From bound states to resonances

Miroslaw Bylicki
Instytut Fizyki, Uniwersytet Mikolaja Kopernika, ul. Grudziadzka 5, 87-100 Torun, Poland
E-mail: mirekb@fizyka.umk.pl

Abstract. There are many quantum systems whose basic properties, e.g. allowed energy values depend on a parameter. The role of the parameter may be played by the size of the system, external-field strength, masses or electric charges of subsystems. When such parameters change the allowed energy levels change. The changes are not only quantitative: the level may leave the discrete range and enter a continuum. In such a case the character of the corresponding state changes from bound stationary state to quasistationary resonance. Moreover, for complex systems, resonances may change character from Feshbach to shape depending on the continua which the resonance energy levels leave or enter, and to which they are coupled. Several such parameterized systems are discussed.

1. Introduction
When thinking about a quantum system like an atom usually we consider it in a bound state or completely unbound, which is often considered as a “nonexistence” state. However, many systems may appear also in resonance states, in which they are temporally bound. They correspond to discrete energy levels embedded in continua, and depending on the coupling to the continua are of two types: the Feshbach and shape resonances. In this paper we will go through several systems whose properties, like existence or nonexistence of bound states or appearance of resonances and character of resonances, depend on some parameters. These properties are directly related to the energy spectrum of the system. Thus what we are going to discuss here is the dependence of the Hamiltonian eigenspectrum, or just specific energy levels, on those parameters.

All the results discussed here have been published elsewhere, hence we will not repeat here unnecessary details but rather we will pay more attention to the changes of the character of a state from bound to resonance or vice versa, and changes in character of resonance from Feshbach to shape.

2. Yukawa potential system
A counterexample to the behavior we want to discuss here is the hydrogenlike system with the nucleus charge, Z, as the parameter: within the whole range of Z no energy level changes its character. If however we consider a potential which is shortened with respect to the Coulomb one, like the Yukawa potential, the energy spectrum changes drastically. Therefore we consider one electron in a spherically symmetric Yukawa potential as the first example [1].

Adding the centrifugal barrier to the Yukawa potential results in an effective radial potential:

\[ V_{\text{eff}}(r) = -\frac{Ze^{-\lambda r}}{r^2} + \frac{l(l+1)}{2r^2}. \]  \hspace{1cm} (1)
By scaling the coordinate $\rho = \lambda r$ one obtains [1]

$$U(\rho) \equiv \frac{1}{\lambda Z} V_{\text{eff}}(r) = \frac{p}{\rho^2} - \frac{e^{-\rho}}{\rho},$$

(2)

where

$$p \equiv \frac{l(l+1)\lambda}{2Z}.$$  

(3)
The shape of the effective potential (2) depends on the parameter \( p \) only (we shall call it the shape parameter). The potential is plotted in figure 1 for several values of \( p \). The important features are the well and the barrier, on which the existence and number of bound states or resonances depend. E.g. one can easily guess that for the increasing \( p \) the number of bound states decreases so that for \( p \geq p_c \approx 0.36 \) there are no bound states. Moreover, for \( p \geq p_o \approx 0.42 \) and there are neither bound states nor resonances. This is discussed in details in [1].

Almost four decades ago Totsuji [2] considered the problem of dependence of the bound Yukawa-potential levels on the screening parameter. Using a quasiclassical approach he provided formulas for the critical screening at which consecutive levels of the orbital angular momentum \( l \) disappear. Stubbins [3] performed quantum mechanical computations for several bound states. The ground state \((l = 0)\) was investigated numerically by Gomes, Chacham, and Mohallem [4]. They found with a high precision that it disappears as a bound state at a critical value of the screening parameter \( \lambda \approx 1.192 \). Those authors did not discuss the fate of the level after crossing the potential asymptote. They simply treat the fact of crossing as “bound-unbound” transition [4].

In [1] the investigations were extended above the continuum threshold. Results of the actual variational computation [1] for the angular momentum \( l = 1, 2, \ldots, 10 \) are shown in figure 2. Every level is pushed up when \( \lambda \) is increasing. Each one reaches the asymptote of the potential at zero, then becomes a resonance, and finally disappears as completely diluted in the continuum. It is interesting that at most one resonance of a given \( l \) exist for a given value of \( \lambda \) (or \( p \)). This can be seen in figure 3 for \( l = 1 \) and it was observed [1] for all investigated values of \( l \) up to \( l = 10 \).

