Semiclassical theory of helium atom

Gregor Tanner and Klaus Richter (2013), Scholarpedia, 8(4):9818. doi:10.4249/scholarpedia.9818 revision #132323 [link to/cite this article]
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Revision as of 11:20, 3 April 2013 by Gregor Tanner (Talk | contribs)

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In memory of our teacher and friend, Dieter Wintgen, who died on the 16th August 1994 at the age of 37 years on the descent from the Weisshorn (4505 m).

Semiclassical theory of helium atom refers to a description of the quantum spectrum of helium in terms of the underlying classical dynamics of the strongly chaotic three-body Coulomb system formed by the nucleus and the two electrons.

Contents

Helium and its role for the development of quantum mechanics

Helium: an atomic three-body problem

The **semiclassical theory of the helium atom** (or other two-electron atoms) follows the idea of computing and understanding the quantum energy levels starting from trajectories of the underlying classical system. In helium, the classical dynamics is given by the pair of interacting electrons moving in the field of the (heavy)

nucleus. Two-electron atoms represent a paradigmatic system for the successful application of concepts of quantum chaos theory and in particular the Gutzwiller trace formula.

Helium, as the prototype of a two-electron atom, is composed of the nucleus with charge Z=2 and two electrons, see Figure 1. The interplay between the attractive Coulomb interaction between the nucleus and the electrons and the Coulomb repulsion between the electrons gives rise to exceedingly complicated spectral features, despite the seemingly simple form of the underlying quantum Hamiltonian. Correspondingly, orbits of the two interacting electrons, when considered as classical particles, are predominantly characterized by chaotic dynamics and cannot be calculated analytically. Hence, helium as a microscopic three-body Coulomb system has much in common with its celestial analogue, the gravitational three-body problem.

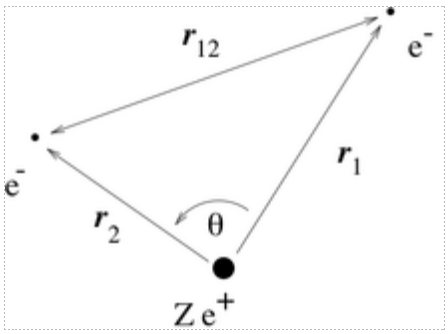

Figure 1: The helium atom composed of two electrons and a nucleus of charge Z=2 (from Tanner et al. 2000)

The failure of the "old quantum theory"

Modern semiclassical theory of the helium atom has its roots in the early days of quantum theory: The observation that atomic spectra consist of discrete lines called for a then novel theoretical approach, a quantum theory for atoms. Bohr's early attempts were formulated in terms of quantum postulates and successfully reproduced the energy levels of hydrogen by requiring periodic (elliptic) Kepler electron motion with quantized radii, respectively momenta p,

$$\oint pdq = nh \qquad (1)$$

(where n is an integer and h Planck's constant). It was natural to try this approach also for helium, the simplest atom with more than one electron. By applying Bohr's ad hoc quantization rule (1) to various periodic orbit configurations of the electron pair motion in helium (see Figure 2), a number of leading physicists of that time, including Bohr, Born, Kramers, Landé , Sommerfeld and van Vleck, tried to compute the ground state energy of helium. However, without success: all models gave unsatisfactory results.

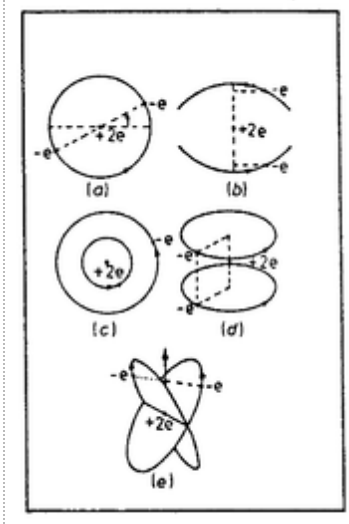

Figure 2: Periodic orbit configurations of the helium electron pair that served as quasi-classical models for the ground state (from Tanner et al. 2000)

