Quantum action variable description of bound and scattering states

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by

Mirley K. Balasubramanya

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TABLE OF CONTENTS

CHAPTER 1. INTRODUCTION ............................................ 1

CHAPTER 2. ACTION VARIABLE IN CLASSICAL MECHANICS 3
  Hamiltonian mechanics and the Hamilton-Jacobi equation ........... 3
  Action-angle variables and periodic motion ........................ 5
  The frequency of a simple harmonic oscillator using \( w - J_c \) .... 7

CHAPTER 3. QUANTUM ACTION VARIABLE .............................. 9
  Quantum Hamilton-Jacobi equation ................................ 9
  Definition of quantum action variable ............................. 10
  Energy levels of the harmonic oscillator .......................... 11

CHAPTER 4. SPHERICALLY SYMMETRIC POTENTIALS ................. 14
  Classical motion ................................................. 14
  Separable solution of the Hamilton-Jacobi equation ............... 15
  Action variables \( J_{\theta c} \) and \( J_{\phi c} \) .......................... 16
  Quantum motion .................................................. 17
  Separation of the quantum Hamilton-Jacobi equation .............. 18
  Action variables \( J_{\theta} \) and \( J_{\phi} \) ............................. 19

CHAPTER 5. COULOMB POTENTIAL - CLASSICAL CASE ............. 22
### Chapter 9. Classical Action Variable - Yukawa Potential

| Location of classical turning points | Case (i): $E \ll -g^2/4L^2$ and $|r_j| \ll L^2/g$ |
|-------------------------------------|--------------------------------------------------|
| Case (ii): $E \approx -g^2/4L^2$ and $r_j \approx r_0 \approx 2L^2/g$ |
| Case (iii): $E \approx E_h$ and $r_j \approx r_h$ |
| Case (iv): $E_h < E < E_w$ and $|r_j| \approx r_h$ |
| Case (v): $\Re(c) < 0$ |
| Case (vi): Western turning points for $E \approx 0$ |

Definitions of the classical momentum function $p_{rc}(r, \mathcal{E}, L)$ and $J_{rc}$

Alternate definition of $J_{rc}$

Features of the Yukawa $J_{rc}$

### Chapter 10. Semiclassical Study - Yukawa Potential

| Nature of $W_{rc}(r, \mathcal{E}, L)$ west of the western turning points |
| Poles for $E < V_0$ |
| Poles for $V_0 < E < 0$ |
| Poles for $E \approx 0$ |
| Poles for $0 < E < V_0$ |
| Poles for $V_h < E < V_w$ |
| Poles for $E > V_w$ |
CHAPTER 11. EXACT STUDY OF THE POLES OF MOMEN-
TUM FUNCTION - YUKAWA POTENTIAL ............. 125
Discussion of the numerical results .................. 125
Summary of the motion of poles with energy .......... 130

CHAPTER 12. QUANTUM ACTION VARIABLE - YUKAWA

Jr on negative energy eigenvalues .................... 136
Modifying the Hamiltonian using \( \epsilon_r \) ............... 137
Exploration of the singularity at \( r = 1/\epsilon_r \) ........ 142
Definition of \( J_r \) .................................. 147

CHAPTER 13. CONCLUSION ............................ 151

ACKNOWLEDGEMENTS ................................ 154

APPENDIX ............................................. 155

Appendix A: Poles of \( p_r \) .......................... 155
Appendix B: Perturbative expansion of \( p_{rc}(r, \mathcal{E}, L) \) .................................. 156

Case (i): \( L = 0 \) ................................... 156
Case (ii): \( L \neq 0 \) ................................... 156

BIBLIOGRAPHY ........................................ 157
LIST OF TABLES

Table 6.1: Coefficients $A$ and $B$ of $\exp(\pm i\frac{W}{h})$ ........................ 48

Table 10.1: Coefficients $A$ and $B$ of $\exp(\pm i\frac{W}{h})$ for $E < V_0$ .......... 108

