leave untouched, however, is a clear conceptual framework within which to understand a number of characteristic effects described in the present paper. These effects appear quite commonly when interacting resonances are involved and are therefore interesting to consider from a broader perspective. As will be argued in the present paper, the Coulomb potential plays a very special role in this respect because of its extraordinary properties in the \mathbf{K} -matrix formulation of Wigner's theory. Furthermore, it is important for the coherence of physics to understand how all the areas in which scattering problems occur are related to each other within a single theoretical scheme. It is argued here that Wigner scattering theory achieves precisely this goal and that the prospects to extend this theory to spectral structures in, for example, metallofullerenes and more complex systems are also excellent.

[★] Contribution to the Topical Issue "Atomic Cluster Collisions (2019)", edited by Alexey Verkhovtsev, Pablo de Vera, Nigel J. Mason, Andrey V. Solov'yov.

^a e-mail: jean-patrick@connerade.com

2 The scattering problem

The scattering problem occurs in many areas of science, extending from nuclear and subnuclear physics [3] to condensed matter. A general scattering theory may therefore be anticipated to apply to atoms, molecules, clusters, and indeed even to biological species under appropriate conditions of excitation. There are situations in the physics of condensed matter to which a scattering model is also relevant [4].

In scattering theory, a projectile is imagined to move towards a target from a very remote past ($t \rightarrow -\infty$) and also from a large distance, where projectile and target are so far separated that the interaction between them tends to zero. The initial wavefunction is thus the product of the projectile wavepacket and one definite state ($|a\rangle$, say) of the target.

At the opposite extreme of time ($t \rightarrow +\infty$), the interaction between projectile and target again tends to zero, leaving the system in some other definite state ($|b\rangle$, say) of the target. The states a and b are referred to as open channels or continuum states, because target and projectile are infinitely separated from each other.

In the presence of a transient interaction, represented by an operator $\mathbf{U}(t_1, t_2)$, the so-called "closed" or discrete bound states of the system become temporarily involved.

We write the scattering matrix \mathbf{S} as

$$\mathbf{S}_{ab} = \langle b | \mathbf{U}(\infty, -\infty) | a \rangle \quad (1)$$

where \mathbf{U} is a unitary operator.

In the scattering process, the probability flow is conserved, i.e. such a scattering matrix must be unitary, which has important consequences.

Although the formulation is extremely general, there is one condition which must be satisfied. The system as a whole must obey a “Schrödinger type” equation, together with the usual asymptotic boundary conditions which apply in quantum mechanics. The reason for referring to a “Schrödinger type” equation is that, as Wigner himself has stressed, this equation does not need to be solved explicitly for the theory to be developed and used. This fact gives great freedom in the way of applying the method.

In numerical applications, to evaluate a scattering matrix, it is convenient to introduce a Wigner sphere (of radius r_0) which must, for practical reasons, “contain” the target. When dealing with short range forces, as in nuclear physics with e.g. the Yukawa potential, “outside” is readily defined. The sphere is simply chosen from the definition of the effective range. For Coulombic forces, the choice would have to be more subtle, except that we can choose to contain within r_0 all the complicated (and unknown) many-body interactions and use a combination of the regular and irregular Coulombic functions outside r_0 , with coefficients to be determined by matching them on the sphere [5]. This approach (which allows a specific derivation of MQDT restricted to Coulombic systems) is not used in the present paper.

The introduction of the Wigner sphere, which is a common feature of numerical methods, has a potential disadvantage in that one might suspect the result to be dependent on the particular choice of r_0 . In principle, therefore, one should check the numerical results by performing computations with different choices of r_0 and making sure that the same result is obtained every time. Since this is a laborious process, it is rarely followed through.

As we argue, following Lane [6] and others [7,8] it is not actually necessary to introduce an interaction or Wigner sphere at all, provided we stay within the analytic structure of the theory and consider only general laws by using an appropriate scattering matrix.

The appropriate matrix is the \mathbf{K} -matrix, we write

$$\mathbf{S} = (\mathbf{1} + \mathbf{K})/(\mathbf{1} - \mathbf{K}) \quad (2)$$

where \mathbf{K} is then real and symmetric, yielding the essential part of the cross-section as

$$\sigma_{aa} = 4K_{aa}^2/(1 + K_{aa}^2) \quad (3)$$

for one open channel and

$$\sigma_{ab} = 4K_{ab}^2/|(1 - K_{aa})(1 - K_{bb}) + K_{ab}^2|^2 \quad (4)$$

for two open channels, etc.