Heisenberg, then a student of Sommerfeld, devised a different trajectory configuration with the electrons moving on perturbed Kepler ellipses on different sides of the helium nucleus; in Figure 3 Heisenberg's sketch of this configuration posted in a letter to Sommerfeld in 1922 is shown. Assuming half-integer quantum numbers in his letter, Heisenberg arrived at a helium ionization potential of 24.6 V very close to the observed value of 24.5 V. However, discouraged by Bohr who did not accept such half-integer orbital quantum numbers, Heisenberg never published his results. Though the good agreement must be considered as accidental, the Heisenberg model came closest to an adequate semiclassical description of the helium ground state. Modern semiclassical theory reveals that the association of energy levels with individual periodic orbits in the old quantum theory was too simple-minded. Indeed, for chaotic systems such as the three-body problem helium, it is the entirety of all periodic orbits which conspire to form the energy levels such as beautifully shown in Gutzwiller's trace formula. For a comprehensive account of the developments of the semiclassical theory for helium up to the year 2000, see Tanner et al. 2000.

The problems and failure of (most of) the attempts to quantize the electron pair motion in helium marked the end of the "old quantum theory" which was subsequently replaced by the "new quantum theory": quantum (wave) mechanics which has proven very successful to this day.

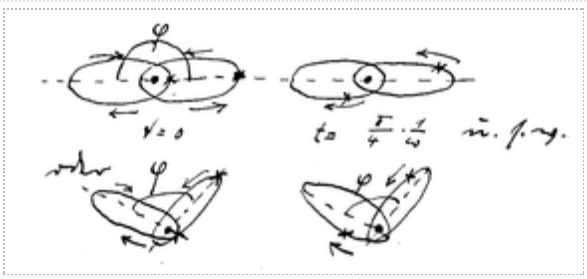

Figure 3: Heisenberg's proposal for Kepler-type electron pair motion in helium (from Tanner et al. 2000)

Spectral properties and quantum-mechanical concepts

By now considerable parts of the rich energy spectrum of the helium atom have been computed quantum mechanically by numerically solving the Schrödinger equation for the two-electron Hamiltonian of helium. To that end, besides the orbital dynamics, the spin degree of freedom of the two electrons has to be considered. The electron spins can be paired antiparallel or parallel leading to the distinction of singlet states (total spin $S = 0$) and triplet states ($S = 1$) often referred to as parahelium and orthohelium, respectively.

Figure 4 depicts, as a representative case, the level diagram of parahelium. The helium states and energy levels can be classified as follows: (i) the ground state and bound singly excited states, (ii) doubly excited resonant states, and (iii) unbound continuum states at energies above the two particle fragmentation threshold that are not considered here. States of category (i) are composed of one electron in a hydrogen-type ground state with quantum number $N = 1$ and the second electron being excited with energy levels (labeled by $n = 1, 2, 3...$) forming a Rydberg series (see Figure 4) converging to the first ionization threshold at an energy of $-Z^2/2$ (in atomic units). In energy region (ii) the doubly excited states have a finite lifetime; they can decay, owing to the mutual repulsive interaction between the electrons, by autoionization where one electron leaves the system while the second one remains bounded to the nucleus. These doubly excited states are organized in doubly infinite level sequences with quantum numbers N and n. As visible in Figure 4, they apparently form individual Rydberg series labeled by the index N, the hydrogen-like principle quantum number of the energetically lower electron. However, closer inspection of the energy region approaching complete fragmentation (i.e. the border to regime (iii)) shows that neighboring Rydberg series perturb each other more and more.

With further increasing energy, these states eventually form a rather dense set of energy levels with seemingly irregular spacings, and the specification of the two-electron states in terms of the quantum numbers (N,n) looses its meaning at such high excitations: At these energies electron-electron interaction gets increasingly important, and hence the concept of quantum numbers (N,n) labeling independent electron states breaks down. The labels (N,n) can be partly replaced by new, though approximate, quantum numbers representing the collective dynamics of the electron pair. However, due to the non-integrability of the three-body Coulomb problem, a clear-cut classification is no longer possible (see Tanner et al. 2000).

