Research plan

Resonances and Rydberg states of atoms in external fields via anharmonic-oscillator semiclassical perturbation theory with complex coefficients

1. Introduction

Effects of external electric and magnetic fields on highly excited atoms have attracted both experimental and theoretical interest, see, for example, the review [1]. For an electric field only, this problem can be easily solved numerically because it is separable (in parabolic coordinates). Several analytical methods were also proposed, see, for example [2], where modifications of the semiclassical WKB method and a perturbation theory were used both for low-lying states and for over the barrier Stark resonances. In the presence of a magnetic field this problem is harder to solve because it is no longer separable. Analytic solutions exist only in the limit of small fields when perturbation theory is applicable. Computations for intermediate and strong fields are done usually by expanding the wave function over a large basis set.

The subject of this research is the development of new advanced methods of perturbation theory that can predict and qualitatively describe new classes of atomic phenomena like resonances over the ionization threshold. Perturbation theory is a usual tool for the ground and lower excited states in weak fields. However, the applied fields can dominate atomic forces for highly excited states, and the resulting spectrum cannot be understood within the framework of traditional perturbation theory (in powers of the field strength). The main idea of the present approach is to use the perturbation theory that is similar to a semiclassical expansion in the theory of molecular vibrations rather than to use a traditional expansion for the perturbed hydrogen atom. Such an approach may become useful in a much broader context, i.e. wherever saddle-point resonances occur [3].

Generally, the results may be useful for astrophysics for detailed analyses of spectra of atoms in interstellar magnetic fields as well as for laboratory studies of highly excited Rydberg atoms.

The general approach to be used here will be described briefly.

2. Semiclassical expansion associated with a potential minimum or complex stationary points

Consider, for example, any quantum Hamiltonian of the form $H = \frac{p^2}{2M} + V(x)$. If the potential $V(x)$ has a minimum at $x = x_0$, then the Hamiltonian is expanded as

$$H = \frac{p^2}{2M} + V_0 + (x - x_0)^2 V_2 + (x - x_0)^3 V_3 + \ldots,$$

and the energy eigenvalues are expanded in powers of $\hbar$, Plank's constant:

$$E = V_0 + (n + \tfrac{1}{2})\omega\hbar + E_2\hbar^2 + E_3\hbar^3 + \ldots,$$

Here, n is an oscillator quantum number, $\omega = \sqrt{2V_2 / M}$ is a frequency of small vibrations around the potential's minimum, and coefficients of this expansion can be calculated to arbitrary order using formulas of Rayleigh – Schrödinger perturbation theory[1].

The present project deals with complex stationary points of the potential when the coefficients V_0, V_2, V_3 etc. are complex numbers. Calculation of the perturbation series remains the same (but it needs complex arithmetic). In this way, complex energies which specify the location and width of resonant states were computed both for spherically-symmetric problems [7] and for a hydrogen atom in parallel electric and magnetic fields [8].

Unlike earlier studies [7, 8], I shall consider the case when a potential supports bound states and in addition has a saddle point or a complex stationary point that gives rise to the series of resonances. So, these resonances may appear as highly excited unstable states or resonances in continuum spectrum.

The prototype of the present study is analysis of asymmetrically doubly excited two-electron atoms („planetary" atoms [9]) within large-dimensional approach [10]. An effective scaled potential for two-electron atom in *D* dimensions

$$V_{\text{eff}}(r_1, r_2, r_3) = -\frac{1}{r_1} - \frac{1}{r_2} + \frac{1/Z}{r_3} + \frac{1}{4}\frac{r_1^2 + r_2^2}{r_1^2 r_2^2 + r_2^2 r_3^2 + r_3^2 r_1^2 - r_1^4/2 - r_2^4/2 - r_3^4/2}$$

has a symmetric minimum (at least for $Z \geq 2$) and seven different asymmetric stationary points listed for $Z = 2$ in the following table [10]:

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[1] Earlier, we developed effective methods of calculation of higher order coefficients [4]. Methods of accelerating of convergence of this series were studied in [5, 6]

No	r_1	r_2	r_3	V_0
1	-5.644	5.580	-1.008	-0.249
2	$-0.018+0.111i$	$0.055+0.020i$	$-0.057-0.024i$	$-11.043+8.764i$
3	$-0.018-0.111i$	$0.055-0.020i$	$-0.057+0.024i$	$-11.043-8.764i$
4	$0.036+0.109i$	$-0.178+0.110i$	$0.110+0.051i$	$2.540+4.522i$
5	$0.036-0.109i$	$-0.178-0.110i$	$0.110-0.051i$	$2.540-4.522i$
6	$0.123+0.354i$	$0.186+0.001i$	$0.151+0.240i$	$-2.654+0.529i$
7	$0.123-0.354i$	$0.186-0.001i$	$0.151-0.240i$	$-2.654-0.529i$