Resonance maxima occur when $\mathbf{K} \rightarrow \pm\infty$, expressing the unitary limit mentioned above, which forces $\mathbf{S}\mathbf{S}^\dagger \leq \mathbf{1}$.

The \mathbf{K} -matrix is especially convenient. It turns out, as Lane has shown [8] that the Coulomb potential is a very special case (similar in some ways to the inverse square law of force and Kepler’s laws in classical mechanics) in that an analytic inversion of the \mathbf{K} -matrix can be performed specifically for this asymptotic law of force. This

unique property allows us to display and verify the general algebraic structure of interacting resonances for this type of potential.

Extending this reasoning, it follows that systems held together by Coulombic forces allow Wigner scattering theory to be tested in a way not accessible for other potentials. In nuclear scattering, for example, such analytic expressions are not available. Therefore, it is of particular interest to study effects which can be displayed using the analytic \mathbf{K} -matrix theory but not otherwise for systems held together by Coulombic potentials.

2.1 The meromorphic pole structure

As implied above, the \mathbf{K} -matrix formulation of Wigner scattering theory is in fact the most general, because it does not depend on the introduction of a Wigner sphere. The \mathbf{K} -matrix is therefore referred to as *external*, i.e. it does not depend on properties internal to the system.

Resonances appear as a sequence of what are called *meromorphic* poles in the scattering cross-section. A meromorphic function may only have finite-order, isolated poles and zeros and no essential singularities within its domain. Meromorphic functions are single-valued and analytic in all but possibly a discrete subset of their domain and, near those singularities, tend to infinity as polynomials. Each one of these poles corresponds to one and only one physical resonance. Since the poles are singularities, their general properties cannot be deduced numerically. That is why analytic theory is the key to understanding their behaviour and also why Coulombic scattering problems provide a unique testing ground for Wigner’s theory.

2.2 Introducing phase shifts

It is convenient to express photoabsorption in terms of phase shifts and to partition the shift into a part due to a given resonance (Δ_0 , say) and a part (δ , say) due to the background continuum. Thus:

$$K = \tan(\delta + \Delta_0). \quad (5)$$

The form of Δ_0 , the phase shift near an isolated resonance is given e.g. by Landau and Lifshitz [9] as a simple pole:

$$\tan \Delta_0 = \Gamma/(2(E_0 - E)). \quad (6)$$

Γ and E_0 are the resonance width and energy respectively. Combining equations (5) and (6) with (3), and writing $q = \cot \delta$ and $\varepsilon = 2(E - E_0)/\Gamma$ we have the well-known Fano formula [10]:

$$\sigma(E) = |D|^2(q + \varepsilon)^2/(1 + \varepsilon^2). \quad (7)$$

There is no essential difference between the nuclear (Breit–Wigner) and atomic (Beutler–Fano) cases. The physics is the same.

The width Γ of the resonance is intrinsic (the lifetime of the excited state) but the asymmetry parameter q depends on δ and hence on the excitation path by which that state is reached.

2.3 The short-range well

In nuclear physics, it is known that, for low-energy scattering from a short-range well, the bound and low-energy scattering spectrum do not depend on the detailed shape of the potential but only on its binding strength. This arises whenever the de Broglie wavelength of the scattered particle is comparable to the range of the well, so that the inverse scattering problem cannot be solved and does not allow the detailed shape of the well to be deduced from the spectrum. One then resorts to effective range theory. It turns out that all short range wells of the same binding strength are equivalent to deduce a general form for parametrising Δ_0 . In particular, we can use the analytic form of the phase shift for a spherical well with angular momentum ℓ [11]. This yields an analytic formula in Bessel functions for Δ_0 . If no background phase shift is present or if it is so small that it can be neglected, the total cross section is then:

$$\sigma(k) = (4\pi/k^2)(2\ell + 1) \sin^2 \Delta_0 \quad (8)$$

where k is the wavevector inside the well. Thus, we can deduce a general form for the profiles of giant resonances (they are neither Breit–Wigner nor Beutler–Fano in shape): let $j_1 = j_\ell, j_2 = j_{\ell-1}, j_3 = j_{\ell-2}, j_4 = j_{\ell-3}$ be the spherical Bessel functions, then the resonant phase shift of the giant resonance is:

$$\tan \Delta_0 = \frac{(zj_1(z')j_2(z) - z'j_1(z)j_2(z'))}{(zj_1(z')j_3(z) + z'j_4(z)j_2(z'))} \quad (9)$$

(where $z = k\alpha, z' = k'\alpha, \alpha$ is the radius of the square well and Δ is its depth so that $\Delta\alpha^2$ is its binding strength). From (9), the resonance profile is readily obtained by using (8) above and examples are shown in Figure 1 [12].