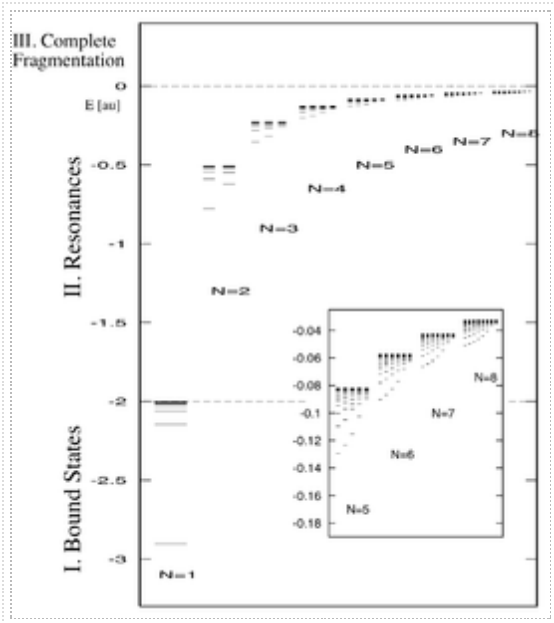

Figure 4: Helium energy level diagram (from Tanner et al. 2000)

The increasing complexity of the energy spectrum close to the helium double ionisation threshold can be experimentally revealed in photo-ionisation measurements. The single photo-ionisation cross section is proportional to the probability of ionising a helium atom by a photon at a given frequency ω. It can be compared directly to experimental data measuring the

electron flux obtained from shining a laser (at sufficiently weak intensity to avoid effects due to multi-photon

ionisation) onto a helium target; a typical photoionisation signal for highly doubly excited helium states is shown in Figure 5 (Jiang et al 2008), exhibiting irregular sequences of peaks from overlapping resonances.

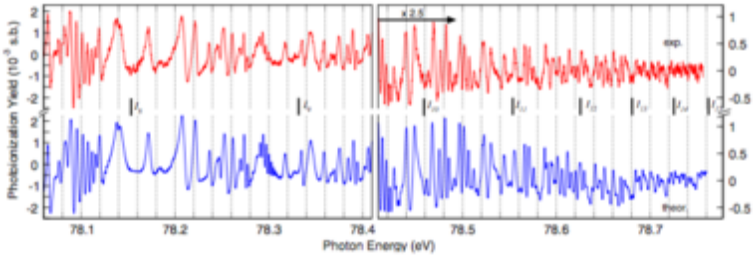

Figure 5: Total photoionisation cross section of helium; Ix refers to the ionisation threshold for the xth Rydberg series (from Jiang et al 2008).

The helium atom - a semiclassical approach

The three-body Coulomb system helium is one of the most complex systems which has been treated fully semiclassically using Gutzwiller's trace formula (Wintgen et al. 1992). The challenge is to describe quantum spectra or photoionisation cross sections of this few particle system in terms of classical trajectories of the nucleus and the two electrons alone. It turns out that the structure of the spectrum is closely linked to features of the underlying classical few-body dynamics such as invariant subspaces in phase space, chaotic or nearly integrable behaviour and the influence of collision events.

The bound and resonance spectrum as depicted in Figure 4 is linked via Gutzwiller's trace formula to the set of all periodic orbits of the system. Furthermore, it can be shown that photoionisation or absorption spectra in atoms are related to a set of returning trajectories, that is, trajectories which start and end at the origin (Du et al. 1988). Note that these orbits are in general only closed in position space and thus not periodic. Interestingly, in helium these are triple-collision orbits, that is, orbits for which both electrons hit the nucleus simultaneously.

A good knowledge of the phase space dynamics is necessary to classify and determine these sets of trajectories.

Classical dynamics

The classical three body system can be reduced to four degrees of freedom (dof) after eliminating the centre of mass motion and incorporating the conservation of the total angular momentum. As the nucleus is about 1800 times heavier than an electron, one can work in the infinite nucleus mass approximation without loosing any essential features. After rescaling and making all quantities dimensionless, one can write the classical Hamiltonian in the form

$$H = \frac{\mathbf{p}_1^2}{2} + \frac{\mathbf{p}_2^2}{2} - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} = \begin{cases} +1 & : \quad E > 0 \\ 0 & : \quad E = 0 \\ -1 & : \quad E < 0 \end{cases} \qquad (2)$$

with nucleus charge $Z = 2$ for helium (Richter et al. 1993). The phase space in Eq. (2) has 6 dof, the dynamics for fixed angular momentum takes place on 4 dof. The $H = +1$ regime corresponds to the region of positive energy where double ionisation is possible. There exist no periodic orbits of the electron pair and one does not find quantum resonance states in this energy regime, see Figure 4. It is the classical dynamics for negative energies, that is H= -1, which shows complex behaviour, chaos, unstable periodic orbits and is linked to the bound and resonance spectrum of helium in Figure 4. Only one electron can escape classically in this energy regime and it will do so for most initial conditions.