The expansion over the symmetric minimum gives rise to 1/*D*-expansion for the ground [11] and lowest excited states [12]. It was found [10] that appropriate stationary point that corresponds to asymmetrically doubly excited two-electron atoms in a large-dimensional limit is the seventh configuration. The energies were calculated as a function of *D* by summation of the complex 1/*D*-expansion. For $Z \geq 2$, the real part of the result of summation agrees with the position of the resonance, and the imaginary part becomes very small.

3. Details of the proposal

The subject of this proposal is a hydrogen atom (or an alkali atom which is almost equivalent to the hydrogen one) in an excited state under external electric and magnetic fields. Firstly, saddle points or complex stationary points of the potential will be searched. Then, complex semiclassical expansions will be developed around these points. Finally, the expansions will be summed and the results will be interpreted and compared with previously studied resonances.

For an atom in an electric field, $V = -1/r - Fz$, and there is only one such point, the Stark saddle point at $z = \sqrt{1/F}$, $V_0 = -2\sqrt{F}$. The proposed approach allows to determine the associated resonances with high precision, however they appear to be very broad and of little interest for the case of pure electric field. The first stage of the research consists of study of evolution of such resonances in the presence of a crossed magnetic field. It is expected that the resonance width will decrease with increasing of a magnetic field. Probably, the resulting resonances will be identical to quasi-Penning resonances studied earlier [13] which are characterized by a triaxial harmonic motion of the electron far apart from the proton [14]. Similar long-lived trapped resonances of a positron in the Coulomb field of a nucleus and in parallel electric and magnetic fields were studied too using anharmonic-oscillator perturbation theory [15].

For an atom in a magnetic field, $V = -1/r + \frac{B^2}{8}\rho^2$ (a paramagnetic term is dropped here because its contribution to the energy is trivial). This potential has a pair of complex-conjugate stationary points at

$z = 0$ and $\rho = \exp(\pm \frac{2}{3}\pi i)(B/2)^{-2/3}$, $V_0 = 2\exp(\pm \frac{1}{3}\pi i)(B/2)^{2/3}$. The second stage of the research consists of detailed study of resonances associated with these stationary points and their interpretation. For lower oscillator quantum numbers, they are very broad ($\mathrm{Im}\, E \sim \mathrm{Re}\, E$), but for higher quantum numbers it may be possible some cancellation of imaginary parts of different terms of the perturbation series as it was found for the helium asymmetric stationary point [10]. These resonances may be closely related to ultranarrow resonances above the ionization threshold that are extensively studied both theoretically [16] and experimentally [17].

Results of this work will provide high accuracy reference data as well as a new classification scheme of higher excited states.

4. Implementation. Timetable

The first stage of the work (resonances associated with the Stark saddle point in crossed electric and magnetic fields) will take 6 months. Firstly, I shall write down the Hamiltonian of a hydrogen atom in electric and magnetic fields in terms of three variables corresponding to normal-mode oscillations around the saddle point. Using my earlier experience in calculating the similar 1/*D*-perturbation series for parallel fields [8, 15] (two independent variables) and for two-electron atoms [10, 18] (three variables), I shall develop a computer program to calculate corresponding anharmonic-oscillator expansion. Then, this perturbation series will be summed for various strengths of electric and magnetic fields, different orientations of fields, and different quantum numbers. Finally, I expect to find general regularities by studying several limiting cases (large and small fields, large quantum numbers etc.). Also, the results will be compared with the known results for quasi-Penning resonances [13, 14].

The second stage (resonances in continuum spectrum of a hydrogen atom in a magnetic field) will take also 6 months. During this stage, I shall probably restrict myself to a magnetic field only. Here, I plan to use my working computer program for 1/*D*-expansion of the diamagnetic hydrogen atom [19]. The only modification will be the use of a complex-conjugate pair of stationary points that appears as a result of solving of the forth-order polynomial equation for the equilibrium radius r_0. Resulting perturbation series will be complex; Padé summation or similar methods will yield precise results as it was found for the expansion around the real minimum that describes circular states in a magnetic field [20]. Results of summation will be studied for the entire range of the field strength and for different quantum numbers.

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