Giant resonances originated in nuclear physics (the liquid drop model) and appear in many-particle problems, even when the system is held together by Coulombic forces. For example, they are a common feature in the spectra of metallic clusters [13] held together by a Woods–Saxon potential (a model potential which also originated from the collective representation in nuclear physics). They are also ubiquitous in the spectra of the fullerenes and metallofullerenes [14].

Giant resonances in all these systems are characterised by the fact that they exhaust all the available oscillator strength allowed by the sum rule in a given channel. They must therefore lie below a $1/k^2$ curve which is termed the *unitary limit* in nuclear scattering, because it is imposed by the unitarity of the \mathbf{S} -matrix, discussed in Section 2 above. The unitary limit results from a fundamental consideration (causality, or the conservation of the probability flow), so is a general property for all scattering problems, whatever the potential or the particles involved. It is exemplified by the family of curves displayed in Figure 1.

2.4 Combining phase shifts

When many resonances occur in a Coulombic channel, their phase shifts are additive. Thus, with N overlapping

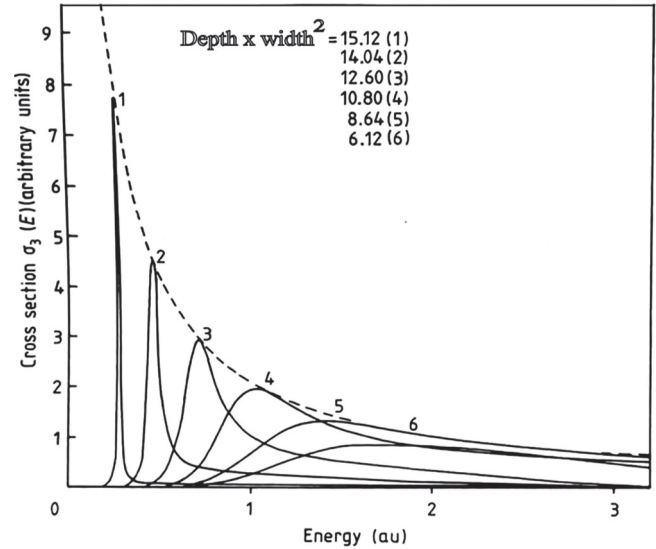


Fig. 1. The evolution of “giant resonances” as a function of binding strength for a short-range well. Note the unitary limit set by the sum rule (shown as a dashed curve).

resonances, we have :

$$K_{\text{res}} = \tan \Delta_0 = \sum_{n=1}^N \left(\frac{\Gamma_n}{2(E_n - E)} \right) \equiv \sum, \text{ say} \quad (10)$$

whence

$$\sigma(E) = 4 \sin^2 \delta \left\{ \left(1 + q \sum^2 \right) / \left(1 + \sum^2 \right) \right\}. \quad (11)$$

The summation over n of course involves only those resonances which actually occur in the physical system. However, atomic physicists are accustomed to a convenient replacement which is not a mathematically exact substitution, viz:

$$\sum \rightarrow \chi \cot \pi(\nu + \mu) \equiv \chi \cot \theta \quad (12)$$

where ν is an energy variable such that

$$E_\infty - E = R/\nu^2. \quad (13)$$

This replacement is almost equivalent to a change of variables, from Γ_n, E_n, E to χ, μ, ν , except that, by introducing a trigonometric function and the running index ν , the “bottom” of the channel becomes undefined, so that this replacement is not quite mathematically exact. However, for sufficiently large values of n , this substitution conveniently reproduces the Rydberg recapitulation [15] characteristic of Coulombic systems. Again, we see that several familiar results of MQDT emerge without the need to solve the Schrödinger equation explicitly or to introduce an interaction sphere of radius r_0 .

