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Periodic orbit theory of broad resonances in two-dimensional hydrogenic Stark effect

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Abstract. The modified version of periodic orbit theory, developed by Robbins for systems which possess discrete symmetries, is used to calculate parameters of broad resonances in the case of two-dimensional hydrogenic Stark effect at energies above the zero field ionization threshold. It is shown that the contribution of single periodic orbits of the system give results that coincide with those of the comparison equation method, also presented in the paper.

1. Introduction

A general theory which, at least in principle, provides a semiclassical description of any system, be it integrable or chaotic in the classical limit, is the periodic orbit theory developed by Gutzwiller (1971) (see also Balian and Bloch (1970), Berry and Tabor (1976), (1977)). In this theory, the so-called oscillatory part of the semiclassical density of states $d^{osc}(E)$ (or response function—trace of Green function $g^{osc}(E)$) is represented as a sum over all periodic orbits of the system (of its classical counterpart). The semiclassical approximations of energy eigenvalues then correspond to poles of, e.g. g(E), on the negative real axis. For integrable systems, the periodic orbit theory has been shown to be equivalent to the standard tori quantization (Berry and Tabor 1976, 1977). On the other hand, for chaotic non-integrable systems, it is often very difficult to extract eigenvalues in this way. The main reason is the exponential proliferation of periodic orbits with long periods. Nevertheless, considerable advances have been made in recent application of periodic orbit theory to calculation of quantum resonances for the classically chaotic three-disc scattering problem (Cvitanović and Eckhardt 1989).

In the present paper we shall use periodic orbit theory (section 2) to calculate parameters of broad resonances in the case of two-dimensional hydrogen atom in uniform electric field at energies above the zero-field ionization threshold (E > 0). At these energies the system allows only one periodic orbit and the periodic orbit 'sum' can easily be calculated. The resonances we shall identify with poles of the response function in complex energy plane. Results thus obtained completely agree with those of the improved WKB (comparison equation) method presented in section 3.

Apart from showing efficiency of periodic orbit theory (of its modified version for systems with discrete symmetry developed by Robbins (1989)) in calculating resonances, our example reveals another important aspect of the theory. It emphasizes that in periodic orbit sum contributions essentially give not periodic orbits themselves, but rather certain manifolds of loops in configuration space having given periodic orbits as a limit. It may happen, as in the present case, that to a single periodic orbit belong more than one manifold of the loops; consequently this orbit gives more than one term in the periodic orbit sum.

Concluding this introduction we note that the theoretical interest in broad resonances arised from their detection in photoionization experiments of rubidium (Freeman *et al* 1978) and hydrogen (Glab *et al* 1985, Rotke and Welge 1986) atoms in electric fields. Many authors have discussed the relation of the single periodic orbit (along field direction) in (three-dimensional) hydrogenic Stark effect with either the oscillations in photoionization spectra near threshold (Bogomolny 1988, Wintgen 1989) or broad resonances i.e. complex poles of *S*-matrix (Kazansky *et al* 1990). However, direct application of the periodic orbit theory to the three-dimensional case is more complicated—apart from separate quantization of the projection of angular momentum onto the field axis, it needs the introduction of complex orbits in the theory. This problem will be addressed in a future publication.

2. Application of periodic orbit theory

The Hamiltonian function of the two-dimensional hydrogen atom in a uniform electric field F reads (throughout this work we set electron mass and charge $m_e = 1$, |e| = 1):

$$H = \frac{1}{2}p_x^2 + \frac{1}{2}p_y^2 - (x^2 + y^2)^{-1/2} + Fx.$$
(1)

The system has simple discrete symmetry: the Hamiltonian function (1) is invariant under reflections through x-axis, $y \rightarrow -y$, i.e. under canonical transformation $(x, p_x, y, p_y) \rightarrow (x, p_x, -y, -p_y)$. Also, as is well known, the system is separable in semiparabolic coordinates:

$$y = uv$$
 $x = (u^2 - v^2)/2$ (2)

in which the Hamiltonian function takes the form

$$H = \frac{1}{u^2 + v^2} \left(\frac{p_u^2}{2} + \frac{p_v^2}{2} \right) - \frac{2}{u^2 + v^2} + F \frac{u^2 - v^2}{2}.$$
 (3)

To make the mapping between u-v and x-y planes (and corresponding phase spaces) one-to-one, we identify the following pairs of points in u-v plane and (u, p_u, v, p_v) phase space:

$$(u, v) = (-u, -v) \qquad (u, p_u, v, p_v) = (-u, -p_u, -v, -p_v).$$
(4)

We see that in semiparabolic coordinates, the reflection through x-axis is formally represented by two mappings, $(u, v) \rightarrow (-u, v)$ and $(u, v) \rightarrow (u, -v)$, but, due to identification (4), they are effectively the same transformation.