Table 10.2: Coefficients $A$ and $B$ of $\exp(\pm i\frac{W}{h})$ for $V_0 < E < 0$ ...... 112
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>The potential and the turning points</td>
<td>6</td>
</tr>
<tr>
<td>3.1</td>
<td>Harmonic oscillator potential and the poles of $p(x)$</td>
<td>12</td>
</tr>
<tr>
<td>5.1</td>
<td>Bound state motion in Coulomb potential</td>
<td>23</td>
</tr>
<tr>
<td>5.2</td>
<td>Variation of the turning points $r_1$ &amp; $r_2$ with energy</td>
<td>27</td>
</tr>
<tr>
<td>5.3</td>
<td>Contour $C$ for evaluating $J_{rc}$ for Coulomb potential</td>
<td>28</td>
</tr>
<tr>
<td>5.4</td>
<td>Dependence of $J_{rc}$ on the particle's energy</td>
<td>30</td>
</tr>
<tr>
<td>5.5</td>
<td>Contours for the modified $J_{rc}$</td>
<td>32</td>
</tr>
<tr>
<td>6.1</td>
<td>The poles of $p_r$ in the complex $r$ plane</td>
<td>34</td>
</tr>
<tr>
<td>6.2</td>
<td>Stokes and anti-Stokes lines from turning point $r_0$</td>
<td>39</td>
</tr>
<tr>
<td>6.3</td>
<td>Stokes lines (broken lines) from turning points $r_1$ and $r_2$ for $E &lt; V_0$</td>
<td>42</td>
</tr>
<tr>
<td>6.4</td>
<td>Definition of $W_{rc1}$ and $W_{rc2}$</td>
<td>44</td>
</tr>
<tr>
<td>6.5</td>
<td>Poles in the complex $r$ plane for $E &lt; V_0$</td>
<td>45</td>
</tr>
<tr>
<td>6.6</td>
<td>Stokes and anti-Stokes lines for $E \approx V_0$</td>
<td>46</td>
</tr>
<tr>
<td>6.7</td>
<td>Stokes and anti-Stokes lines for $V_0 &lt; E &lt; 0$</td>
<td>47</td>
</tr>
<tr>
<td>6.8</td>
<td>Variation of $T(E)$ with energy in $T$ plane</td>
<td>50</td>
</tr>
<tr>
<td>6.9</td>
<td>Movement of a southern pole with energy</td>
<td>52</td>
</tr>
</tbody>
</table>
Figure 6.10: Variation of $T'(E)$ with energy in $T'$ plane .......... 53
Figure 6.11: Movement of a northern pole with energy ............ 54
Figure 6.12: Collective movement of poles with energy .......... 55
Figure 6.13: Stokes and anti-Stokes lines for $E \approx 0$ ............ 56
Figure 6.14: Stokes and anti-Stokes lines for $E > 0$ ............ 57
Figure 6.15: Motion of the southern and northern poles with increasing energy ........................................... 57
Figure 6.16: First three southern poles of $p_r$ computed using the WKB approximation for the Coulomb wave function 60
Figure 6.17: First three southern poles of $p_r$ computed using the WKB approximation for the Coulomb wave function with smaller $\epsilon_E$ 61
Figure 6.18: Ten southern poles of $p_r$ in the complex $r$ plane computed using the WKB approximation for the Coulomb wave function 62
Figure 6.19: First northern pole of $p_r$ computed using the WKB approximation for the Coulomb wave function .......... 63
Figure 6.20: First northern pole of $p_r$ computed using the WKB approximation for the Coulomb wave function with smaller $\epsilon_E$ .... 64
Figure 6.21: Ten northern poles of $p_r$ in the complex $r$ plane computed using the WKB approximation for the Coulomb wave function 65
Figure 7.1: First three southern poles of $p_r$ obtained by numerical integration of the Schrödinger equation for the Coulomb potential 69
Figure 7.2: First three southern poles of $p_r$ obtained by numerical integration of the Schrödinger equation for the Coulomb potential 70
Figure 7.3: First three southern poles of $p_r$ with constant $\epsilon_E$ .......... 70
Figure 7.4: Second southern pole of $p_r$ for three successively higher values of angular momentum ........................................ 71

