Quantum Anomaly Dissociation of Quasibound States Near the Saddle-Point Ionization Limit of a Rydberg Electron in Crossed Electric and Magnetic Fields

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Abstract

In the combination of crossed electric and magnetic fields and the Coulomb field of the atomic nucleus the spectrum of the Rydberg electron in the vicinity of the Stark saddle-point are investigated at a quantum mechanical level. The results expose a quantum anomaly dissociation: quasibound states near and above the saddle-point ionization limit predicted at the semi-classical level disappear at a quantum mechanical level.

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Twenty years ago Clark et al. [1] claimed that the combination of crossed electric and magnetic fields and the Coulomb field of the atomic nucleus can lead to the localization of the Rydberg electron in the vicinity of the Stark saddle-point. When the characteristic parameter $\omega^2_t > 0$ in the classical equation of motion the electron motion is periodic in an elliptical orbit. Such orbits give rise to electron states which are localized above the saddle-point and whose spectrum is that of a harmonic oscillator. Divergent hyperbolic trajectories are obtained in the case when $\omega^2_t < 0$. The classical equation of motion includes both type of solutions. The periodic orbits are unstable with respect to small perturbations, thus assume the character of quasibound states. Ref. [1] focused attention on the energy region near the ionization threshold for the first time in literature. The distinctive character of this portion of the spectrum makes it an attractive target of experimental investigation. Their treatment is semi-classical. The determination of the lifetimes of these states and their associated transition moments awaits a full quantum mechanical treatment.

The full quantum mechanical treatment of the above-ionization-threshold spectra of atoms in crossed electric and magnetic fields can be investigated globally and locally. In literature there were a lot of works focused on the global aspect of this problem, for example, see Main and Wunner [2], Main, Schwacke and Wunner [3], etc. and references there in. Clark et al [1] considered, classically, the local aspect of the above system.

In this Letter we investigate the local aspect of the above system for Clark’s case [1] at a quantum mechanical level. The results reveal a quantum anomaly dissociation: bound states which exist at a semi-classical level may disappear at a quantum mechanical level. For the present example, we find that quasibound states of the harmonic type above the saddle-point ionization limit predicted in Ref. [1] do not exist at a quantum mechanical level. This explains the reason that non of the suggested experiments yet has been realized.

Let the constant electric field $\mathbf{E} = -E \mathbf{i}$, and the uniform magnetic field $\mathbf{B}$ aligning the $x_3$ axis. We can choose a gauge so that the corresponding vector potential $A_i$ reads $A_i = \frac{1}{2} \epsilon_{ij} B_j \hat{x}_j$, where $\epsilon_{ij}$ is a 2-dimensional antisymmetric unit tensor, $\epsilon_{12} = -\epsilon_{21} = 1$, $\epsilon_{11} = \epsilon_{22} = 0$. In the combination of the crossed uniform magnetic and electric fields, and the Coulomb field of the atomic nucleus the Hamiltonian $H$ of the Rydberg electron,
globally, reads (the summation convention is used henceforth)
\[
H = \frac{1}{2\mu} \dot{p}_i^2 - \frac{e^2}{\tilde{r}} - \frac{1}{2} \omega_c \epsilon_{ij} \tilde{p}_i \tilde{x}_j + \frac{1}{8} \omega_c^2 \tilde{x}_i^2 - eE \tilde{x}_1, \quad (i, j = 1, 2)
\]
where \( \tilde{r} = (\tilde{x}_1^2 + \tilde{x}_2^2 + \tilde{x}_3^2)^{1/2} \), and \((\tilde{x}_1, \tilde{x}_2, \tilde{x}_3)\) are the coordinates of the electron centered about the atomic nucleus. In the above \( \mu \) and \( -e \) are, respectively, the mass and the electric charge of the electron; The magnetic cyclotron frequency \( \omega_c = eB/\mu c \).