We wish to calculate response function g(E) (i.e. trace of Green function) of our system at energies E > 0 using periodic orbit theory. We use the variant of the theory appropriate for systems with discrete symmetries developed by Robbins (1989). His main result for the so-called oscillatory part of symmetry-projected semiclassical response function reads:

$$g_m^{sc}(E) = \frac{d_m}{i\hbar} \sum_l \frac{\bar{T}_l}{|K_l|} \sum_{n=1}^{\infty} \chi_m(g_l^n) \frac{\exp[in(\bar{S}_l(E)/\hbar - \bar{\mu}_l \pi/2)]}{|\bar{A}_l^n - I|^{1/2}}.$$
 (5)

Here, χ_m designates the character of the *m*th irreducible representation (with dimension d_m) of the given discrete symmetry group. The *l* sum is taken over primitive periodic

orbits (i.e. single traversals of periodic orbits) of the system, but in the reduced phase space, while the sum over *n* accounts for iterations of the primitive orbit (for the definition of the reduced phase space we refer readers to Robbins article (1989)). \overline{T}_i is the period, \overline{S}_i is the action of the *l*th primitive orbit, \overline{A}_i is a matrix which represents the Poincare surface-of-section map linearized around the *l*th orbit; all these quantities are defined on reduced phase space. The group element g_i depends on the relation between *l*th primitive orbit in full phase space and its projection on reduced phase space (see Robbins 1989). $\overline{\mu}_i$ is an integer related to the number of caustics crossed by the orbit and finally, $|K_i|$ is the order of the subgroup K_i of the symmetry group which leaves each point of the *l*th orbit (in full phase space) invariant.

To apply equation (5) to our system we have to define reduced phase space, irreducible representation of symmetry group and find periodic orbits. Our group consists of identity element I and reflection R of x-y plane through x-axis, and of course $R^2 = I$. It has two irreducible one-dimensional representations: one is isomorphic to the group itself, we shall designate it by – (because in space of wavefunctions, states with odd parity transform according to this representation) and the other representation has only identity element and we designate it by + (because wavefunctions with even parity transform according to this representation). We have:

$$d_{-} = d_{+} = 1$$
 $\chi_{-}(I) = 1$ $\chi_{-}(R) = -1$ $\chi_{+}(I) = \chi_{+}(R) = 1.$ (6)

Reduced phase space we simply define by giving the corresponding reduced configuration space (see Robbins 1989) which is represented by, e.g., upper half of x-y plane with x-axis as boundary. In u, v coordinates, reduced configurational space is given by region u > 0, v > 0 with positive u and v half-axes as boundaries.

To find periodic orbits (in reduced phase space) corresponding to Hamiltonian function (3) we have to solve corresponding equations of motion. After introducing new time-like variable τ with $d\tau = dt/(u^2 + v^2)$, it can be easily shown that equations of motion corresponding to Hamiltonian function (3) at energy E > 0 and in time t are equivalent to equations of motion in time τ of two separated one-dimensional systems with the following Hamiltonian functions:

$$H_{1} = \frac{p_{u}^{2}}{2} - Eu^{2} + \frac{F}{2}u^{4} = 2\beta$$
(7*a*)

$$H_2 = \frac{p_v^2}{2} - Ev^2 - \frac{F}{2}v^4 = 2(1 - \beta)$$
(7b)

where β is a separation constant. We see that the motion in u, p_u variables is bounded and the action and period (in reduced space u > 0 and in time τ) of that motion are given by:

$$S(E,\beta) = \oint p_u \, \mathrm{d}u = 2 \int_0^{u_r} (2Eu^2 + 4\beta - Fu^4)^{1/2} \, \mathrm{d}u \tag{8a}$$

$$T(E,\beta) = \oint du/p_u = 2 \int_0^{u_r} (2Eu^2 + 4\beta - Fu^4)^{-1/2} du$$
 (8b)

where $u_i > 0$ is the turning point—the zero of the first integrand. The motion in variables v, p_v is unbounded so that Hamiltonian function (3) allows only one periodic orbit which corresponds to a unique fixed point of Hamiltonian (7b), for which:

$$v_{\rm c} = 0$$
 $p_{\rm c} = 0$ $\beta_{\rm c} = 1.$ (9)

In u-v plane this orbit lies on u-axis. Similarly in x-y plane orbit lies on positive x-axis and it is invariant under reflections through x-axis, hence:

$$|K_{\rm c}| = 2.$$
 (10)

In order to investigate stability of the fixed point (9) we expand Hamiltonian function (7b) in its vicinity by introducing variables $\delta p = p_v - p_c$, $\delta v = v - v_c$, and obtain for the quadratic part:

$$\delta^2 H_2 = (\delta p^2)/2 + \omega_c^2 (\delta v)^2/2 \qquad \omega_c^2 = -2E.$$
(11)

We see that the fixed point is unstable and hyperbolic. Therefore the Hamiltonian function (1) allows only one periodic orbit at positive energies, which is unstable, lies on positive x-axis and whose action S_c , period T_c and instability angle w_c are given by:

$$S_{\rm c}(E) = 2 \int_0^{u_{\rm c}} (2Eu^2 + 4 - Fu^4)^{1/2} \, \mathrm{d}u \qquad T_{\rm c}(E) = 2 \int_0^{u_{\rm c}} (2Eu^2 + 4 - Fu^4)^{-1/2} \, \mathrm{d}u \qquad (12a)$$

$$w_{\rm c}(E) = T_{\rm c}\sqrt{2E}$$
 $u_{\rm c}^2 = E/F + (E^2/F^2 + 4/F)^{1/2}.$ (12b)

It seems that in our case the l sum in equation (5) consists of only one term corresponding to the unique periodic orbit of the system. But apart from the fact that our periodic orbit lies on the border of the reduced phase space (because of this the calculation of g_i and denominator in equation (5) is not trivial), there is another reason preventing the straightforward application of equation (5). We recall that in Gutzwiller theory periodic orbits arise when the stationary phase method is used to calculate the trace of semiclassical approximation of the Green function, whose diagonal element G(q, q; E) is represented as sum over loops in configuration space (loops are trajectories that start and end at the same point of configuration space). Then, there is the assumption that to each isolated periodic orbit corresponds a unique manifold of loops lying close to that orbit and having it as the limit. However, the analysis of classical motion shows that to our periodic orbit belong two topologically distinct manifolds of loops: one has $\beta < 1$ and the other $\beta > 1$, while as we know for periodic orbit $\beta = 1$. Both manifolds give their own contribution to the periodic orbit sum (5) and both correspond to our periodic orbit which is, in a sense, degenerated. In other words, when applying equation (5), it is necessary to calculate quantities $(S_l, g_l, A_l...)$ that actually correspond to loops infinitesimally close to periodic orbit. The representatives of these two manifolds of loops in reduced u-v space and corresponding trajectories in full x-y configurational space are sketched in figures 1 and 2. We see that there is only one, but very important, difference between them: all loops with $\beta < 1$ reflect once from the u-axis while loops with $\beta > 1$ never reach the u-axis. These reflections from u- and v-axes are essential because these axes are at the same time boundaries of the reduced configurational space and the symmetry axes.