Figure 7.5: Northern poles of $p_r$ obtained through numerical integration of the Schrödinger equation for the Coulomb potential .... 72

Figure 8.1: Contour $C'$ for the definition of $J_r$ for all energies .......... 75

Figure 8.2: Poles of $p_r$ for eigenvalue $E = E_2$ ............................. 77

Figure 8.3: Common angular momentum states for Coulomb potential .......................... 79

Figure 8.4: Variation of $J_r$ with energy for Coulomb potential .......... 80

Figure 9.1: Effective Yukawa potential as a function of real $r$ ............. 82

Figure 9.2: Motion of $r_1$ and $r_2$ with energy ............................... 85

Figure 9.3: Computed motion of $r_1$ and $r_2$ with energy for the range $E = 2V_0$ to $E \geq V_0$ with $R = 1$ ....................... 86

Figure 9.4: Motion of $r_2$ and $r_3$ with energy ............................... 88

Figure 9.5: Computed motion of $r_2$ and $r_3$ with energy for the range $E = 2V_0$ to $E \geq V_{w}$ with $R = 1$ .................... 89

Figure 9.6: Motion of the western turning points with energy ............ 90

Figure 9.7: Computed motion of the western turning points with energy for the range $E = 2V_0$ to $E \geq V_{w}$ with $R = 1$ ................ 91

Figure 9.8: Motion of the western turning points with energy for $E \approx 0$ . 93

Figure 9.9: Branch cuts of $p_{\alpha\beta}(r, E, L)$ and the contour $C$ for for $E < E_h$ 95

Figure 9.10: Branch cuts of $p_{\alpha\beta}(r, E, L)$ and the contour $C$ for for $0 < E < E_w$ .................................................. 96

Figure 9.11: Branch cuts of $p_{\alpha\beta}(r, E, L)$ and the contour $C$ for $E > E_w$ 97
Figure 9.12: Contour $C'$ for the definition of $\tilde{J}_{rc}$ .......................... 101

Figure 10.1: Stokes and anti-Stokes lines for $E < V_0$ ................................. 106
Figure 10.2: Poles of $p_r$ for $E < V_0$ ......................................................... 110
Figure 10.3: Stokes and anti-Stokes lines for $V_0 < E < 0$ ............................ 111
Figure 10.4: Poles of $p_r$ for $V_0 < E < 0$ .................................................. 114
Figure 10.5: Stokes and anti-Stokes lines for $E \approx 0$ ..................................... 116
Figure 10.6: Poles of $p_r$ for $E \approx 0$ ........................................................... 117
Figure 10.7: Stokes and anti-Stokes lines for $0 < E < V_0$ ............................. 119
Figure 10.8: Stokes and anti-Stokes lines for $V_h < E < V_w$ .......................... 120
Figure 10.9: Poles of $p_r$ for $V_h < E < V_w$ .............................................. 121
Figure 10.10: Stokes and anti-Stokes lines for $E > V_w$ ................................. 123
Figure 10.11: Poles of $p_r$ for $E > V_w$ .......................................................... 124