Symmetries and invariant subspaces

The equations of motion derived from the Hamiltonian (2) are invariant under the transformation $(\mathbf{r}_1, \mathbf{r}_2) \rightarrow (-\mathbf{r}_1, -\mathbf{r}_2)$, as well as $(\mathbf{r}_1, \mathbf{r}_2) \rightarrow (\mathbf{r}_2, \mathbf{r}_1)$. The symmetries give rise to invariant subspaces in the full phase space. Trajectories which start in such a subspace will remain there for all times thus reducing the relevant degrees of freedom of the dynamics. Invariant subspaces are thus an extremely useful tool to study classical dynamics in a high dimensional phase space. The subspace most important for

a semiclassical treatment is the collinear eZe space where the electrons move along a common axis at different sides of the nucleus, see Figure 6. The dynamics in this space describes the spectrum near the ground state as well as some of the Rydberg series in the energy spectrum, Figure 4. Furthermore, the photoionisation spectrum is dominated by the collinear dynamics. Heisenberg's early success is indeed related to the similarity of his 'periodic orbit' in Figure 3 with the shortest periodic orbit in the eZe space. We will discuss the most important properties of the dynamics in this subspace in more detail below. Other subspaces are, for example, the collinear dynamics of both electrons on the same side of the nucleus giving rise to 'frozen planet states' (Richter et al. 1992) and the so-called Wannier ridge space with $\mathbf{r}_1 = \mathbf{r}_2; \mathbf{p}_1 = \mathbf{p}_2$, which is, however, unstable with respect to perturbations away from the subspace and thus less relevant for the spectrum. It plays an important role as a gate-way for ionisation processes, see Lee et al. 2005, Byun et al. 2007. For a more detailed description of the dynamics in other invariant subspaces, see Tanner et al. 2000 and references therein.

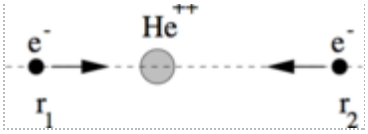

Figure 6: The collinear eZe configuration

Symbolic dynamics in the eZe collinear space

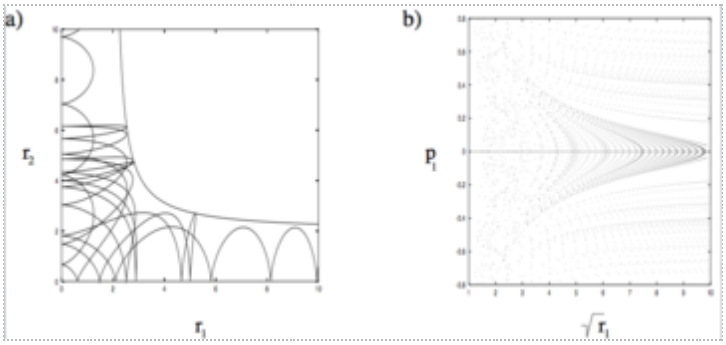

Figure 7 : a) A typical orbit in the eZe - space; b) trajectory in the Poincaré surface of section $r_2 = 0$ (from Tanner et al. 2000)

The dynamics in the eZe collinear space turns out to be fully chaotic with a binary symbolic dynamics. The two degrees of freedom are the distances $r_i, i = 1, 2$ of electron i from the nucleus - a typical trajectory is shown in Figure 7. Note that the axis $r_i = 0$ corresponds to binary collisions, that is, the electron "i" collides with the nucleus - see also the next section for a discussion of collision events. One electron can escape (ionise) to infinity leaving the other electron in a regular Kepler ellipse around the nucleus. Interestingly, escape can only occur after both electron come close to the nucleus simultaneously to allow for momentum transfer between the light particles. The triple collision (discussed below) serves thus as the gateway to electron ionisation. The dynamics is nearly regular having a small, but positive Lyapunov exponent, if the electrons are far apart (that is, $r_1 \gg r_2$ or vice versa), see the Poincaré surface of section in Figure 7b).