By some algebra, one finds:

$$\sigma(\theta) = |\mathbf{D}|^2 \frac{\tan^2 \pi\nu + 2B \tan \pi\nu + B^2}{\tan^2 \pi\nu + 2C \tan \pi\nu + D^2} \quad (14)$$

with

$$\begin{aligned} B &= \frac{q\chi + \tan \pi\mu}{1 - q\chi \tan \pi\mu} \\ C &= \frac{(1 - \chi^2) \tan \pi\mu}{1 + \chi^2 \tan^2 \pi\mu} \\ D^2 &= \frac{\chi^2 \tan^2 \pi\mu}{1 + \chi^2 \tan^2 \pi\mu}. \end{aligned} \quad (15)$$

Equation (14) is known in quantum defect theory as the Dubau–Seaton formula [16–18]. It represents a full Rydberg manifold of interacting resonances in a “flat” continuum with three shape parameters B, C , and D of which only B depends on q . One also finds that $q = \{1/\chi\} \tan \pi(\beta - \mu)$, where $B = \tan \pi\beta$. The constant $|\mathbb{D}|^2$ is a dipole operator.

2.5 General trends within a channel

Some general rules concern the trends of the parameters. Thus:

- Γ_n scales as $1/(n - \mu)^3$ for an asymptotically Coulombic potential;
- one zero in the cross section occurs between each resonance;
- χ is necessarily negative for all $E_1 < E < E_\infty$ since

$$\chi = \frac{1}{\cot^2 \pi(\nu + \mu)} \frac{2R}{\pi\nu} \sum_{n=1}^N \left(\frac{\Gamma_n}{2(E_n - E)^3} \right) \quad (16)$$

and Γ_n is necessarily positive.

Close to the unitary limit, where the cross section rises to its allowed maximum, narrow resonances can only appear in the form of $q=0$ “windows”.

For channels 1 and 2, we have

$$K = \frac{(\Sigma_1 + \Sigma_2) + \xi(1 - \Sigma_1 \Sigma_2)}{(1 - \Sigma_1 \Sigma_2) - \xi(\Sigma_1 + \Sigma_2)} \quad (17)$$

in the notation introduced above for equation (11), with $\xi = (q_1 + q_2)/(q_1 q_2 - 1)$.

Two dimensional QDT graphs for this case are not the same as for a double sequence of bound states although both may look the same topologically: for bound states, avoided crossings tend to zero as the interaction strength tends to zero. This is not the case for resonances, which have intrinsic widths. This point is discussed and illustrated in reference [19].

The connecting equations from \mathbf{K} -matrix to MQDT formulations are (15) above for the constants B, C , and D in (14). The constant μ is termed the quantum defect. For $q = 0$, we have a sequence of symmetric “window” resonances (or antiresonances). Again, in (12), the tangent replacement formula is not exact. It has no “bottom end” i.e. there is no low energy bound as for the summation over n which starts from the lowest resonance. Likewise, there is no such thing as a “flat” continuum over the full range of energies because, in reality, there is a threshold at the “bottom” of any continuum.

2.6 Hybrid or complex systems

Hybrid systems, such as metallofullerenes, involve an interplay between a short-range potential as in Section 2.3 above and the Coulombic channels described of Section 2.4. Often, the fullerene “cage” yields the “giant resonance” and the endohedral atom provides Coulombic states, with the excited electron either inside the cage or outside the system. Conversely, any form of “cage” in a metallofullerene produces so-called confinement resonances [20], which can overlap in energy with an atomic giant resonance. All such cases can be handled by adding phase shifts in the same style as above.

For example, we can couple a Rydberg series of fine resonances Γ_n to a broad Giant resonance Γ_G . This problem is treated in [21] by essentially the same formalism as above. It is slightly more complex, depending on the magnitude of the coupling strength, but in the weak coupling limit, the essential result is that the combined cross section is proportional to:

$$\frac{(\mathbb{D} + \mathfrak{d})^2}{(1 + \mathfrak{d}^2)(1 + \mathbb{D}^2)} \frac{\tan^2 \pi\theta + 2B \tan \pi\theta + B^2}{\tan^2 \pi\nu + 2C \tan \pi\nu + D^2} \quad (18)$$

where $\theta = \pi(\nu + \mu)$

$$\tan \mathbb{D} = \frac{\Gamma_G}{2(E_G - E)}$$

$$\begin{aligned} \tan \Delta_0 &= \chi \cot \theta \text{ and} \\ \mathfrak{d} &= \tan \delta, \end{aligned}$$

δ being a background phase shift. Also:

$$B = \frac{\chi}{\mathbb{D} + \mathfrak{d}}$$

$$C = \frac{\chi \mathbb{D}}{1 + \mathbb{D}^2}$$

$$D^2 = \frac{\chi^2}{1 + \mathbb{D}^2}. \quad (19)$$

We recognise the second factor in (18) as the Seaton–Dubau formula of reference [18]. The first term depends only on \mathbb{D} and \mathfrak{d} , i.e. from (19), it contains only information on the giant resonance and background phases. When \mathbb{D} is constant and $\mathfrak{d} \rightarrow 0$, we simply recover the Seaton–Dubau formula.