Figure 11.1: First two southern poles of $p_r(r, \varepsilon, l)$ for $V_0 < E < V_w$ and
\[ l = 1, \quad g = 23 \] ................................................................. 127
Figure 11.2: First two southern poles of $p_r(r, \varepsilon, l)$ for $V_0 < E < V_w$ and
\[ l = 1, \quad g = 23 \] ................................................................. 128
Figure 11.3: First five southern poles of $p_r(r, \varepsilon, l)$ for $V_0 < E < V_w$ and
\[ l = 1, \quad g = 23 \] ................................................................. 129
Figure 11.4: First four southern poles of $p_r(r, \varepsilon, l)$ for $V_0 < E < V_w$ and
\[ l = 1, \quad g = 55, \text{ with four bound states} \] ....................................... 131
Figure 11.5: First five southern poles of $p_r(r, \varepsilon, l)$ for $V_0 < E < V_w$ and
\[ l = 2, \quad g = 55 \text{ with three bound states} \] ....................................... 132
Figure 11.6: First three southern poles of $p_r(r, \xi, l)$ for $V_0 < E < V_w$ and
$l = 3, \quad g = 55$ with one bound state and a resonant state . . 133

Figure 11.7: Northern and northwestern poles of $p_r(r, \xi, l)$ for $V_0 < E <$
$V_w$ and $l = 1, \quad g = 20$ with two bound states . . . . . . . 134

Figure 12.1: Poles of $p_r$ for the energy eigenvalue $E = E_3$ . . . . . . . . . . . . . 137
Figure 12.2: Stokes (broken lines) and anti-Stokes lines for $V_0 < E < 0$ . . 140
Figure 12.3: Poles of $P_r(r, \xi, l, \epsilon_r)$ for $V_0 < E < 0$ . . . . . . . . . . . . . 141
Figure 12.4: Integration paths for the modified Schrödinger equation . . 143
Figure 12.5: Zeroes of $U(r, \xi, l, \epsilon_r)$ in the neighborhood of $1/\epsilon_r$ . . . . . . . 144
Figure 12.6: Contours used in the definition of $J_r(\xi, l, \epsilon_r)$ . . . . . . . . . . . . . 149
CHAPTER 1. INTRODUCTION

Classical periodic systems can be described elegantly in terms of their action and angle variables which constitute a set of canonically conjugate momenta and coordinates. The Hamiltonian of such systems is a function of the action variables only. These action variables, like angular momentum and energy, are a measure of the total motion of periodic systems. The angle variables evolve linearly in time, advancing by one unit every cycle. The period of such systems can be found using the functional relationship between the action variable and the other constants of the motion without requiring a complete solution of the dynamical equations. Delaunay invented action and angle variables in classical mechanics. This canonical set of coordinates and momenta arise in the Hamilton-Jacobi form of classical mechanics. They also assumed importance in early quantum mechanics; the Wilson-Sommerfeld quantization rules involved the quantization of action variables to explain the bound state spectra. These rules, however, suffered from the same inadequacy as the Bohr quantization conditions; they were ad hoc. With the establishment of the wave and matrix forms of quantum mechanics the construction of action variables in the quantum context were essentially dropped. Leacock and Padgett [1] built a form of quantum mechanics, equivalent to the Schrödinger theory, that involved the formulation of a quantum version of the action variable. The bound states of a system were characterized by
the quantization of the action variable which, in turn, led to the quantization of the system's energy.

Systems that admit both bound and scattering states may display the phenomenon of resonant scattering. Quantum resonance is characterized by a maximum in the delay time of the scattering process. Their resemblance to bound states, which have an infinite delay time, is striking. Leacock and Nanayakkara [2] have explored the unified description of bound and scattering states of two particles interacting via the Coulomb potential, using the action variable. It required the extension of the notion of the action variable to scattering states (which are aperiodic). The classical definition of the action variable as $\frac{1}{2\pi} \oint pdq$ over an orbit in phase space is unsatisfactory; it cannot be extended to scattering states. Neither can it provide leads to define action variables for the corresponding quantum scattering states. An action variable was successfully defined for the Coulomb potential that had the same form for all states of the system, bound and scattering. In this thesis we show that one can define an action variable for particles that interact through the Yukawa potential, both classically and quantum mechanically. This potential, unlike the Coulomb one, admits resonant scattering states. It will also be shown that the method is general and can be employed for all long range central potentials that cut off sufficiently smoothly. This work is a prelude to the construction of particle resonances in terms of the radial action variable.
CHAPTER 2. ACTION VARIABLE IN CLASSICAL MECHANICS

In this chapter we review the role of action\( (J) \)-angle\( (\omega) \) variables in classical mechanics. Their definitions and utility are illustrated using the one dimensional harmonic oscillator.