The symbolic dynamics for the chaotic eZe - configuration maps each trajectory one-to-one onto a binary symbol string. The symbols are defined through binary collisions, that is,

- 1 if a trajectory crosses the line $r_1 = r_2$ between two collisions with the nucleus, (i.e. $r_1 = 0$ or $r_2 = 0$);
- 0 otherwise.

Note that the symbolic dynamics is closely related to the triple collision, that is, the boundaries of the partition are given by trajectories starting in or ending at the singular point $r_1 = r_2 = 0$ (triple collision manifolds).

The symbolic dynamics fully describes the topological properties of the phase space; periodic orbits, for example, can be characterised by a periodic symbol string $\overline{a} = \ldots aaaa \ldots$ where a is a finite binary symbol string. There are infinitely many periodic orbits and they are all unstable with respect to the dynamics "in" the collinear plane. Some examples are shown in Figure 8. The number of periodic orbits increases exponentially with the code length and thus with the period of the orbits. The 'asymmetric stretch' orbit $\overline{1}$ is the shortest orbit in this subspace. The asymptotic periodic orbit $r_1 \equiv \infty, p_1 \equiv 0$ corresponds to the notation $\overline{0}$ in the binary code.

Collisions, regularisation and the triple collision

Collisions are an important feature in few-body

dynamics as described above. There is in particular a fundamental difference between two-body (or binary) collisions and many-body collisions where more than two particles collide simultaneously. Binary collisions can be regularised, that is, the dynamics can be continued through the singularity after a suitable transformation of the time and space variables. A popular regularisation scheme is the Kustaanheimo-Stiefel transformation which preserves the Hamiltonian structure of the equations. Binary collisions do not add instability to the classical dynamics.

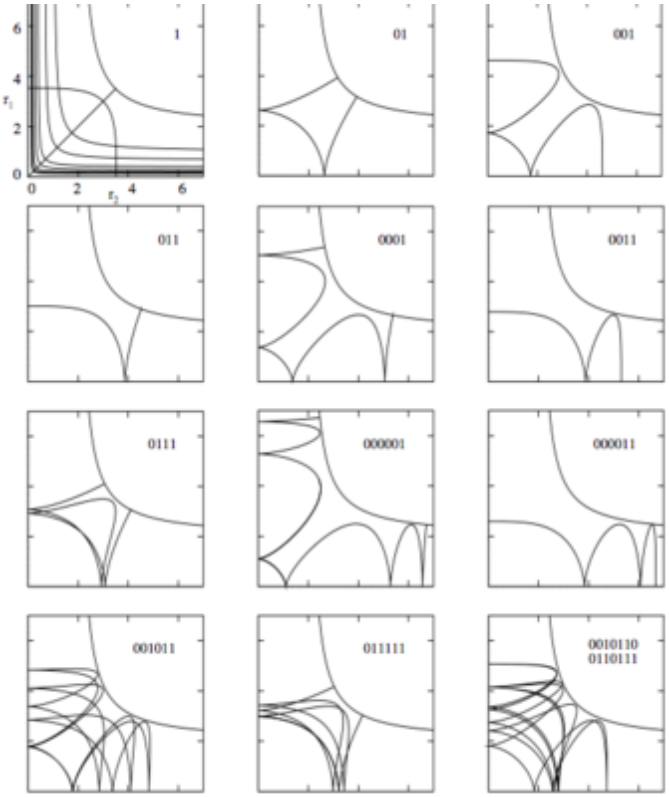

Figure 8: Representative periodic orbits of the helium electron pair in the eZe - space (from Wintgen et al. 1992)

This is in contrast to triple collisions where both electrons hit the nucleus simultaneously. The triple collision is a non-regularisable singularity, that is, there is no unique way to determine the fate of a trajectory after it has encountered a triple collision. The manifold of all orbits coming out of or going into a triple collisions - the so-called triple collision manifold (Waldvogel 2002) - plays an important role in tessellating the full phase space and provides the symbolic dynamics in the eZe space. Triple collision orbits always move along the so-called Wannier orbit $r_1 = r_2$|when encountering the singularity. The triple collision singularity thus acts as an infinitely unstable fixed point; a closer analysis shows that the singularity itself has a non-trivial structure and topology which can be illuminated using McGehee transformation techniques.