A particle trap using static fields must confine the electron about the Stark saddle-point where the net electric force vanishes. We therefore consider, locally, the Schrödinger equation in coordinates centered about the saddle point rather than about the atomic nucleus. The coordinate of the saddle point is \( x_{10} = \sqrt{e/E} \). In this coordinate system the coordinates of the electron are \((x_1, x_2, x_3)\). The electrostatic potential is given by \( \Phi = e/[(x_1 + x_{10})^2 + x_2^2 + x_3^2]^{1/2} + E(x_1 + x_{10}) \). A harmonic approximation of the potential in the region around the saddle point is enough. For small \( x_1, x_2 \) and \( x_3 \) the electrostatic potential is approximated by \( \Phi = -\frac{1}{e} V_c - \frac{1}{2} \omega_z^2 (-2x_1^2 + x_2^2 + x_3^2) \), where \( V_c = -2e\sqrt{eE} \) is the energy of the classical ionization limit in the presence of the electric field, and \( \omega_z^2 = e^2/\mu x_{10}^3 \) is the axial frequency. The Hamiltonian \( H \) of this system can be decomposed into a 2-dimensional Hamiltonian \( H_\perp \) and a one-dimensional harmonic Hamiltonian \( H_z \) with the axial frequency \( \omega_z \): \( H = H_\perp + H_z \). The 2-dimensional Hamiltonian \( H_\perp \) is, locally, the type of a quasi-Penning trap
\[
H_\perp = \frac{1}{2\mu} (p_i - \frac{1}{2} \mu \omega_z \epsilon_{ij} x_j)^2 + \frac{1}{2} \mu \omega_z^2 (-2x_1^2 + x_2^2) + V_c = \frac{1}{2\mu} p_i^2 - \frac{1}{2} \mu \epsilon_{ij} p_i x_j + \alpha_1 x_1^2 + V_c, \quad (2)
\]
where \( \alpha_1 = \mu (\omega_c^2 - 8\omega_z^2)/8, \alpha_2 = \mu (\omega_c^2 + 4\omega_z^2)/8 \). The magnetic field should be strong enough to satisfy a condition \( \omega_c^2 > 8\omega_z^2 \) so that \( \alpha_1 > 0 \). At the semi-classical level the magnetic field \( B \) itself enters into the classical equation of motion. At a quantum mechanical level the vector potential \( A_i \) enters into the Schrödinger equation. Comparing Eq. (2) with the coefficients \( \omega_i^2 \) of \( x_i \) terms in the classical equation of motion in Ref. [1], it shows that the coefficients \( \alpha_i \) of \( x_i^2 \) terms in the Schrödinger equation include more information [4].

In the following discussions the starting point is the Hamiltonian (2), that is, we shall take the Hamiltonian (2) as the definition of the model of the (local) quasi-Penning trap without making further reference to the original (global) Hamiltonian (1).
This system is unlike the case in Ref. [5–7]. Because of lacking symmetry in the above crossed electric and magnetic fields, the situation of this system is involved. We find that this system is solved by the following ansatz. We define the canonical variables $X_{\eta}$ and $P_{\eta}$ ($\eta = a, b$) as

\[
X_a \equiv \sqrt{\mu \Omega_1/2} x_1 - \sqrt{1/2} \mu \Omega_1 \omega_1 p_2, \quad X_b \equiv \sqrt{\mu \Omega_2/2} x_1 + \sqrt{1/2} \mu \Omega_2 \omega_2 p_2,
\]
\[
P_a \equiv \sqrt{\omega_1 \omega_2} p_1 + \sqrt{\mu \Omega_1 \omega_1} (\omega_2 - \omega_1) x_2,
\]
\[
P_b \equiv \sqrt{\omega_1 \omega_2} p_1 - \sqrt{\mu \Omega_1 \omega_1} (\omega_2 - \omega_1) x_2.
\]

In the above the parameters $\Omega_{1,2}$ and $\omega_{1,2}$ are, respectively, defined as

\[
\Omega_{1,2} \equiv \{ \pm (\alpha_2 - \alpha_1) + [(\alpha_2 - \alpha_1)^2 + \mu \omega_c^2 (\alpha_1 + \alpha_2)]^{1/2} \}/\mu \omega_c,
\]
\[
\omega_{1,2} \equiv (\Omega_1 + \Omega_2)(2\Omega_{1,2} + \omega_c)/4\Omega_{1,2}.
\]

