Binding of resonant states in a magnetic field

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We report the theoretical prediction of the phenomenon of turning a *shape* resonance into a bound state in the presence of a magnetic field. A model potential for a multishell spherical quantum dot is used in the study. Sharp changes of the resonance width are observed when the magnetic field is increasing. It is shown that for some critical value of the field, the above-threshold resonant states undergo an abrupt transformation to bound states. The effect is explained and the influence of a magnetic field on the width of atomic shape resonances is discussed. [S0163-1829(99)05947-0]

I. INTRODUCTION

In this paper we deal with an unusual phenomenon of turning a quasistationary state of an electron in a quantum dot into a bound state under an applied constant homogeneous magnetic field. The motivation for the investigation of this effect is twofold: Firstly, the study of the energy structure of quantum dots is important because of their possible applications in electronic and optoelectronic devices.[1,2] In particular, a knowledge of the resonance states of quantum dots is necessary for a proper description and interpretation of tunneling processes in novel one-electron devices.[2,3] Secondly, the impetus comes from atomic physics. It was shown by Bylicki, Themelis, and Nicolaides,[4] who first studied autoionizing resonances of H^- in a magnetic field, that for some strength of the field, the resonance level may cross the continuum threshold causing a change in its energy width. Apart from a possible case of smooth variation of the width with respect to the field strength, two extreme situations after such a crossing are thinkable. Depending on the relation to the open and closed channels, the resonance wavefunction either delocalizes, i.e., the resonance disappears, or quite oppositely, it becomes bound.

Recently, Ho[5] and Bylicki and Nicolaides[6] considered the case of the hydrogen negative ion $^1P^o$ resonance in a magnetic field. This state, having the energy position just above the $n=2$ hydrogen level (the second threshold for the continuum), belongs to the category of *shape* resonances. The existence, i.e., the wave-function localization, and dynamic properties of *shape* resonances are, in the first approximation, determined by an effective one-electron potential containing a barrier,[7] so they appear because of the particular shape of the effective potential.[8] (Therefore such resonances are referred to as *shape* resonances). The results obtained by Ho[5] show that the width of the $^1P^o$ resonance decreases monotonically and smoothly with an increasing field B, reaching, for $B=658$ Teslas (T), a value twelve times smaller than in the absence of the magnetic field. The computation[5] was not carried out for stronger fields. The extrapolation from Ho's results suggests that, apparently, the state is bound for fields stronger than 700 T. Let us note, however, that such a result is not intelligible. This state cannot be bound at such field values, since its energy is still well above the $n=1$ continuum threshold. A result similar to that for $^1P^o$ of Ref. 5 was also obtained by Ho[9] for the $^3P^o$ H^- *shape* resonance lying above the $n=3$ H threshold. On the other hand, in a recent computation by Bylicki and Nicolaides[6] the $^1P^o$ H^- *shape* resonance was followed up to a field of about 140 T at which its energy level was reached by one component of the $n=2$ threshold (the threshold splits in the field). For stronger fields the state disappeared from their computation, i.e., either it had changed so abruptly that it was impossible to follow the change, or it disappeared physically, i.e., the localization was destroyed. Thus, the transformation of the $^1P^o$ H^- resonance under the applied magnetic field is far from being determined and understood.

In the case of many-electron atoms a theoretical investigation of resonant states requires large scale calculations to account for electron correlation effects as well as for many open-channel continuum contributions. In the presence of an external field, the problem is even more complicated and computationally larger due to the breaking of spherical symmetry. Hence, in a case like the $^1P^o$ H^- *shape* resonance in a magnetic field, where the resonance energy level crosses the continuum thresholds, obtaining reliable quantitative results is indeed difficult. However, the *shape* resonance is, in the first-order approximation, determined by a local barrier-well potential for the electron scattered in the field of nucleus and the remaining electrons. Thus, avoiding additional complications due to electron correlation and many open channel continua, one can investigate at least some leading features of the influence of a magnetic field on the energy position and width of *shape* resonances by using a model potential.