For a discussion of the Kustaanheimo-Stiefel and McGehee transformations in the context of three body Coulomb problems, see Richter et al. 1993 and Lee et al. 2005, respectively.

Semiclassical periodic orbit quantisation

The Gutzwiller trace formula marked a milestone in the development of semiclassical theories. It relates the spectrum of a quantum system to the set of all periodic orbits of the corresponding classical system in terms of a Fourier-type relation where the eigenenergies and the actions of the classical periodic orbits act as Fourier-pairs. The classical dynamics of the eZe collinear configuration can be used for a quantisation of an important part of the helium spectrum due to a 'lucky' coincidence: It turns out that the electron motion in the vicinity of the collinear space is stable in all degrees of freedom perpendicular to the eZe space. The electrons carry out a regular bending-type vibration while performing chaotic motion in the collinear degrees of freedom. This makes it possible to use the periodic orbits of the eZe configuration for a semiclassical description of parts of the spectrum for angular momentum L=0 including the ground state. The existence of this connection can be shown by Fourier methods. By inverting the Gutzwiller trace formula using Fourier

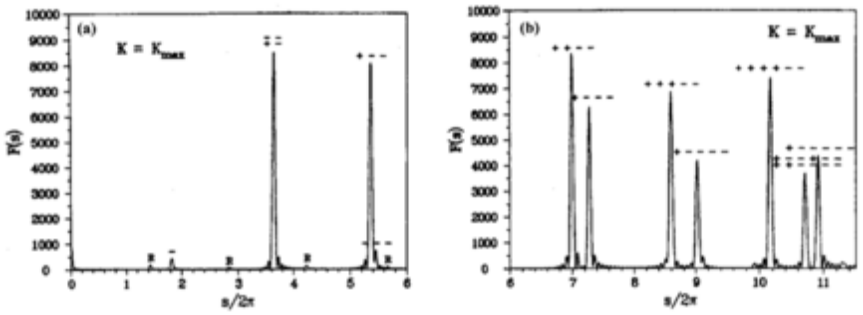

Figure 9: The Fourier transformed part of the spectrum associated with the eZe space (here denoted K_{max}|) - the binary code (+,-) refers to the code (0,1) introduced above (from Qiu et al. 1996)

connection can be shown by Fourier methods. By inverting the Gutzwiller trace formula using Fourier transformation, one obtains an *action spectrum* related to the full quantum energy spectrum as shown in Figure 9 (Qui et al. 1996). The energy scaling relation for the classical actions

$$S_{po} = \frac{1}{\sqrt{|E|}} \tilde{S}_{po}, \tag{3}$$

has been used here, where $\tilde{S}_{po}$ is the action of a periodic orbit (po) at fixed energy $E = -1$, see (2). The quantum spectrum used in Figure 9 has been obtained from full 3D numerical calculations (Bürgers et al. 1995) and semi-empirical formulas based on approximate quantum numbers. (For more details on approximate quantum numbers, see Tanner et al. 2000).

Each of the peaks in Figure 9 can be identified with a periodic orbit of the classical two-electron dynamics; furthermore all these periodic orbits lie in the eZe space confirming the statement that large parts of the quantum spectrum are determined by this invariant lower dimensional subspace - a truly amazing result. At last the periodic orbits Niels Bohr was looking for have been found and they are quite close to the solution proposed by Heisenberg which he himself did not dare to publish! For a full blown semiclassical quantisation, one needs information of as many periodic orbits as possible - these can be obtained systematically using the symbolic dynamics in the eZe space. The most extensive semiclassical calculations so far made use of all periodic orbits up to length 16 ($2^{16} = 65536$ orbits) together with cycle expansion techniques to obtain energies as listed in Tab 9 (Wintgen et al. 1992). Pushing the semiclassical calculation to even higher energies is hampered by the exponential increase of the number of periodic orbits with increasing (symbol) length in chaotic systems - a general obstacle for semiclassical quantisation techniques.