The above definitions give that $\Omega_{1,2} > 0$, $\omega_2 > 0$. From $\omega_2 - \omega_1 = \omega_c (\Omega_1 + \Omega_2)^2/4\Omega_1 \Omega_2 > 0$, it follows that $\omega_2/\omega_1 = \Omega_1 (2\Omega_2 + \omega_c)/\Omega_2 (2\Omega_1 - \omega_c) > 1$, which shows $(2\Omega_1 - \omega_c) > 0$, hence $\omega_1 > 0$. These results confirm that the definitions of $X_{\eta}$ and $P_{\eta}$ are meaningful. Furthermore, the canonical variables $X_{\eta}$ and $P_{\eta}$ satisfy $[X_{\eta}, P_{\rho}] = i\hbar \delta_{\eta\rho}$ ($\eta, \rho = a, b$) and $[X_a, X_b] = [P_a, P_b] = 0$, which show that modes $a$ and $b$ are fully decoupled at the quantum mechanical level. Finally, we define the parameters $\omega_{a,b}^2$ as

\[
\omega_{a,b}^2 \equiv \Omega_{1,2} \omega_{1,2} (\omega_c = 2\Omega_{2,1})/(\Omega_1 + \Omega_2).
\]

From Eqs. (3)-(5) it follows that the Hamiltonian $H_\perp$ in Eq. (2) decouples into two modes

\[
H_\perp = H_a + H_b + V_c,
\]
\[
H_{a,b} = \frac{1}{2} P_{a,b}^2 + \frac{1}{2} \omega_{a,b}^2 X_{a,b}^2.
\]

Eq. (5) shows that $\omega_b^2 > 0$. The mode $b$ is a harmonic oscillator with the unit mass. It is worth noting that

\[
\omega_c - 2\Omega_2 = \{ (\omega_c^2 + 3\omega_z^2) - [(\omega_c^2 + 3\omega_z^2)^2 - 8\omega_c^2 \omega_z^2]^{1/2} \}/\omega_c > 0,
\]

from which Eq. (3) also gives that $\omega_a^2 > 0$. The possibility of $\omega_a^2$ can’t be changed through tuning external parameters like the magnetic field $B$ and/or the electric field $E$. The
Schrödinger equation of the mode $a$ reads

$$i\hbar \frac{\partial}{\partial t} \psi_a(X_a, t) = \left( \frac{1}{2} p_a^2 - \frac{1}{2} \omega_a^2 X_a^2 \right) \psi_a(X_a, t).$$  \hspace{1cm} (8)

In the above the system (2) is solved exactly.

At the quantum mechanical level the normalization conditions of wave functions of bound states are a key point. The minus sign of the $X_a^2$ term in Eq. (8) elucidates that normalized wave functions $\psi_a(X_a, t)$ of bound states of the mode $a$ do not exist, thus for the whole system normalized wave functions $\Psi(X_a, X_b, t) = \psi_a(X_a, t) \psi_b(X_b, t)$ of bound states do not exist either. Thus it is impossible to locate an electronic state. This observation reveals the phenomenon of the quantum anomaly dissociation that quasibound states predicted in Ref. [1] do not exist at the quantum mechanical level.

**Discussions** - (i) The conclusion about the quantum anomaly dissociation applies only, locally, to the Hamiltonian (2) of the system in the region above the saddle point.

**Globally**, the Hamiltonian of the system is Eq. (1). Main and Wunner [2], Main, Schwacke and Wunner [3] et al. performed, full quantum-mechanically, numerical calculation of the system (1). The results showed the existence of quite a few bound states near or above the ionization threshold. The features of these bound states are different from the bound states predicted by Clark et al. [1]. For Clark’s case the energy spectrum associated with the periodic elliptical orbits is the type of a harmonic oscillator.

(ii) Glas, Mosel and Zint showed that [8] in the cranked oscillator model when the parameters satisfy certain conditions the square of frequencies of the two decoupled modes are positive. The bound states exist. The situation of the Hamiltonian (2) is different from the cranked oscillator. All the parameters of the Hamiltonian (2) depend on the external magnetic field $B$ and/or the electric field $E$. Their relations are fixed. Eq. (7) shows that the sign of $\omega_a^2$ and in turn the minus sign of the term $X_a^2$ in Eq. (8) can’t be changed through tuning the external magnetic field $B$ and/or the electric field $E$. Thus at the quantum mechanical level the bound states of the harmonic type corresponding to the classical periodic elliptical orbit predicted by Clark et al. [1] disappear exactly.

Up to now the quantum anomaly dissociation exposed in the Hamiltonian (2) is the only example. At the present the clarification of general conditions leading to such a
phenomenon is an open issue. Studies on this subject are important for experimental atomic physics which are based on the semi-classical treatment.

Note in revised version - Since submitting this paper, Connerade group has reached the same conclusion experimentally as the one in this paper [9]. However, they do find the states near the minimum of the outer well. They have lifetimes which seem to fit tunnelling rate between the two wells. The features of these states are different from the ones predicted by Clark et al. [1].

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