In figure 4 the widths of the \( l = 1 \) levels are plotted. They are zero for bound states. After a level has entered the continuum its width increases rapidly and smoothly. Such regular behavior is due to the structureless character of continuum. These resonances are due to the shape of the potential. They are called shape resonances.

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure3.png}
\caption{Energies \( \varepsilon = -\log(1.3V_{\text{max}} - E) \) of the \( l = 1 \) Yukawa-potential states versus the potential-shape parameter \( p \). The dotted line at the bottom is the potential minimum, dashed line is the top of the potential barrier and the full line parallel to the latter one is the asymptote of the potential \((E = 0)\). Full points are used above the asymptotic value in order to emphasize the resonance character of the level.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.4\textwidth]{figure4.png}
\caption{Widths \( \Gamma \) of the \( l = 1 \) Yukawa-potential resonances versus the potential-shape parameter \( p \). For the energy values below the potential asymptote (see figure 3) the widths are equal to 0, not shown in the figure. The width curves start at 0 for levels at the potential asymptote. For energies increasing above the asymptote the widths increase very rapidly by many orders of magnitude.}
\end{figure}
3. Two-electron quantum dot

Now we consider a two-electron semiconductor quantum dot (QD) [5]. The electrons interact by Coulomb repulsion and are attracted by a short range potential (of the solid state origin; conduction band profile) which is just a spherically symmetric rectangular well: \( V(r) = -V_o \) for \( r \leq R \) and \( V(r) = 0 \) for \( r > R \). Thus the Hamiltonian is

\[
H = -\frac{\hbar^2}{2m^*} (\Delta_1 + \Delta_2) + V(r_1) + V(r_2) + \frac{e^2}{cr_{12}}.
\]

The effective mass, \( m^* \), and the dielectric constant, \( \epsilon \), are assumed to be uniform within the whole structure.

Bound states of this system and dependence of their energies on the size of QD were investigated by Szafran, Adamowski, and Bednarek [6]. Very accurate variational computations covering also the resonance region were performed by Bylicki, Jaskólski, Stachów, and Díaz [5]. Some results of [5] are presented in figures 5 and 6. The effective Rydberg \( R_o \) and the effective Bohr radius \( a_o \) units are used.\(^1\) In figure 5 the energy levels are plotted against the QD radius \( R \). One can see that when \( R \) is decreasing every level leaves the white area where it is bound and enters the grey area where it is coupled to unbound states. Some levels are pushed so high that they are embedded in a multiple continuum. In such a case the resonance state associated to it may decay in many channels, each one connected to one continuum \( nls l' \). Decay in the \( nls l' \) channel consists in ejection of one electron with the kinetic energy \( \epsilon \) and the angular momentum \( l' \) and leaving the other electron in the \( nl \) bound state. Such a decay process may be called autoionization.

The probabilities of autoionization per unit of time, given by the widths \( \Gamma \), are presented in figure 6. For a state having the critical energy position at the \( 1s \) continuum threshold, the autodecay probability is equal to zero. The width increases monotonically when the resonance level is getting deeper into the continuum, when \( R \) is decreasing. The dependence of the width on the QD size is specific to a given state. In particular, it depends on the relation between the leading electron configuration of the resonance and the continuum configurations. The widths of the \( 1s^2 \) and \( 1s2s \) states increase rapidly but smoothly with decreasing \( R \). These states are strongly coupled to the \( 1s\varepsilon s \) unbound continuum states. Therefore their widths reach quickly large values (of about \( 10^{-2} \)eV) and the levels disappear before reaching next continuum threshold. This behavior is very similar to the behavior of the Yukawa resonances of previous section.