N	n	$j=1$	$j=4$	$j=8$	$j=12$	$j=16$	$-E_{qm}$
1	1	3.0970	2.9692	2.9001	2.9390	2.9248	2.9037
2	2	0.8044	0.7714	0.7744	0.7730	0.7727	0.7779
2	3		0.5698	0.5906	0.5916	0.5902	0.5899
2	4				0.5383	0.5429	0.5449
3	3	0.3622	0.3472	0.3543	0.3535	0.3503	0.3535
3	4			0.2812	0.2808	0.2808	0.2811
3	5			0.2550	0.2561	0.2559	0.2560
3	6				0.2416	0.2433	0.2438
4	4	0.2050	0.1962	0.1980	0.2004	0.2012	0.2010
4	5		0.1655	0.1650	0.1654	0.1657	0.1657
4	6			0.1508	0.1505	0.1507	0.1508
4	7			0.1413	0.1426	0.1426	0.1426

Figure 10: Quantum eigenvalues obtained from cycle expansion techniques using periodic orbits up to length j; the exact quantum results are given in the last column (in atomic units), from Wintgen et al. (1992).

Photoionisation cross sections

Information about atomic spectra is often experimentally obtained through measurements of the photo excitation or ionisation, see Figure 5 for helium. An expression for the photo-ionisation cross section can be written in terms of the retarded Green function *G(E)* of the full three particle problem, that is,

$$\sigma(E) = -\frac{4\pi}{c}\, \omega\, \Im\langle D\phi_0 | G(E) | D\phi_0 \rangle \tag{4}$$

where c is the speed of light, ϕ_0 is the initial state wave function and $D = \mathbf{\Pi} \cdot (\mathbf{r}_1 + \mathbf{r}_2)$ is the dipole operator with $\mathbf{\Pi}$, the polarization of the incoming photon. Using again Gutzwiller's expression for the Green function in terms of classical trajectories, one can relate the cross section to classical trajectories of the three-body dynamics.

Semiclassical methods are particularly useful when considering the cross section in the limit $E \to 0$, that is, at the double ionisation threshold. Especially the regime just below the threshold with $E < 0$ is not accessible both to experiments and to fully numerical calculations due to the large density of resonances. Using a semiclassical closed orbit theory together with a semiclassical treatment of triple collision orbits, one can make detailed predictions here; in particular, the cross section can be written in the form (Byun et al 2007, Lee et al 2010)

here, in particular, the cross section can be written in the form (Byun et al. 2007; Lee et al. 2010)

$$\sigma(E) \approx \sigma_0 + \frac{8\pi^2\omega}{c} |E|^{\mu} \Re\left[2\pi i \sum_{\mathrm{CTCO}_\gamma} a_\gamma e^{i\tilde{S}_\gamma/\sqrt{E}-i\pi\nu_\gamma/2}\right], \quad (5)$$

where σ_0 gives a smooth background contribution and the sum is taken over all *closed triple collision orbits* (CTCO), that is, trajectories which start and end in the triple collision. It can be shown that CTCOs are part of the eZe sub-space. Furthermore, $\tilde{S}$ is the classical action at energy $E = -1$ as given in (3) and a_γ is an energy independent coefficient related to the stability of a given CTCO away from the triple collision. Most remarkably is the energy scaling due to the exponent μ, (for details see Lee et al. 2010),

$$\mu = \mu_{eZe} + 2\mu_{wr} = \frac{1}{4}\left[\sqrt{\frac{100Z-9}{4Z-1}} + 2\sqrt{\frac{4Z-9}{4Z-1}}\right], \quad (6)$$

which can be obtained through a stability analysis of the triple collision itself. Here, wr relates to a contribution from the so-called *Wannier Ridge* dynamics, an invariant subspace of the full dynamics where the two electrons are always at the same distance from the nucleus. The exponents are related to Siegel exponents (see Waldvogel 2002) or Wannier exponents (Wannier 1953). The energy scaling describes the decay of the fluctuations in the photoionisation cross section towards the threshold as can be seen in Figure 5.