For the general case, however, the shape parameters of the fine resonances Γ_n are no longer constant as in the Dubau–Seaton problem. Their variation with energy expresses the influence of the Giant resonance on the Coulombic channel. This is readily related to the profile index q of reference [22]:

$$q = \frac{B - C}{(D^2 - C^2)^{1/2}} = \frac{1 - \mathbb{D}\mathfrak{d}}{\mathbb{D} + \mathfrak{d}}.$$

Thus, in the weak-coupling limit, the variation of q is determined entirely by the giant resonance and background phase shifts. Note in particular that $q = 0$ when

$\mathbb{D} = 1/d$ which is also the condition for a maximum in the first factor of expression (18), i.e. when

$$E = E_G - \frac{\Gamma_G}{2 \cot \delta}.$$

For small δ , this is detuned only slightly from E_G , the giant resonance energy. In general, q tends to zero at the peak intensity of the giant resonance, because of the unitary limit mentioned above. About this value, \mathbb{D} and therefore also q change sign.

While the treatment just described is quite general, there is an important limitation to this approach: it does not allow for the possibility of relative movement of an endohedral atom with respect to the confining cage, in which case, of course, phase shifts are no longer simply additive.

2.7 Novel effects from the K-matrix

I now turn to several novel effects which can only be well understood by starting from the fully analytic approach applied to Coulombic systems. These are (i) q -reversals, (ii) vanishing widths, (iii) perturbative stabilisation, and (iv) vanishing fluctuations. They are, however, quite general and all the indications are that they will appear in many scattering problems (experimental or numerical) and for many systems. Because they can only be fully characterised in a Coulombic potential, the study of Coulombic systems is particularly relevant to Wigner scattering theory.

2.7.1 The q -reversal

As already mentioned, the symmetry of resonances can flip over as a result of inter-channel interactions. This can happen more than once. A q -reversal was first observed in Nuclear Physics [23], where of course the potential is non-Coulombic. It is termed the Robson effect. Somewhat later, but independently, it was observed in atomic physics [24]. Additional characteristics associated with this effect emerged more clearly after further experimental examples had been uncovered. They confirm predictions from Wigner's theory.

When the q -reversal is due to a broad intruder state E_G which exhausts available oscillator strength within its own channel, antiresonances are observed near the peak in the cross section. This of course is simply a manifestation of the unitary limit.

The existence of q -reversals immediately raises the questions: (a) just how many will appear in a given channel and (b) should there always be a q -reversal when an intruder state is present? Such questions can be answered by analytic theory and there are general theorems relating to the maximum number of q -reversals (see e.g. Fig. 2).

2.7.2 Vanishing Widths

The vanishing width effect corresponds to the stabilisation of an excited state against particle decay by the action of

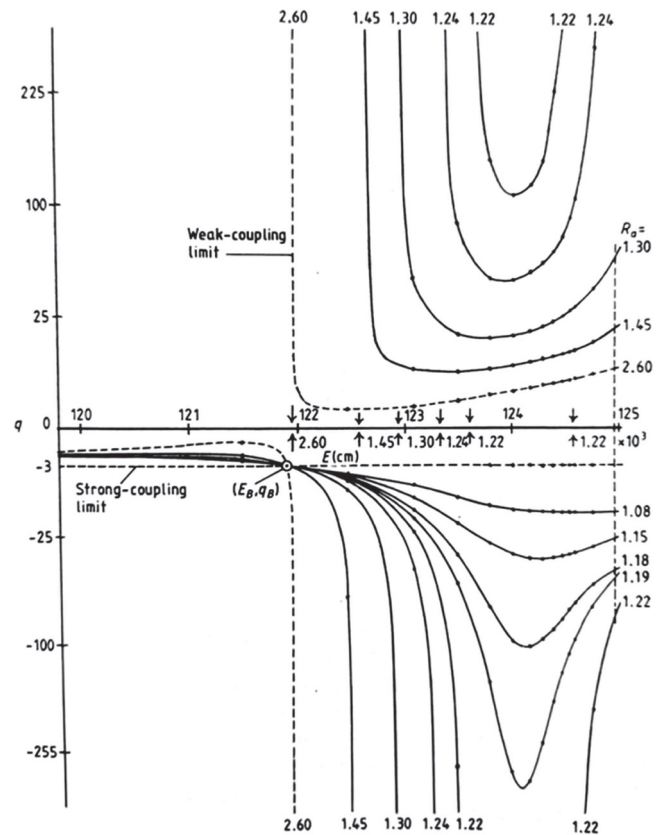


Fig. 2. The picture shows the variation of the q -parameter in a channel perturbed by a broad intruder state, as a function of energy for different coupling strengths. At weak coupling, there is just one reversal. As the strength increases, there can be two. The second one is less stable and occurs only for a limited range. At very high coupling, there are no q reversals and the q is just that of the perturber.

a perturbation. Such stabilisation effects occur, not only in particle, but also in radiative decay, in the case of the half-scattering (photoabsorption) problem.