The behavior of the \( 1p^2 \) and \( 1d^2 \) \( 1S^o \) states is different. These states are weakly coupled to the \( 1s\varepsilon s \) continuum. After a rapid increase, corresponding to the position just above the \( 1s \) threshold, the widths stabilize at values of the order of \( 10^{-4} \)eV. Only after getting into the \( 1p\varepsilon p \) continuum the width of the \( 1p^2 \) level jumps up and the level disappears soon (for the QD size for which the one-electron \( 1p \) state gets lost). The opening of the \( 1p\varepsilon p \) continuum does not affect significantly the width of the \( 1d^2 \) level. It increases a bit and then remains stable at \( 3 \times 10^{-4} \)eV until the level has reached the \( 1d\varepsilon d \) continuum at \( R = 1.62a_o \). These continuum states are strongly coupled to the \( 1d^2 \) configuration. Hence, the width increases rapidly for \( R < 1.6a_o \).

The relationship between the continuum electron configurations and the resonance configuration is the main criterion for distinguishing between the so-called Feshbach and shape resonances. The ones whose configurations are closely related to the configurations of the continuum in which they are embedded, are of the shape type. They decay easily and their widths are large. The configuration of a Feshbach resonance is not related to the background

\(^1\) The effective Rydberg \( R_o = m^* \kappa^2 \epsilon^4 / 2\hbar^2 \epsilon^2 \) and the effective Bohr radius \( a_o = \epsilon \hbar^2 / m^* \kappa \epsilon^2 \), where \( \kappa = 1/4\pi \epsilon_o, \epsilon_o \) is the vacuum permittivity and \( \epsilon \) is the electron charge. We assumed also \( m^* = 0.1m_o \) and \( \epsilon = 5 \). The depth of the potential well has been taken as \( V_o = 10R_o \).
continuum configurations. Hence the decay must involve reconfiguration of the system remaining after it. Therefore, the lifetimes of Feshbach resonances are relatively longer than those of shape resonances. As one can see from the discussion above, in our system we have resonances of both categories. Moreover, most of them change the character from Feshbach to shape when the QD size decreases and the levels enter into the proper continua. One can state that every resonance evolving down the QD size starts as a bound state and reaches the shape stage before disappearing. Some states like those of 1s\textit{n}u\textit{l} configurations miss the Feshbach phase.

The Feshbach and shape resonance concepts are simplified models only. Real complex systems are more complicated due to the electron-correlation effects mixing the open and closed channels. Nevertheless, from the discussion above it is seen how well these models work and are physically meaningful in cases like the present one.

**Figure 5.** Energies of two-electron \( S^e \) bound and resonance states vs the quantum dot radius. Open circles are used for singlet states and full points for triplet ones. The levels are labeled with the leading electron configurations. The 1\( s \), 1\( p \), 1\( d \), and 2\( s \) one-electron levels constitute continua thresholds. The area above the 1\( s \) level is shadowed to indicate the energy continuum.

**Figure 6.** Widths of two-electron \( 1S^e \) resonance levels vs the QD radius. The labels are used as in Fig. 5. Vertical bars placed on a given line indicate the QD size values for which the corresponding resonance level crosses the excited oneelectron levels (consecutively: 1\( p \) and 1\( d \)) and enters higher continua. Drastic change of the slope of the line associated with such a crossing is due to the Feshbach-to-shape change of the resonance character.

4. One-electron quantum dot in a magnetic field
In this section we discuss one electron in a spherical quantum dot consisting of three concentric shells of different semiconducting materials, as considered by Bylicki and Jaskólski in [7], where it is called spherical quantum dot quantum well (SQDQW). The quantum dot is modeled by a spherically symmetric potential for the electron motion constituted by the conduction band-edge profile, presented in figure 7. This system is subjected to a static homogeneous magnetic field directed along the \( z \) axis. Thus the Hamiltonian is\(^2\)

\[
H = -\frac{\hbar^2}{2m^*}\Delta + V(r) + \frac{e^2}{8m^*}B^2\rho^2,
\]

\(^2\) The linear magnetic term is neglected here as being additive; it does not influence the energy level position with respect to the continuum threshold; see [7].
where $\rho^2 = x^2 + y^2$.

**Figure 7.** Conduction band-edge profile constituting the radial potential $V(r)$ for the electron motion in SQDQW. The dotted line shows the energy level of a near-threshold resonance state at $E_0 = 78\text{meV}$ with a width $\Gamma_0 = 7.4\text{meV}$, appearing for $a = 8\text{nm}, b = 2.5\text{nm}$, $V_1 = 0.37\text{eV}, V_2 = 0.13\text{eV}$ and $m^* = 0.041m_0$.