The CTCOs can in fact be seen in cross section data using a Fourier transformation of Eqn. (5). The data shown in Figure 11 are obtained from a 1D eZe cross section calculations (Byun et al. 2007) and show a nice one-to-one correspondence between peaks and triple collision trajectories.

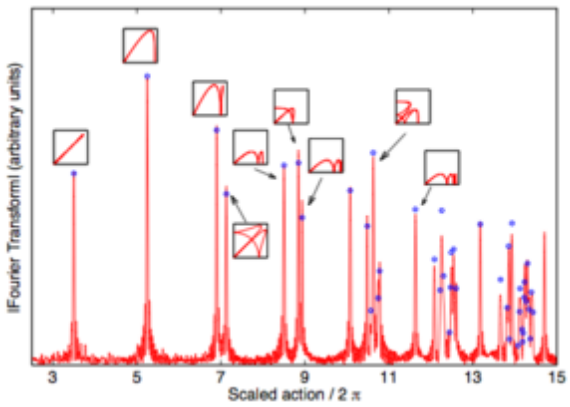

Figure 11: Fourier transform of cross section data; the peaks can be related to the CTCOs depicted in the insets (from Byun et al. 2007).

Experimental and numerical studies confirm that the dominant contribution to the cross section signal is given by the collinear eZe dynamics (Jiang et al. 2008) as predicted by the semiclassical analysis.

Recent developments and open questions

Exploring the full phase space - approximate symmetries and global structures

Helium has provided a prime example where experimental and numerical results of the *quantum* 3-body problem give clear hints about interesting structures in the phase space of the classical dynamics. However, the story is not finished yet - at the time of writing (2013), large areas of the full 7 dimensional classical phase space are unexplored and the connection between *approximate* quantum numbers (Herrick's quantum numbers - see Lee et al. 2005, Sano 2010) is still unclear. This also opens up interesting links to celestial mechanics and triple collision encounters in three-body gravitational problems as discussed at the workshops on Few Body Dynamics in Atoms, Molecules and Planetary Systems (http://www.pks.mpg.de/~fbd10/) in Dresden in 2010 and Celestial, Molecular, and Atomic Dynamics (CEMAD) (http://www.pims.math.ca/scientific-event/130729-cmad2) in Victoria in 2013.

Highly doubly excited states - recent advances

The world record of experimentally accessing and numerically calculating highly doubly excited states in helium is currently held (in 2013) by Jiang et al. 2008 for total cross sections reaching helium resonances up to the ionisation thresholds N=17 and Czasch et al. 2005 for partial cross sections reaching N=13. Going even higher in the spectrum or considering helium under electromagnetic driving (Madronero et al. (2008)) is a formidable challenge asking for new numerical techniques to deal with the large basis sets necessary and experimental techniques to reach the resolutions required. Unusually for atomic physicists, the rewards may lie in looking at the Fourier transforms of their data.

Double ionisation of helium for strong laser fields and ultra-short pulses - probing correlated electron-electron dynamics

Studying double ionisation (DI) of helium by looking at the classical dynamics of the two electrons as they escape form the nucleus has a long history: Already in 1953, Wannier predicted an unexpected energy scaling of the DI cross section near the threshold governed by exponents similar to those found in Eq.(6). Interesting recent effects being considered are electron-electron correlation effects in strong laser fields and in attosecond pulses. In the strong field case, rescattering can lead to a large contribution to the DI cross section from ionisation events where both electrons escape from the nucleus along the same direction (Prauzner-Bechcicki et al. 2007). Two-photon DI in ultra-short pulses, on the other hand, shows a preference for back-to-back electron escape due to electron-electron repulsion (Feist et al. 2009). These and many other scenarios can be studied using classical electron dynamics.

Semiclassics for many-body problems

While helium represents a prime example for the success of semiclassics for an interacting few body system, generalizations to other many-body problems remain as a future challenge.

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Reviewed by (http://www.scholarpedia.org/w/index.php?title=Semiclassical_theory_of_helium_atom&oldid=132323) : Bertrand Georgeot, Laboratoire de Physique Theorique, CNRS, Universite Paul Sabatier, Toulouse

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Accepted on: 2013-04-03 11:20:55 GMT (http://www.scholarpedia.org/w/index.php?title=Semiclassical_theory_of_helium_atom&oldid=132323)

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