II. MODEL

In this paper, we chose to investigate a quantum dot, which also is referred to as an *artificial atom* because of the similarities of its energy structure to the energy spectrum of real atom. The quantum dot is represented here by a simple barrier-well potential (Fig. 1). The energy position of a *shape* resonance, shown schematically in Fig. 1 as dotted line, corresponds to the energy of resonant tunneling of carriers in a quantum dot. The advantage of this model is that (i) it is easy to deal with computationally to high numerical accuracy, and (ii) it can be realized as a chemically synthesized multishell semiconductor nanocrystal,[3,10] so that theoretical predictions can be verified experimentally. The use of a semiconductor

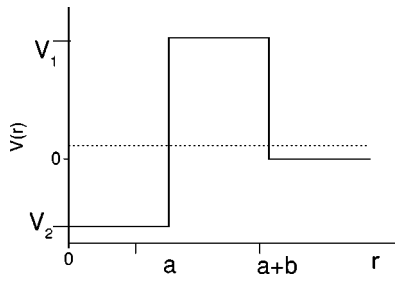

FIG. 1. Conduction band-edge profile constituting the radial potential $V(r)$ for the electron motion in SQDQW. The dotted line shows the energy position of a near-threshold resonances state.

environment to study the resonance state dependence on the magnetic field gives the possibility of applying fields attainable in the laboratory, while for atoms a similar study would require fields stronger by several orders of magnitude.

More specifically, we considered a spherical quantum-dot quantum well (SQDQW) system consisting of three concentric shells of different semiconducting materials. The most internal core, of radius a, is built of a material whose energy gap between the valence and conduction band is small. The middle shell, a barrier of thickness b, consists of a cap of a wider-gap semiconductor. The bottom of the conduction band in the core is at V_2 and in the middle shell is equal to V_1 (see Fig. 1). The external macroscopic shell is again built of a small gap material; its conduction band edge is placed between V_1 and V_2 levels. The bottom of the conduction band of the outer shell, constitutes the continuum threshold and is chosen to be zero of the energy scale. As a particular realization of such a quantum dot one can consider a structure built of caps of $Ga_x In_{1-x}As$, $Al_x In_{1-x}As$ and $Ga_y In_{1-y}As$ with properly chosen compositions (x and y) of Ga and Al atoms in In As.[11–13]

We investigated only the electron states and we worked within the one-band effective mass approximation. The electron effective mass m^* was, for simplicity, considered as being homogeneous in the whole system.[11] The conduction band-edge profile, shown in Fig. 1, constitutes a spherical potential $V(r)$, for the electron motion. The Hamiltonian of the electron in a spherical quantum dot and static homogeneous magnetic field $B=B_z$ is

$$H=\frac{\hbar^2}{2m^*}\Delta+V(r)+\frac{e^2}{8m^*}B^2\rho^2, \tag{1}$$

where $\rho^2=x^2+y^2$.[14] Since the magnetic field breaks the spherical symmetry of the dot, the orbital angular momentum is not a constant of motion and the eigenstates of H can be labeled by the magnetic quantum number M and parity π. The consecutive states of a given M and parity are numbered by n, i.e., M_n^π.

III. METHOD

As a tool for finding the resonance energy position, E, and the energy width, Γ, we applied the complex eigenvalue Schrödinger equation (CESE) approach,[15] which is a fast convergent (as the size of basis set is considered) method involving complex coordinate rotation technique as a way of handling with the resonance boundary conditions. A review of applications of the CESE method to atomic resonances can be found in Refs. 16 and 17. The method was also applied to the study of resonant tunneling in low-dimensional structures,[12,13,18] and in this context was described in detail in Refs. 12 and 13.

Here we summarize briefly only the most important features of the CESE approach: The resonance wave function can be divided into two terms,

$$\Psi=\Psi_{loc}+\chi_{asympt}. \tag{2}$$

The localized part, Ψ_{loc}, is square integrable and describes the quasibound character of the state, whereas χ_{asympt} takes care of the proper asymptotic behavior of the state, i.e., it is responsible for the decay of the resonance. Since the decaying resonance function contains asymptotically only an outgoing wave, the corresponding eigenvalue of the Hamiltonian is complex, $\epsilon=E-i\Gamma/2$, with the imaginary part determining the decay probability, Γ. Because of different properties of Ψ_{loc} and χ_{asympt}, they require to be represented in different basis sets. In our calculations the localized part was expanded in a basis of the usual Slater-type orbitals (STO) of real coordinates, while the asymptotic part was represented by STO's of the complex rotated coordinate $re^{-i\theta}$ (r is the radial coordinate). The use of such a complex coordinate regularizes the wave function, i.e., makes it square integrable.