An account of all topologically different loops follows: for each integer *n* there are two manifolds of loops with action and period infinitesimally close to nS_c and nT_c . Any loop from the first manifold has $\beta < 1$ and reflects *n* times from the *v* axis and once from *u* axis, while loops with $\beta > 1$ also reflect *n* times from *v* axis and do not reflect from *u* axis. Two manifolds of loops give different results only for elements g_c and matrix $\overline{A_c}$ of equation (5) while in both cases

$$\tilde{\mu}_{c} = 1 \tag{13}$$



Figure 1. (a) and (b) represent loops with $\beta < 1$ in reduced u-v configurational space. The loop given in (a) is close to one traversal of periodic orbit (which lies along the u-axis) while the loop in (b) corresponds to two traversals of periodic orbit. Both loops reflect once from u-axis. Corresponding trajectories in the full x-y plane are given in (c) and (d). Here both trajectories cross once positive x-axis. We see, as shown in figure (d), that loop (or periodic orbit) in reduced space does not necessarily correspond to loop (or periodic orbit) in full space. Actually, starting and ending points of trajectory in full space coincide up to the symmetry transformation (see Robbins 1989).

(in our case $\bar{\mu}_c$ simply reduces to the number of turning points of *u*-motion traversed during one period T_c). It is obvious that matrix $\bar{A}^n_>$ corresponding to loops with $\beta > 1$ has for eigenvalues $\exp(nw_c)$ and $\exp(-nw_c)$ hence

$$|\bar{A}_{>}^{n} - I|^{1/2} = 2\sinh(nw_{c}/2) \tag{14a}$$

while because of the reflection from *u*-axis matrix $\bar{A}_{<}^{n}$ belonging to loops with $\beta < 1$ has for eigenvalues $-\exp(nw_{c})$ and $-\exp(-nw_{c})$ hence

$$|\bar{A}_{<}^{n} - I|^{1/2} = 2\cosh(nw_{c}/2).$$
(14b)

Now we explain how to calculate the group element g_i of equation (5) corresponding to a given trajectory in reduced space of our case. It represents the ordered product of group elements belonging to the given trajectory. We say that a group element belongs to the trajectory if it represents reflection through axis which is boundary of reduced space and from which the trajectory reflects. In our case, if trajectory reflects from u and v axes s times then the corresponding group element is \mathbb{R}^{s} . Therefore:

$$g_{>}^{n} = \mathbf{R}^{n} \qquad g_{<}^{n} = \mathbf{R}^{n+1}.$$
 (15)

Now, we can calculate two symmetry projected response functions $g_{+}^{sc}(E)$ and $g_{-}^{sc}(E)$



Figure 2. Same as figure 1 but for loops with $\beta > 1$. Here, in (a) and (b) trajectories never reach the u axis in reduced u-v space, or, in (c) and (d), never cross the positive x-axis in the x-y plane.

of our system. Using equations (6), (10), (12)-(15) in equation (5) one obtains:

$$g_{+}^{sc}(E) = \frac{T_{c}(E)}{2i\hbar} \sum_{n=1}^{\infty} \left(\frac{\exp[in(S_{c}(E)/\hbar - \pi/2)]}{2\sinh(nw_{c}(E)/2)} + \frac{\exp[in(S_{c}(E)/\hbar - \pi/2)]}{2\cosh(nw_{c}(E)/2)} \right)$$
(16a)

$$g_{-}^{sc}(E) = \frac{T_{c}(E)}{2i\hbar} \sum_{n=1}^{\infty} \left((-1)^{n} \frac{\exp[in(S_{c}(E)/\hbar - \pi/2)]}{2\sinh(nw_{c}(E)/2)} + (-1)^{n+1} \frac{\exp[in(S_{c}(E)/\hbar - \pi/2)]}{2\cosh(nw_{c}(E)/2)} \right).$$
(16b)

Expanding the functions in denominators according to formulae:

$$[2\sinh(x/2)]^{-1} = \sum_{k=0}^{\infty} \exp[-(k+1/2)x]$$
(17*a*)

$$[2\cosh(x/2)]^{-1} = \sum_{k=0}^{\infty} (-1)^k \exp[-(k+1/2)x]$$
(17b)

then changing formally the order of sums in n and k and finally summing up geometric series in index n, one obtains:

$$g_{\pm}^{\rm sc}(E) \sim \frac{T_{\rm c}}{\mathrm{i}\hbar} \sum_{k=0}^{\infty} \frac{\exp(\mathrm{i}\theta_k^{\pm})}{1 - \exp(\mathrm{i}\theta_k^{\pm})}$$
(18*a*)

$$\theta_k^+ = S_c/\hbar - \pi/2 + i(2k+1/2)w_c \qquad \theta_k^- = S_c/\hbar - 3\pi/2 + i(2k+3/2)w_c. \qquad (18b)$$

