Stokes lines, quantum defects and the Yukawa potential

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Abstract. Phase-integral and Newton-Raphson methods are used to calculate real turning points, energy eigenvalues and hence quantum defects ($\mu_{n,l}$). Stokes and anti-Stokes lines are traced using a complex Newton-Raphson method.

1. Introduction
We wish to generalize our recent work [1, 2] in which complete information was obtained for the Stokes constants associated with both crossing and non-crossing parabolic-cylinder functions. The emphasis is on strong coupling of Whittaker functions $M_{\kappa,\mu}(z)$ and $W_{\kappa,\mu}(z)$ where all three parameters $|\kappa|$, $|\mu|$ and $|z|$ may be large and where we have a double pole as well as two transition points. In this respect we wish to generalize previous work on the semiclassical treatment of quantum defect theory [3]–[7] and relate the quantum defect in the Rydberg formula

$$E = -\frac{0.5Z^2}{(n - \mu)^2}$$

(1)

to the Stokes phenomenon. This work is applicable to ion-atom collisions at low velocities of impact and also to multichannel quantum defect theory.

2. Yukawa Potential
We consider the Yukawa or screened Coulomb potential

$$V(r) = -Ze^2e^{-\alpha r}/r$$

(2)

and also the modified Coulomb potential of Linnaeus [7] to calculate real turning points and energy eigenvalues. Here $e$ is the electron charge, $\alpha$ is a small screening parameter and $Z$ is the product of the charges of the two (possible highly charged) ions. The Yukawa potential is of particular interest to nuclear physicists as it is a good approximation to the strong force between nucleons. We begin with the time-independent radial Schrödinger equation

$$\frac{d^2}{dr^2}u_{nl}(r) + R(r)u_{nl}(r) = 0$$

(3)
where \( R(r) = \frac{2m}{\hbar^2} (E_{nl} - V(r)) - \frac{l(l+1)}{r^2}. \) (4)

We use a 1st order phase integral approximation, where \( q(r) \) is given by

\[
q(r) = Q(r) \sum_{i=0}^{N} Y_{2i}
\]

and \( Y_0 = 1. \) (5)

\( Q(r) \) is the base function and is chosen as

\[
Q(r) = R(r) - \frac{1}{4r^2}.
\] (7)

For bound states \( Q(r) \) has a second order pole at the origin and two positive zeros, \( t_1 \) and \( t_2, \) which are the generalized classical turning points.

3. Numerical Work

We calculate the real turning points of \( Q(r) \) using a Newton-Raphson method.

\[
Q^2(r) = 2E - \frac{4Ze^{-\alpha r}}{r} - \frac{(l + \frac{1}{2})^2}{r^2}
\]

where \( E = -\frac{Z^2}{2(n - \mu)^2}. \) (8)

Using these turning points we calculate the energy eigenvalues and hence the quantum defect \( \mu \) for each \( n, l \) level using a Newton-Raphson method and the Bohr-Sommerfeld rule

\[
\int_{t_1}^{t_2} Q(s)ds = (n - l - \frac{1}{2})\pi
\] (10)

If the screening parameter \( \alpha \) is small then we can treat the exponential as a small perturbation to the Coulomb potential:

\[
e^{-\alpha r} \approx 1 - \alpha r + O(\alpha^2)
\] (11)

Comparing the resulting equation with equation (1) and assuming \( \alpha \) and \( n \) are small we can write

\[
\mu \approx n \left( 1 - \frac{1}{\sqrt{1 - \frac{2\alpha n^2}{Z}}} \right).
\] (12)

Using a binomial expansion we can write this as

\[
\mu \approx n \left[ 1 - \left( 1 + \frac{1}{2} \left( \frac{2\alpha n^2}{Z} \right) + \frac{3}{8} \left( \frac{2\alpha n^2}{Z} \right)^2 + \cdots \right) \right].
\] (13)

Table 1 shows the quantum defects obtained by taking the first three terms of the expansion compared with those obtained using Newton-Raphson methods.