Hamiltonian mechanics and the Hamilton-Jacobi equation

The time evolution of a mechanical system is governed by its Hamiltonian \( H \) which is a function of the \( n \) coordinates \( x_i \), the \( n \) conjugate momenta \( p_i \) and the time \( t \). The dynamics of such a system is determined by Hamilton's equations of motion

\[
\dot{x}_i = \frac{\partial H(x_i, p_i, t)}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H(x_i, p_i, t)}{\partial x_i}.
\]  

(2.1)

The Hamiltonian of a particle moving in one dimension under the influence of a potential \( V(x) \) is given by

\[
H = p^2 + V(x).
\]  

(2.2)

The units of mass have been so chosen that \( 2m = 1 \). We maintain these units throughout for convenience. It can be shown [3] that such a Hamiltonian is a constant of the motion and is the total energy \( E \) of the system. Thus,

\[
p^2 + V(x) = E.
\]  

(2.3)
Transformations \((x, p) \rightarrow (X, P)\) that preserve the form of Hamilton's equations are termed *canonical transformations*. One such transformation is generated by the generating function \(W(x, P)\):

\[
p = \frac{\partial W(x, P)}{\partial x}, \quad X = \frac{\partial W(x, P)}{\partial P}.
\]  

(2.4)

If this transformation transforms the Hamiltonian into a function of \(P\) only, then, using (2.1),

\[
\dot{X} = \frac{\partial H(P)}{\partial P} = \text{constant} \Rightarrow X(t) = \left[\frac{\partial H(P)}{\partial P}\right] t + X_0
\]  

(2.5)

\[
\dot{P} = -\frac{\partial H(P)}{\partial X} = 0 \Rightarrow P(t) = P = \text{constant}.
\]  

(2.6)

Thus \(X\) and \(P\) evolve very simply in time, the former linearly and the latter a constant. \(W(x, P)\), which generates a canonical transformation in which the new coordinate \(X\) is cyclic, is called *Hamilton's characteristic function*. It satisfies the *Hamilton-Jacobi equation* which is obtained by using (2.4) in (2.3):

\[
W_x(x, P) + V(x) = E(P)
\]  

(2.7)

where the subscript \(x\) denotes partial differentiation with respect to \(x\).

The use of this method to solve the dynamical problem then involves the following steps:

(i) Define the new constant momentum \(P\),

(ii) Integrate (2.7) to obtain \(W(x, E(P))\),

(iii) Obtain \(x(X, P)\) and \(p(X, P)\) using (2.4),

(iv) Express \(X_0\) and \(P\) in terms of the initial values \(x_0\) and \(p_0\).
Action-angle variables and periodic motion

The method of Hamilton-Jacobi is particularly suited to the study of periodic or bound motion. By a particular choice of the new momentum $P$ one obtains the period of the motion without requiring a complete solution of the dynamical problem. The new coordinate and momentum are chosen to be

$$X = \omega, \quad P = J_c,$$  \hspace{1cm} (2.8)

with

$$J_c = \frac{1}{2\pi} \oint p(x, E) dx,$$  \hspace{1cm} (2.9)

where $p(x, E)$ is obtained by solving for $p$ from (2.3) and the integral is done over one cycle of the periodic motion. The subscript $c$ refers to the classical problem. A similar momentum is defined in the corresponding quantum problem and it will be referred to as $J$. Since $J_c = J_c(E)$ we can invert it to obtain $H = E = E(J_c)$. Using (2.1) we get,

$$\dot{\omega} = \frac{\partial H(J_c)}{\partial J_c} \Rightarrow \omega(t) = \left[\frac{\partial H(J_c)}{\partial J_c}\right] t + \omega_0$$  \hspace{1cm} (2.10)

It can be shown [3] that the angular frequency of the periodic motion is

$$\omega = \dot{\omega} = \frac{\partial H(J_c)}{\partial J_c}.$$  \hspace{1cm} (2.11)

Thus the problem of finding the frequency of periodic motion is reduced to that of doing the integral (2.9).