From the last equation we immediately see that response functions $g_{\pm}(E)$ have poles in complex plane whenever $\theta_k^{\pm} = 2s\pi$, s, $k = 0, 1, 2, \ldots$ Therefore for resonances with even parity we have the condition:

$$S_{c}(E) = (2s+1/2)\pi\hbar - i\hbar(2k+1/2)w_{c}(E) \qquad s, k = 0, 1, 2, \dots$$
(19a)

while for resonances with odd parity we have:

$$S_{c}(E) = (2s+3/2)\pi\hbar - i\hbar(2k+3/2)w_{c}(E) \qquad s, k = 0, 1, 2, \dots$$
(19b)

3. Comparison equation method

In this section we shall identify broad resonances with complex values of energy for which the Schrödinger equation has solutions in the form of the 'outgoing waves' in $\pm v$ directions (see Grozdanov *et al* 1988). To Hamiltonian function (3) corresponds the following Schrödinger equation:

$$\left(\frac{\hbar^2}{2(u^2+v^2)}\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right)+\frac{2}{u^2+v^2}-F\frac{u^2-v^2}{2}+E\right)\Psi(u,v)=0.$$
 (20)

We allow variables u and v to take all positive and negative values, but because of identification (4) of points in configurational space we impose the following condition on the wavefunction Ψ :

$$\Psi(u, v) = \Psi(-u, -v). \tag{21}$$

The assumption that Φ has the form $\Psi(u, v) = \psi_1(u)\psi_2(v)$ permits separation into two ordinary differential equations:

$$\hbar^2 \frac{d^2 \psi_1}{du^2} + (2Eu^2 - Fu^4 + 4\beta)\psi_1 = 0$$
(22a)

$$\hbar^2 \frac{d^2 \psi_2}{dv^2} + (2Ev^2 + Fv^4 + 4(1 - \beta))\psi_2 = 0.$$
(22b)

The last two equations we shall solve using the comparison equation method. Before doing it we note that according to the preceding section we expect that resonances at energies E > 0 are related to the periodic orbit which lies along x-axis and has $\beta = 1$. Therefore we seek solutions of equations (22*a*, *b*) for which

$$\beta = 1 + \gamma \hbar \qquad \gamma = O(1). \tag{23}$$

For comparison equations we take the following:

$$\hbar^2 \frac{d^2 \phi_1}{dz^2} + (\mu - z^2) \phi_1 = 0$$
(24a)

$$\hbar^2 \frac{d^2 \phi_2}{dw^2} + (\hbar \nu + w^2) \phi_2 = 0.$$
(24b)

As is well known linearly independent solutions of last two equations are given respectively by:

$$\phi_1^{\pm}(z) = D_{(\mu/\hbar - 1)/2}(\pm \sqrt{2}z/\sqrt{\hbar})$$
(25a)

$$\phi_2^{\pm}(w) = D_{(\pm i\nu - 1)/2}(\sqrt{2}w \ e^{\pm i\pi/4}/\sqrt{\hbar})$$
(25b)

where D is parabolic cylinder function (see Abramowitz and Stegun 1970). Now we seek the solutions of equations (22*a*, *b*) in the form

$$\psi_1^{\pm}(u) = (z'(u))^{-1/2} \phi_1^{\pm}(z(u)) \tag{26a}$$

$$\psi_2^{\pm}(v) = (w'(v))^{-1/2} \phi_2^{\pm}(w(v))$$
(26b)

with the expansions

$$z(u) = z_0(u) + \hbar z_1(u) + \dots \qquad \mu = \mu_0 + \hbar \mu_1 + \dots \qquad (27a)$$

$$v(v) = w_0(v) + \hbar w_1(v) + \dots \qquad v = v_0 + \hbar v_1 + \dots \qquad (27b)$$