For a general set of levels, arbitrarily spaced, an exact **K**-matrix inversion to obtain analytic expressions for the cross section cannot be performed. For Coulombic states, in the presence of both radiative decay to a channel γ and particle decay to a channel a , both the interaction strength H_n and the widths $\Gamma_n^{1/2}$ have the same variation with n . Thus the coupling strength $\mu_a \equiv \Gamma_{na}^{1/2}/H_n$ is independent of n , which is why an exact result can be written down for $\sigma(E - E_B)$, where E_B stands for a general broad perturber, in terms of the six real parameters E_B , Γ_{Ba} , $\Gamma_{B\gamma}$, μ_a , μ_γ , and $K_{\gamma\gamma}$. For the case where radiative widths γ are very small and the background can be neglected, the full result simplifies to:

$$\sigma(\varepsilon) = \frac{(\varepsilon + q\Gamma_B/2)^2}{(\varepsilon + \Sigma)^2 + \left\{ \left(\mu_a \Gamma_B^{1/2} + \mu_a^2 \varepsilon / 2 \right) \Sigma - \Gamma_B^2 \right\}^2}$$

where $\varepsilon = (E - E_B)$ is the detuning from the broad intruder state B . The full expression, distinguishing

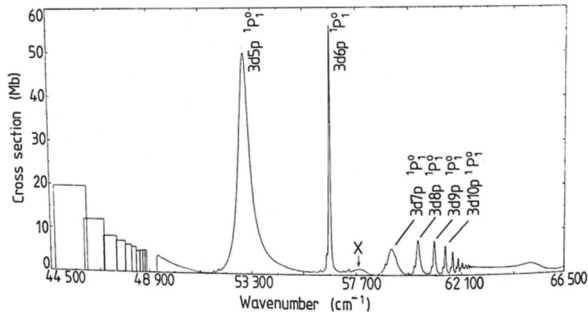


Fig. 3. Vanishing particle width in the 3d np series of Ca. The effect occurs at $n = 6$.

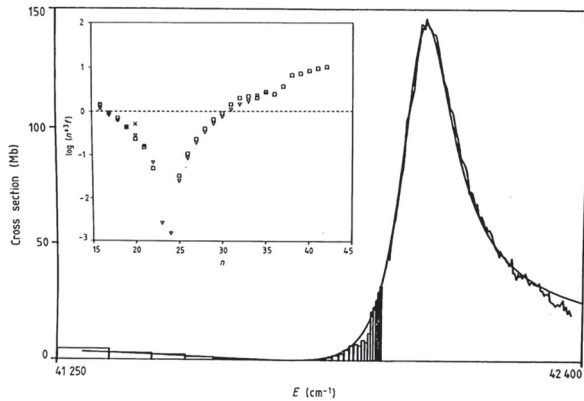


Fig. 4. Vanishing radiative width in the principal series of Ba: radiation is quenched close to the apparent zero of a Beutler–Fano or Breit–Wigner resonance which is continuous across the threshold.

radiative from particle widths, is given in reference [25] and is significantly more complex.

Vanishing widths can occur either in the particle decay (autoionisation) channel, as illustrated in Figure 3 [26] or in the radiative channel (stabilisation against radiative decay or enhanced lifetime) as shown in Figure 4 [27].

2.7.3 The fluctuation operator

In Nuclear Physics, fluctuations are studied directly through the variance

$$\text{var } \sigma \equiv \langle \sigma(E)^2 \rangle - \langle \sigma(E) \rangle^2$$

which constitutes an observable. Strictly, it is of fourth order in elements of the \mathbf{S} -matrix, but Moldauer’s theorem states that fluctuations in total cross section for a given entrance channel are only of second order:

$$\text{var } \sigma_a = 2\{\langle |S_{aa}|^2 \rangle - \langle S_{aa} \rangle^2\}.$$

Thus, the fluctuations themselves behave like a cross section. In particular, they are continuous across a threshold. We are familiar with the situation that fluctuations often disappear at the threshold as $n \rightarrow \infty$ (whence the Gailitis averaging procedure [28]) but the interesting question is whether they can also pass through zero at an energy which does not coincide with any threshold.