An equivalent definition of $J_c$, which can be generalized to nonperiodic motion as well as quantum motions, is

$$J_c = \frac{1}{2\pi} \oint p_c(x, E) dx,$$  \hspace{1cm} (2.12)
Figure 2.1: The potential and the turning points
where \( p_c(x, E) \) is an analytic function of \( x \) (considered complex) defined by

\[
p_c(x, E) = \left[ E - V(x) \right]^\frac{1}{2}.
\] (2.13)

The classical turning points \( x_1 \) and \( x_2 \) are defined by \( p_c(x_1, E) = p_c(x_2, E) = 0 \). These two real turning points are the branch points of \( p_c(x, E) \). There is a branch cut connecting \( x_1 \) and \( x_2 \). \( p_c(x, E) \) is chosen as that branch of the square root which is positive along the bottom of the cut. The contour \( C \) encloses counterclockwise the two turning points \( x_1 \) and \( x_2 \). A graph of the potential and the branch cut are shown in Figure 2.1.

The contour integral definition of \( J_c \) is more than a mathematical trick. It will be shown in later chapters that such a definition is necessary in order to analytically continue the definition of \( J_c \) to positive energy states. It is also essential for defining the quantum counterpart of \( J_c \).

**The frequency of a simple harmonic oscillator using \( w - J_c \)**

We now illustrate the use of action-angle variables by obtaining the frequency of a particle moving in one dimension in the simple harmonic potential \( V(x) = x^2 \). The contour \( C \) can be deformed continuously into a circle \( C_0 \) centered at \( x = 0 \) in the region external to the turning points. Here \( x_1 = -x_2 \) and, in the region \( |x| > |x_1| \), \( p_c(x, E) \) has the form

\[
p_c = \left[ E - x^2 \right]^\frac{1}{2} = ix - iE/2x + \ldots,
\] (2.14)

and by residue theorem and definition (2.12)

\[
J_c = \frac{E}{2}.
\] (2.15)
Inverting this, we get

\[ E = E(J_c) = 2J_c \quad \Rightarrow \quad \omega = \frac{\partial E}{\partial J_c} = 2, \quad (2.16) \]

which is indeed the angular frequency of a simple harmonic oscillator of mass 1/2 and spring constant 2.
CHAPTER 3. QUANTUM ACTION VARIABLE

In this chapter we review quantum Hamilton-Jacobi theory. We show that the exact bound state energies of the quantum harmonic oscillator can be obtained using a quantum action variable $J$ whose definition closely resembles that of $J_C$.

Quantum Hamilton-Jacobi equation

Leacock et al. [1] have constructed a version of quantum mechanics which parallels the classical Hamilton-Jacobi theory. We consider systems whose Hamiltonian is of the form

$$\hat{H} = \hat{p}^2 + \hat{V}(\hat{x}).$$  \hfill (3.1)

Here, a hat denotes a linear operator. The measurable values of the observables $\hat{H}$, $\hat{p}$, $\hat{x}$, etc. are their eigenvalues. We write the equations of a quantum canonical transformation in terms of the eigenvalues and functions of eigenvalues. Using the quantum characteristic function $W(x, P)$ these transformation equations are

$$p = \frac{\partial W(x, P)}{\partial x}, \quad X = \frac{\partial W(x, P)}{\partial P} \hfill (3.2)$$

The quantum Hamilton-Jacobi equation is postulated as

$$-i\hbar W_{xx}(x, E(P)) + W_x^2 = E(P) - V(x), \hfill (3.3)$$

$$\hat{p}^2 + \hat{V}(\hat{x}).$$
where subscript refers to partial differentiation. Physical boundary conditions have to be imposed on $W(x, E(P))$ to complete its definition. We note that this equation resembles the classical Hamilton-Jacobi equation (2.7) but for the first term involving $\hbar$.