When choosing the basis set we took advantage of the well-defined geometry of the system. Since we knew that the resonance wave function should be localized inside the well, we chose the nonlinear parameters of the real STO's so as to localize them within the well in the sense of the mean value of r. The complex rotated STO's, representing the asymptotic part of the wave function, were distributed outside the well.[19] The Hamiltonian matrix built from such a basis set is non-Hermitian; its eigenvalues are complex and, as functions of parameter θ, form the so called θ-trajectories on the complex energy plane.[22] These complex eigenvalues of the Hamiltonian matrix, which correspond to resonances should be independent of the complex rotation parameter θ, if the basis set was complete. The basis sets actually used are finite and incomplete, so the eigenvalues may be θ dependent. The complex roots that stabilize against the variation of θ correspond to the resonance states. Their values at the stabilization points of θ trajectories are considered as being the best approximations to the complex energies of the resonances, ϵ. In our computation the basis set was also optimized with respect to other nonlinear parameters so as to obtain the best θ stabilization.

IV. RESULTS AND DISCUSSION

We performed calculations of the resonance spectra for two different symmetries in two slightly different SQDQW systems. The $M^\pi=0^e$ symmetry states were investigated in SQDQW defined by $a=7$, $b=2.5$ nm, $V_1=0.37$, $V_2=0.1$ eV and $m^*=0.041m_0$. The 1^o states were studied for a system determined by $a=8$, $b=2.5$ nm, $V_1=0.37$, $V_2=0.13$ eV and $m^*=0.041m_0$. The values of the effective mass m^* and band offset parameters, V_1 and V_2, correspond to SQDQW built of previously mentioned $Ga_x In_{1-x}As$ and $Al_x In_{1-x}As$ materials.[11,13] The thickness of layers was cho-

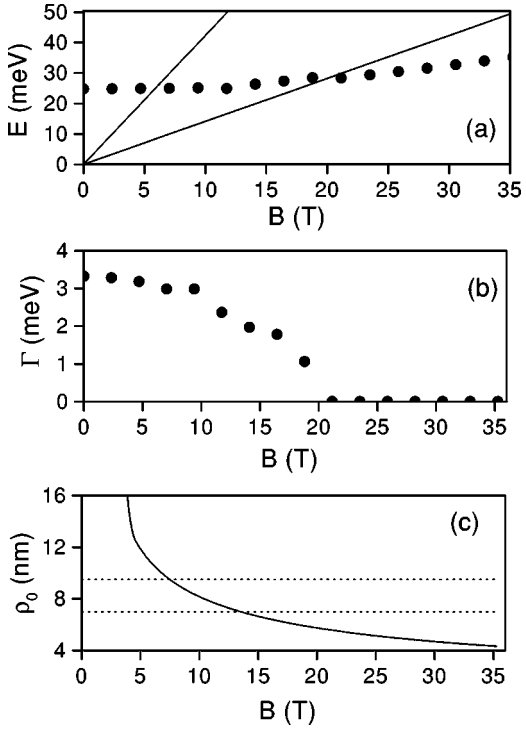

FIG. 2. The 0_1^e resonance of SQDQW defined by $a=7$, $b=2.5$ nm, $V_1=0.37$, and $V_2=0.1$ eV (see Fig. 1). (a) Energy position, E (full points), versus magnetic field B. The solid lines show the two lowest Landau energy levels [Eq. (3)] constituting continuum thresholds. (b) Width, Γ, vs magnetic field. (c) Radius $\rho_o=[(2|M|+1)\hbar/eB]^{1/2}$ (solid line) of the the maximum-charge-density cylinder of the lowest Landau state. Dotted lines mark the position of the barrier-shell.