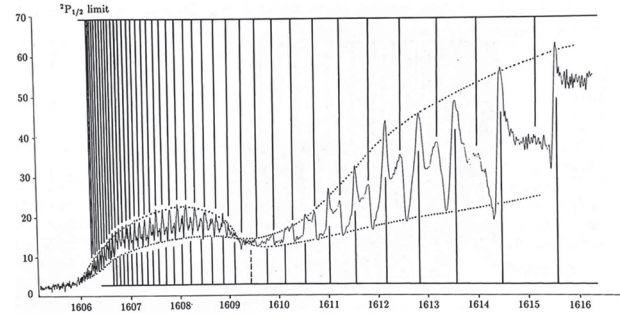


Fig. 5. Example of vanishing fluctuations at an energy removed from the limit of a Rydberg series. Such fluctuations tend to occur at an energy close to a broad perturber.

2.7.4 Vanishing fluctuations

A novel effect predicted from Wigner’s theory is the disappearance of fluctuations at an energy removed from any threshold. In calculations with a single open channel, fluctuations vanish for a system of narrow resonances $\Gamma_n/D_n \rightarrow 0$ (where D_n is the level spacing). We find $E_{vf} = E_B - H_n \Gamma_B^{1/2} / \Gamma_n^{1/2}$ in this case, which shows that the vanishing point lies close to an intruder level Γ_B . For more than one open channel, the situation is more complex.

An example of this kind is shown in Figure 5 [29]. It occurs in the heavily mixed Rydberg system of levels converging on the $6p_{1/2}$ threshold of Ba I.

3 Conclusion

Wigner’s scattering theory offers a unified theoretical framework within which resonances can be described and their interactions studied over scale sizes ranging at least from Nuclear physics to clusters and even to larger systems. It turns out that systems held together by Coulombic forces play a very special role, in that the \mathbf{K} -matrix formulation of Wigner’s theory then leads to an analytic representation of resonances in terms of meromorphic poles. Once this representation is identified, it becomes possible to explore the full range of variation of the parameters and to explore new effects the existence of which is not immediately apparent from numerical simulations. Several such effects have been found in this way. They are also present in other systems with different potentials and can be searched for both in numerical simulations and in experimental spectra.

For all these reasons, and also in the interest of the unity of physics, the theory of resonances should be discussed in the general frame of Wigner scattering theory. The method applies to all quantum mechanical systems and to all potentials (short or long range).

The study of interacting meromorphic poles via such characteristic effects as symmetry or q -reversals, unitary limits, vanishing widths, vanishing fluctuations, and perhaps further properties is a challenging new area.

The generality of scattering theory is ultimately an expression of causality, as Wigner has emphasised [30].

Because of its generality, Wigner scattering theory is extremely robust. For example, systems exist with both giant resonances due to a short range part of the potential and overlapping resonances due to a Coulombic outer range. They all turn out to obey general rules described in the present paper.

Some general effects have been omitted from this paper, as being less likely to occur in large systems, for example those due to perturbation by an antiresonance and the appearance of “universal crossing points” which are more relevant in connection with atoms and with laser-induced continuum structure [31]. Another omission from the present report is the Wigner–Eisenbud time delay in resonant coulomb scattering [32]. In this connection, we note a recent theoretical investigation of the Wigner photoemission time delay from endohedral anions $A@C_{60}$ as a function of increasing charge [33], which suggests that this is also a promising direction of investigation.

Metallofullerenes whose Rydberg states can even straddle the boundary between the inner and outer regions of the fullerene are expected to provide especially interesting examples. It may also prove possible to observe cases in which narrow confinement resonances due to a molecular cavity lie close to broad resonances of a confined atom. As they pass “through” the broad resonance, at least one q -reversal is to be expected in the weak coupling limit.

At the present time, it is not yet possible to trap such large and complex systems and “freeze” them for study by high resolution laser spectroscopy. However, such experimental progress is likely in the future and, when it comes, effects described in the present paper and their analysis by \mathbf{K} -matrix theory will become increasingly relevant.