A new function $p(x, E)$, called the quantum momentum function, is defined as below:

$$p(x, E) = \frac{\partial W(x, E)}{\partial x}. \quad (3.4)$$

$p(x, E)$ is the quantum analogue of the classical momentum function $p_c(x, E)$ defined in Chapter 1. Using this in (3.3) we obtain an equation for $p(x, E)$:

$$-i\hbar \frac{\partial p(x, E)}{\partial x} + p^2(x, E) = E - V(x) = p_{c2}(x, E). \quad (3.5)$$

We note that this quantum momentum function reduces to $\pm p_c$ defined by (2.13) in the limit of $\hbar \to 0$. The physical boundary condition on $p(x, E)$ is

$$\lim_{\hbar \to 0} p(x, E) = p_c(x, E). \quad (3.6)$$

Equation (3.5), along with (3.6), can be viewed as the defining equation for $p(x, E)$ which we will use in the definition of quantum action variable $J$. The relation between eq. (3.5) and the Schrödinger equation is shown in [1] ; we utilize it in Chapter 6.

**Definition of quantum action variable**

Further development of the quantum theory of action-angle variables requires the definition of a new momentum $P$ which we call the quantum action variable $J$. It is defined as a contour integral in the complex $x$ plane,

$$J = \frac{1}{2\pi} \oint_C p(x, E) dx, \quad (3.7)$$
with the counterclockwise contour $C$ enclosing the two turning points, as shown in Figure (2.1). (3.5) and (3.6) imply $p(x, E)$ has poles of residue $-i\hbar$ (see Appendix A) between the two turning points. The number of these poles is 0, 1, 2, ... for the ground state, first excited state, second excited state, ... etc. respectively. Since the contour $C$ encloses these poles, the residue theorem leads to the quantization of $J$:

$$J = J(E) = n\hbar. \quad (3.8)$$

Inverting this, we obtain the system's energy eigenvalues:

$$E = E(n\hbar). \quad (3.9)$$

As will be shown in the next section the integral (3.7) can be done without obtaining a solution of (3.5) all over the complex $x$ plane. The energy eigenvalues can thus be obtained without solving any dynamical equation.

**Energy levels of the harmonic oscillator**

We now illustrate the use of the quantum action variable by obtaining the energy levels of a particle moving in one dimension in the harmonic potential $V(x) = x^2$. To evaluate $J$ from (3.7) we deform the contour $C$ into $C_0$, which is a circular contour centered at $x = 0$ enclosing the turning points $x_1$ and $x_2$, and evaluate the integral along $C_0$. Writing $p(x, E)$ and $p_c(x, E)$ on $C_0$ as

$$p(x, E) = a_1 x + a_0 - a_{-1} / x + \ldots \quad \text{and}$$

$$p_c(x, E) = b_1 x + b_0 - b_{-1} / x + \ldots$$

where $b_1 = i$, $b_0 = 0$, $b_{-1} = -iE/2$, ... from (2.14).
Figure 3.1: Harmonic oscillator potential and the poles of $p(x)$
Substituting these in (3.5) we get

\[ a_1^2 = b_1^2, \quad a_0 = 0, \quad a_{-1} = (1/2a_1)[2b_1 b_{-1} + i\hbar a_1], \quad \ldots \]  

(3.10)

The boundary condition (3.6) requires \( a_1 \) to be \( +b_1 \) and not \( -b_1 \). Thus, from (3.10),

\[ a_1 = i, \quad a_0 = 0, \quad a_{-1} = -i/2(E - \hbar), \quad \ldots \]  

(3.11)

Using (3.11) in (3.7) we get, via the residue theorem,

\[ J = ia_{-1} = (E - \hbar)/2, \]

and from (3.8) we have

\[ J(E) = (E - \hbar)/2 = n\hbar, \]  

(3.12)

and so \( E = 2\hbar(n + 1/2) \) which are the energy eigenvalues of a quantum harmonic oscillator with angular frequency \( \omega = 2 \).