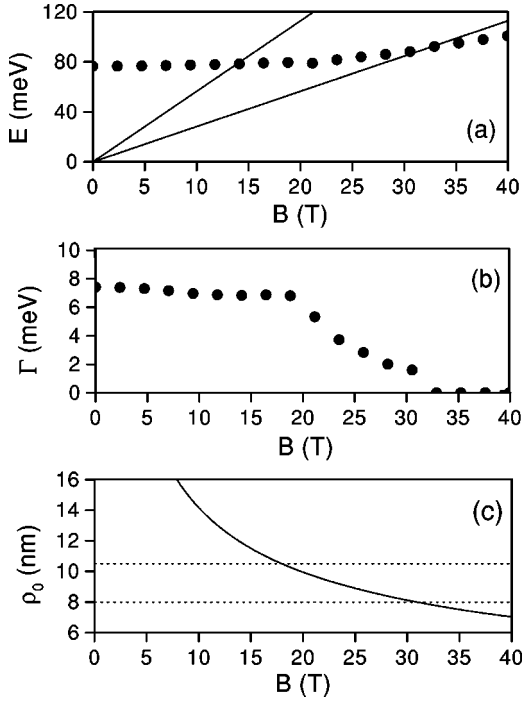

FIG. 3. The same as in Fig. 2, but for the 1_1^o state of SQDQW determined by $a=8$, $b=2.5$ nm, $V_1=0.37$, and $V_2=0.13$ eV.

sen within a practically attainable range and to guarantee the presence of very-near-threshold resonances (see Fig. 1). The magnetic field was varied in the range from 0 up to 40 T. The energy spectrum of both symmetries had several resonance levels. The parameters, E and Γ, of high-lying resonances changed smoothly with respect to the variation of the field strength and Γ did not reach zero for any field. They were not of interest in this paper.

We have focused our attention on the lowest resonances, 0_1^e and 1_1^o, having energy levels just above the continuum threshold.[23] The results obtained for the 0_1^e and 1_1^o states are presented in Figs. 2 and 3, respectively. Two characteristic features in the variation of the resonance widths versus magnetic field are easily seen in Figs. 2(b) and 3(b): First, the widths change very slightly for weak fields up to some critical value of the field, depending on the case, 9 T for 0_1^e and 19 T for 1_1^o, at which they start decreasing rapidly. Next, for fields stronger than 21 T in the case of 0_1^e, or 32 T for the 1_1^o state, the value of the width is exactly equal to zero. This means that the nonstationary states have been transformed into completely *bound* states.

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 a nonstationary state of our system. The decay process corresponds to the tunneling of the electron out of 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,

$$E_n=\frac{B}{m^*}(|M|+n+\tfrac{1}{2}), \tag{3}$$

and of the kinetic energy, E_{kin}, 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) from the dot, the channels associated with the Landau levels $E_n \leqslant E$ are *open*, i.e., energetically accessible, while the others are *closed*.

The field-induced increase of the energy of a 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. 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 Figs. 2(b) and 3(b). The slowly increasing energy positions of the 0_1^e and 1_1^o states are shown as functions of B in Figs. 2(a) and 3(a), respectively. For comparison, the lowest two Landau energy levels are displayed in both cases. One can see that the 0_1^e and 1_1^o energies fall below the lowest Landau level for the fields $B\geqslant 21$ T and $B\geqslant 32$ T, respectively. This means that all the decay channels are closed, the decay rate Γ drops to zero [see Figs. 2(b) and 3(b)] and the states become bound. It is noteworthy that the observed binding effect occurs for near threshold resonances and may not happen for higher lying states.

An additional comment is needed to explain the other effect, i.e., a sharp decrease of the resonance width, Γ, observed for the field $B>9$ T in the 0_1^e case and for $B>19$ T in the 1_1^o case. Let us note, that apart from the Landau state energy, there is another important feature characterizing Landau channels and potential scattering in the presence of a magnetic field. This is the radius $\rho_o=[(2|M|+1)\hbar/eB]^{1/2}$ 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, $R_D \equiv a+b$. These characteristics are presented in Figs. 2(c) and 3(c). If the Landau state is *diffuse*, i.e., if $\rho_o \gg R_D$, 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, ($B>9$ T for 0_1^e or $B>19$ T in the 1_1^o case), then $\rho_o<R_D$, which means that the lowest Landau state is forced into the dot. From Figs. 2(a) and 3(a) 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 of the dot is the field direction. This leads to a sharp decrease of the resonance width, which is clearly seen in Figs. 2(b) and 3(b).