**Figure 8.** Dependence of the lowest $M = 1$ odd state of SQDQW on the magnetic field (SQDQW parameters as given in the caption of figure 7.)

(a) Energy position, $E$ (full points), versus magnetic field $B$. The solid lines show the two lowest Landau energy levels (eq. 4) constituting continuum thresholds.
(b) Width, $\Gamma$, vs magnetic field.
(c) Radius $\rho_0 = [(2|M| + 1)\hbar/eB]^{1/2}$ (solid line) of the the maximum-charge-density cylinder of the lowest Landau state. Dotted lines mark the position of the barrier-shell.

Let us focus our attention on a specific case: the lowest state corresponding to the $M = 1$ value of the $z$-component of angular momentum and to odd parity. For the potential parameters chosen in [7] (see figure 7) this state is a resonance having the energy level just above the continuum threshold. The results obtained [7] for it are presented in figure 8 as a function of the magnetic field $B$. From figure 8a one can see that the absolute position of the energy level increases very slowly. In figure 8b two features are easily seen: First, the width changes very slightly for fields up to a critical value of 19T, at which it starts decreasing rapidly. Next, for fields stronger than 32T, the width is exactly equal to zero. This means that the nonstationary state has been transformed into a completely bound state.

A detailed explanation of the observed effects is given below. Let us first recognize the structure of the continuum channels open for the decay of our resonance. The decay process corresponds to the tunneling of the electron out off the dot through the barrier shell. In the field-free case ($B = 0$) the energy of the electron moving outside the dot consists of the kinetic energy, exclusively. When the field is on ($B \neq 0$) the electron motion in the plane perpendicular to the field direction is quantized and bound, i.e., the electron is trapped in a Landau state. Its
total energy $E$ consists of the Landau state energy,

$$E_n = \frac{\hbar e B}{m^*} \left( |M| + n + \frac{1}{2} \right), \quad (4)$$

and of the kinetic energy of the asymptotic motion along the field axis. The energy continuum breaks into an infinite number of channels, each one associated with a single Landau level. For the electron, of a given energy $E$, that tunnels out (or is scattered) off the dot, the channels associated with the Landau levels $E_n < E$ are open, i.e., energetically accessible, while the others are closed.

The field-induced increase of the energy of the quasibound state is governed by the quadratic term of the Hamiltonian. When the field increases, more and more channels get closed because the Landau levels (the thresholds of the continua) rise up linearly with $B$, i.e., for small fields, faster than the resonance energy. (Two lowest Landau energies are shown in figure 8a.) Reduction of the number of open channels with an increasing magnetic field manifests itself in the lowering of the width of the resonance state as shown in figure 8b. One can see that the energy of our state falls below the lowest Landau level for the fields $B > 32T$. This means that all the decay channels are closed. Therefore the decay rate $\Gamma$ drops to zero (see figure 8b) and the state becomes bound.

An amazing feature is the sharp decrease of the resonance width, $\Gamma$, observed for the field $B > 19T$. It seems to be not correlated with any Landau channel. However, we should note, that apart from the Landau state energy, there is another important property characterizing the Landau channels and the potential scattering in the presence of a magnetic field. This is the radius $\rho_0$ of the cylinder at which the charge density in the lowest Landau state reaches its maximum, and its relation to the quantum dot size defined as the external radius of the barrier shell, $R_D = a + b$. These characteristics are presented in figure 8c. If the Landau state is diffuse, i.e., if $\rho_0 > R_D$, the electron can tunnel from the quantum dot in any direction. Increasing the field, the Landau states get squeezed and if the field is strong enough, $B > 19T$, then $\rho_0 < R_D$, which means that the lowest Landau state is forced into the dot. From figure 8a one can see that for fields of that strength, the lowest Landau channel is the only open one and the only way open for the electron to get out off the dot is the field direction. This leads to a sharp decrease of the resonance width seen in figure 8b.