For $z_0(u)$ we obtain the standard equation:

$$\int_{0}^{z_{0}} (\mu_{0} - s^{2})^{1/2} ds = \int_{0}^{u} (2Et^{2} - Ft^{4} + 4\beta)^{1/2} dt$$
(28a)

while the condition of continuity of $z'_0(u)$ on real axis gives:

$$\int_{0}^{\sqrt{\mu_{0}}} (\mu_{0} - s^{2})^{1/2} ds = \mu_{0} \pi/4 = \int_{0}^{u_{1}} (2Eu^{2} - Fu^{4} + 4\beta)^{1/2} du$$
(28b)

$$u_t^2 = E/F + (E^2/F^2 + 4\beta/F)^{1/2}.$$
 (28c)

On the other hand for $w_0(v)$ we obtain:

$$w_0(v) = \operatorname{sgn}(v) \left[2 \int_0^{|v|} (2Et^2 + Ft^4)^{1/2} \, \mathrm{d}t \right]^{1/2}$$
(29*a*)

while the condition of continuity of $w_1(v)$ on real axis gives:

$$\nu_0 = \frac{4(1-\beta)}{\hbar\sqrt{2E}}.$$
(29b)

Now using the asymptotic behaviour for large argument of function D (Abramowitz and Stegun 1970) one finds that the condition for functions $\phi_1^{\pm}(z)$ to be quadratically integrable reads:

$$\mu_0/\hbar - 1 = 2n_1$$
 $n_1 = 0, 1, 2, ...$ (30*a*)

or, from (28b)

$$2\int_{0}^{u_{t}} (2Eu^{2} - Fu^{4} + 4\beta)^{1/2} dt = (n_{1} + 1/2)\pi\hbar \qquad n_{1} = 0, 1, 2, \dots$$
(30b)

and in that case for the wavefunctions $\psi_1^{\pm}(u)$ we obtain, up to the first order in \hbar :

$$\psi_{1n_1}^{\pm}(u) = (z_0'(u))^{-1/2} D_{n_1}(\pm \sqrt{2} z_0(u) / \sqrt{\hbar}).$$
(31a)

From the last and equation (28a) we have equalities

$$\psi_{1n_1}^+(u) = (-1)^{n_1} \psi_{1n_1}^-(u) \qquad \qquad \psi_{1n_1}^+(-u) = (-1)^{n_1} \psi_{1n_1}^+(u). \tag{31b}$$

Again using the asymptotic behaviour for large argument of function D one finds that the condition for functions $\phi_2^+(w)$ to represent an outgoing wave reads

$$i\nu_0 - 1 = 2n_2$$
 $n_2 = 0, 1, 2, ...$ (32*a*)

or, from (29b)

$$\beta = 1 + i\hbar\sqrt{E/2}(n_2 + \frac{1}{2})$$
 $n_2 = 0, 1, 2, ...$ (32b)

and in that case for the wavefunctions $\psi_2^+(v)$ we obtain, up to the first order in \hbar :

$$\psi_{2n_2}^+(v) = (w_0'(v))^{-1/2} D_{n_2}(\sqrt{2}w_0 \,\mathrm{e}^{-\mathrm{i}\pi/4}/\sqrt{\hbar}). \tag{33a}$$

When condition (32*a*) is fulfilled, the function $\phi_2^-(w)$ represents an incoming wave. From (33*a*) and (29*a*) we have equality

$$\psi_{2n_2}^+(-v) = (-1)^{n_2} \psi_{2n_2}^+(v). \tag{33b}$$

We see that our system has resonances for (complex) values of energy for which are simultaneously fulfilled conditions (30b) and (32b) and in that case the wavefunction of resonance is given by:

$$\psi_{n_1n_2}(u, v) = \psi_{1n_1}^+(u)\psi_{2n_2}^+(v). \tag{34}$$

Now, the condition (21) together with the equalities (31b) and (33b) implies that integers n_1 and n_2 can be either simultaneously even or odd, i.e. either

$$n_1 = 2s, \ldots$$
 $n_2 = 2k, \ldots$ $s, k = 0, 1, 2, \ldots$ (35a)

for resonances with even parity, or

$$n_1 = 2s + 1, \ldots$$
 $n_2 = 2k + 1, \ldots$ $s, k = 0, 1, 2, \ldots$ (35b)

for resonances with odd parity. One can easily show that (30b) and (32b) together with the condition (35a)[(35b)] are up to first order in \hbar equivalent with (19a)[(19b)].

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