In summary, we have shown that near-threshold *shape* resonances can become bound in a magnetic field. To our best knowledge this effect was not reported earlier. We have explained the effect in terms of the different field dependence of the energy positions of the quasibound states and continuum thresholds. The observed phenomenon of turning a quasistationary state into a bound state may occur in any system of one charged particle in a barrier-well potential. We feel strongly that the present results, showing that the abrupt changes of the width are correlated with breaking through the continuum thresholds, give some insight into the problem of stabilizing atomic *shape* resonances in a magnetic field.[5,6,9] Let us also note, that the effect of the formation of a bound state from a resonance state may be of fundamental importance in the investigation of transport phenomena in low-dimensional nanostructures. Since the binding of a resonance state means the suppression of resonant tunneling through this state, the magnetic field could be used to control (to switch on/off) the tunneling current in electronic devices built of quantum dots.

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[1] U. Woggon, *Optical Properties of Semiconductor Quantum Dots* (Springer Verlag, Berlin, 1997); J. Lumin. **70**, 1 (1996); special issue on Spectroscopy of Isolated and Assembled Semiconductor Nanocrystals.

[2] L. Kouvenhoven and Ch. Marcus, Phys. World **11**, 35 (1998); M. Devoret and Ch. Glatti, *ibid.* **11**, 29 (1998).

[3] D. L. Klein, R. Roth, A. K. L. Lim, A. P. Alivisatos, and P. L. McEuen, Nature (London) **389**, 699 (1997); A. P. Alivisatos, Science **271**, 933 (1996).

[4] M. Bylicki, S. I. Themelis, and C. A. Nicolaides, J. Phys. B **27**, 2741 (1994).

[5] Y. K. Ho, Phys. Lett. A **230**, 190 (1997).

[6] M. Bylicki and C. A. Nicolaides (unpublished).

[7] J.-P. Connerade, *Highly Exited Atoms* (Cambridge University Press, Cambridge, 1998), p. 167.

[8] This is in contrast with the Feshbach resonances, which are caused by the coupling between the closed and open channels, and therefore, their appearance cannot be explained by a one-electron potential model.

[9] Y. K. Ho, J. Phys. B **31**, 1191 (1998).

[10] A. Mews, A. Eychmüller, M. Giersig, D. Schoos, and H. Weller, J. Phys. Chem. **98**, 934 (1994); D. Schooss, A. Mews, A. Eychmüller, and H. Weller, Phys. Rev. B **49**, 17 072 (1994).

[11] J. A. Porto, J. Sanchez-Dehesa, L. A. Cury, A. Nagaret, and J. C. Portal, J. Phys.: Condens. Matter **6**, 887 (1994).

[12] M. Bylicki, W. Jaskólski, and R. Oszwałdowski, J. Phys.: Condens. Matter **8**, 6393 (1996).

[13] W. Jaskólski and M. Bylicki, Vacuum **48**, 235 (1997).

[14] The linear Zeeman term is omitted because of its trivial additive character.

[15] C. A. Nicolaides, Y. Komninos, and Th. Mercouris, Int. J. Quantum Chem. **S15**, 355 (1981).

[16] C. A. Nicolaides, Th. Mercouris, Y. Komninos, and I. D. Petsalakis, Int. J. Quantum Chem. **51**, 529 (1994).

[17] M. Bylicki, Adv. Quantum Chem. **32**, 207 (1998).

[18] M. Bylicki and W. Jaskólski, Acta Phys. Pol. A **94**, 271 (1998).

[19] This way of choosing basis set functions is related to an idea introduced by Nicolaides and Beck (Ref. 20) and then by Simon (Ref. 21), and known as the exterior complex scaling.

[20] C. A. Nicolaides and D. R. Beck, Phys. Lett. **65A**, 11 (1978).

[21] B. Simon, Phys. Lett. **71A**, 211 (1979).

[22] Typical θ trajectories corresponding to continuum, bound and resonant states can be found in Ref. 12.

[23] We chose the levels nearest to the threshold because their response to weak fields, measured in terms of the level position with respect to the threshold, is more pronounced than for the others. This was also the reason for choosing different SQDQW systems for different symmetries.