It should be stressed that the binding effect discussed here occurs for a near threshold resonance. The binding is due to the fact that the localized resonance level and the Landau levels (the continuum thresholds) depend on the magnetic field in different ways: the former one quadratically and the latter linearly. Such an effect may not happen for higher lying states.

5. **Lithium isoelectronic sequence**

Another case we should consider here are isoelectronic sequences of atoms. With the atomic number, $Z$, changing along the sequence the energy spectrum changes. For $Z$ decreasing so that the elements of the sequence change from positive ions to neutrals and then to negative ions, many of levels change from bound ones to resonances. In extreme cases the only localized states are resonances. Such a case is the lithium isoelectronic sequence. For Li [8] and still for He$^-$ [9] there is a bound state of $^4S_o$ symmetry which can be assigned to the $2p^3$ electron configuration. Its energy lies below the $2p^2 \, ^3P_e$ level. Thus the state is bound in a nonrelativistic approximation. In fact it is embedded in a continuum to which it is coupled weakly by a relativistic interaction of spin-orbit type only. From this point of view it is a Feshbach-type relativistic resonance. For the hydrogen doubly negative ion, H$^{--}$, the level is pushed above the $2p^2 \, ^3P_e$ level of H$^-$ [10,11]. It is embedded in the $2p^2 \varepsilon p \, ^4S_o$ continuum to which it is strongly coupled via interelectron Coulomb repulsion. Therefore it is a very broad shape resonance.
The $2p^3\,^4S^o$ resonance being the lowest temporally localized state of $H^{-\infty}$ provides the only chance for this ion to be observed. Unfortunately the resonance lifetime is so short that $H^{-\infty}$ has not been observed yet.

6. Summary

The discussion presented in this paper reminds us that nonexistence of bound states of a quantum system does not imply the nonexistence of the system itself. It may live for finite time in a temporally localized resonance state. Being dependent on a parameter (e.g. the spatial size of the system or an external field strength) the energy spectrum of the system may be transformed so that some of bound states become resonances or vice versa, in accordance to the changes of the parameter. This makes preparing systems of needed properties possible. For instance, one can build a quantum dot of such a size that the allowed energies appear at the levels one wishes. Another very important implication of this that an external electric and/or magnetic field can be used to tune the system. Especially the magnetic field can be used to stabilize systems like quantum dots or atoms. The author believes that such a stabilization by a magnetic field may help in experimental observations of fragile systems such as negative ions.

References

[1] Bylicki M, Stachów A, Karwowski J and Mukherjee P K 2007 The resonance levels of the Yukawa potential Chem. Phys. 331 346
[2] Totsuji H 1971 Theory of critical screening radius of energy levels of hydrogen-like atoms in plasmas J. Phys. Soc. Japan 31 584
[3] Stubbins C 1993 Bound states of the Hulthén and Yukawa potentials Phys. Rev. A 48 220
[4] Gomes O A, Chacham H and Mohallem J R 1994 Variational calculations for the bound-unbound transition of the Yukawa potential Phys. Rev. A 50 228
[5] Bylicki M, Jaskólski W, Stachów A and Diaz J 2005 Resonance states of two-electron quantum dots Phys. Rev. B 72 075434
[6] Szafran B, Adamowski J and Bednarek S 1999 Ground and excited states of few-electron systems in spherical quantum dots Physica E (Amsterdam) 4 1
[7] Bylicki M and Jaskólski W 1999 Binding of resonant states in a magnetic field Phys. Rev. B 60 15924
[8] Aagento T, Andersen T and Chung K T 1984 Optical emission from the (2p2p2p) $^4S^o$ states in three-electron systems J. Phys. B: At. Mol. Opt. Phys. 17 L433
[9] Bylicki M and Pestka G 1996 Bound states of He$^-$ J. Phys. B: At. Mol. Opt. Phys. 29 L353
[10] Sommerfeld T, Riss U V, Meyer H-D and Cederbaum L S 1996 Evidence for a Resonance State of H$^2-$ Phys. Rev. Lett. 77 470
[11] Bylicki M and Nicolaides C A 1998 The H$^2-$ $^4S^o$ spectrum has at least two resonance states J. Phys. B: At. Mol. Opt. Phys. 31 L685