The same \mathbf{K} -matrix methods can also be extended to study β -parameters observed by electron scattering. The study of overlapping resonances [34] in this context is an area to be developed, and is also accessible to analysis by \mathbf{K} -matrix theory. Lastly, I have omitted results for multiphoton excitation, which allows resonances to be “transported” in energy and embedded in other channels by strong laser fields. These are given in reference [25].

Publisher’s Note The EPJ Publishers remain neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Open Access This is an open access article distributed under the terms of the Creative Commons Attribution License (<https://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

References

1. M.J. Seaton, Rep. Prog. Phys. **46**, 167 (1983)
2. E. Wigner, L. Eisenbud, Phys. Rev. **72**, 29 (1947)

3. P.A. Moldauer, Phys. Rev. **157**, 907 (1967)
4. S.C. Lovatt, B.L. Gyorffy, G.Y. Guo, J. Phys.: Condens. Matter **5**, 8005 (1993)
5. A.F. Starace, *Photoionisation and Other Probes of Many-Electron Interactions* (Plenum Press, New York, USA, 1976)
6. A.M. Lane, J. Phys. B: At. Mol. Phys. **17**, 2213 (1984)
7. Y. Komninos, C.A. Nicolaides, Z. Phys. D **4**, 301 (1987)
8. A.M. Lane, J. Phys. B: At. Mol. Phys. **19**, 253 (1986)
9. L.P. Landau, E.M. Lifshitz, *Quantum Mechanics* (Addison Wesley, Reading, MA, USA, 1965)
10. U. Fano, Phys. Rev. **124**, 1866 (1961)
11. N.F. Mott, H.S. Massey, *The Theory of Atomic Collisions*, 3rd edn. (Clarendon Press, Oxford, UK, 1965)
12. J.P. Connerade, J. Phys. B: At. Mol. Phys. **17**, L165 (1984)
13. C. Brechignac, J.P. Connerade, J. Phys. B: At. Mol. Opt. Phys. **27**, 3795 (1994)
14. J. Berkowitz, J. Chem. Phys. **111**, 1446 (1999)
15. R.S. Mulliken, J. Am. Chem. Soc. **86**, 3183 (1964)
16. J. Dubau, M.J. Seaton, J. Phys. B: At. Mol. Phys. **17**, 381 (1984)
17. A. Giusti-Suzor, U. Fano, J. Phys. B: At. Mol. Phys. **17**, 215 (1984)
18. J.P. Connerade, J. Phys. B: At. Mol. Phys. **16**, L329 (1983)
19. J.P. Connerade, J. Phys. B: At. Mol. Opt. Phys. **26**, 4041 (1993)
20. J.P. Connerade, V.K. Dolmatov, S.T. Manson, J. Phys. B: At. Mol. Opt. Phys. **33**, 2279 (2000)
21. J.P. Connerade, A.M. Lane, J. Phys. B: At. Mol. Phys. **20**, L181 (1987)
22. J.P. Connerade, A.M. Lane, M.A. Baig, J. Phys. B: At. Mol. Phys. **18**, 3507 (1985)
23. B.A. Robson, *Nuclear Interactions* (Springer Verlag, Berlin, 1978)
24. J.P. Connerade, Proc. R. Soc. London A **362**, 361 (1978)
25. J.P. Connerade, A.M. Lane, Rep. Prog. Phys. **51**, 1439 (1988)
26. U. Griesmann, Shen-Ning, J.P. Connerade, K. Sommer, J. Hormes, J. Phys. B: At. Mol. Phys. **21**, L83 (1988)
27. J.P. Connerade, A.M. Lane, Rep. Prog. Phys. **51**, 1439 (1988)
28. M.Gailitis, Sov. Phys. JETP **17**, 1328 (1963)
29. J.P. Connerade, S.M. Farooqi, J. Phys. B: At. Mol. Opt. Phys. **24**, L331 (1991)
30. E.P. Wigner, Rendiconti della Scuola Internazionale di Fisica “Enrico Fermi”, XXIX Corso, in *Relazione di dispersione e loro rapporto con il principio della causalità* (Academic Press, New York and London, 1964), Vol. 40
31. J.P. Connerade, J. Phys. B: At. Mol. Opt. Phys. **24**, L513 (1991)
32. E.P. Wigner, Phys. Rev. **98**, 145 (1955)
33. A. Kumar, H.R. Varma, P.C. Deshmukh, S.T. Manson, V.K. Dolmatov, A. Kheifets, Phys. Rev. A **94**, 043401 (2016)
34. J.P. Connerade, V.K. Dolmatov, J. Phys. B: At. Mol. Opt. Phys. **30**, L181 (1997)