By treating the exponential as a small perturbation to the Coulomb potential we obtain values for \( \mu_{n,l} \) comparable to those obtained using Newton-Raphson methods. Although it must be noted that in using the perturbation method the values of \( \mu \) do not depend on the value of the orbital angular momentum quantum number \( l.\)
Table 1. Quantum defects obtained using perturbation and Newton-Raphson methods for the Yukawa potential ($\alpha = 0.01, Z = 1$)

| n | $\mu$ (Perturbation theory) | $\mu$ (Newton-Raphson) |
|---|----------------------------|-------------------------|
| 1 | 0.01015                    | 0.0100820481            |
| 2 | 0.08460                    | 0.0825419460            |
| 3 | 0.30645                    | 0.2899826253            |
| 3 | 1                          | 0.2916132163            |
| 3 | 2                          | 0.2948868630            |
| 4 | 0.83456                    | 0.7296675105            |
| 4 | 1                          | 0.7341921940            |
| 4 | 2                          | 0.7433050744            |
| 4 | 3                          | 0.7571360419            |
| 5 | 0.91406                    | 1.5491950836            |
| 5 | 1                          | 1.5601851808            |

4. Stokes and Anti-Stokes Lines

The next stage involves tracing the Stokes and anti-Stokes lines around the turning points. The Stokes lines are defined by

$$\Re \int_{r_0}^{r} Q(r)dr = 0.$$  \hspace{1cm} (14)

where $r_0$ is one of the turning points $t_1$ or $t_2$. We begin by determining the initial directions of the Stokes lines around each of the turning points by expanding $Q^2(s)$ in a Taylor expansion around $t_1$ and $t_2$. For $t_2$ we have

$$Q^2(s) = Q^2(t_2) + \frac{dQ^2(t_2)}{ds}(s - t_2) + \frac{d^2Q^2(t_2)}{ds^2} \frac{(s - t_2)^2}{2!} + \cdots.$$  \hspace{1cm} (15)

Neglecting higher order terms we have

$$Q(s) = \sqrt{\frac{d}{ds}Q^2(t_2)(s - t_2)}.$$  \hspace{1cm} (16)

After some manipulation we find that this equation can only be satisfied if the initial angles of the Stokes lines around $t_1$ are $\pm \frac{\pi}{3}, \pi$ and around $t_2$ are $0, \pm \frac{2\pi}{3}$. We then trace the Stokes lines away from the turning points, changing variable from $r$ to $\theta$

$$s = t_2 + \hat{R} \exp(i\theta)$$  \hspace{1cm} (17)

where $\hat{R}$ is a small constant, this way we approximate the Stokes line by a series of short straight lines. For fixed $\theta$ and varying $R$ we have a straight line,

$$ds = e^{i\theta}d\hat{R}.$$  \hspace{1cm} (18)

A complex Newton-Raphson method is used to determine the angle, $\theta$ of each successive part of the Stokes line,

$$\theta_{n+1} = \theta_n - \frac{f(\theta_n)}{f'(\theta_n)}.$$  \hspace{1cm} (19)
A similar procedure is used to trace the anti-Stokes lines which are defined by

\[ \Im \int_{r_0}^{r} Q(r)dr = 0. \]  

(20)

Figure 1 shows the arrangement of the Stokes and anti-Stokes lines for the Yukawa potential with \( \alpha = 0.01 \).

![Figure 1. Stokes and anti-Stokes lines for the Yukawa potential](image)

5. Future Work

This work could be extended to look at the connection formulae for this potential in order to obtain the exact Stokes constants associated with each Stokes line. Then it may be possible to find a connection between the quantum defects and the Stokes constants.

This project can be extended further by looking at the Stokes constants and quantum defects associated with other potentials, such as the Wood-Saxon potential

\[ V(r) = -\frac{Z}{r} - \frac{Ze^{-\alpha r}}{r}. \]  

(21)

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