This method is general and can be used to find the energies of any bound system. For those potentials for which the integral (3.7) cannot be obtained in the closed form we can use asymptotic methods developed by Leacock [4].
CHAPTER 4. SPHERICALLY SYMMETRIC POTENTIALS

The motion of a particle moving in a spherically symmetric potential $V(r)$ is considered in this chapter. The first part examines the classical motion and the second part the quantum motion. The classical Hamiltonian of the particle is expressed in terms of spherical polar coordinates $(r, \theta, \phi)$ and their conjugate momenta $(p_r, p_\theta, p_\phi)$ as

$$H = p_r^2 + \frac{1}{r^2} \left( p_\theta^2 + \frac{p_\phi^2}{\sin^2 \theta} \right) + V(r). \quad (4.1)$$

The quantum Hamiltonian for this system is obtained by replacing the classical coordinates and momenta by the corresponding Hermitian operators. It is shown in this chapter that such a three dimensional problem, both classical and quantum, can be transformed into three one dimensional problems.

Classical motion

We show, first, that the motion can be separated into $r$, $\theta$ and $\phi$ motions. We define, for a particle with total energy $E$, total angular momentum $L$ and azimuthal angular momentum $L_\phi$, classical momentum functions $p_r(r, E, L)$, $p_\theta(\theta, L, L_\phi)$ and $p_\phi(\phi, L_\phi)$ with complex arguments $r$, $\theta$ and $\phi$ respectively. These definitions are analogous to the definition of momentum function in the one dimensional case. These complex momentum functions are then used to construct the action variables $J_r$, $J_\theta$
Separable solution of the Hamilton-Jacobi equation

A canonical transformation is made to a new set of coordinates and momenta $(X_r, X_\theta, X_\phi, P_r, P_\theta, P_\phi)$ such that the Hamiltonian is cyclic in the new coordinates $X_r, X_\theta$ and $X_\phi$. The generator of this transformation is Hamilton's characteristic function $W_C(r, \theta, \phi, P_r, P_\theta, P_\phi)$. The equations of canonical transformation are

$$\begin{align*}
p_r &= \frac{\partial W_C}{\partial r}, \\
p_\theta &= \frac{\partial W_C}{\partial \theta}, \\
p_\phi &= \frac{\partial W_C}{\partial \phi}, \\
X_r &= \frac{\partial W_C}{\partial P_r}, \\
X_\theta &= \frac{\partial W_C}{\partial P_\theta}, \\
X_\phi &= \frac{\partial W_C}{\partial P_\phi}.
\end{align*}$$

(4.2)

The Hamilton-Jacobi equation for $W_C$, given (4.1) and (4.2), is

$$\left(\frac{\partial W_C}{\partial r}\right)^2 + \frac{1}{r^2}\left[\left(\frac{\partial W_C}{\partial \theta}\right)^2 + \frac{1}{\sin^2 \theta}\left(\frac{\partial W_C}{\partial \phi}\right)^2\right] + V(r) = E, \quad (4.3)$$

where $E$ is the particle's constant energy. This equation is separable if we let

$$W_C = W_{rc}(r, E, L) + W_{\theta c}(\theta, L, L_\phi) + W_{\phi c}(\phi, L_\phi),$$

$L$ and $L_\phi$ being separation constants. These constants and $E$ are functions of the new momenta, $P_r, P_\theta$ and $P_\phi$, which will be defined later. Then, (4.3) can be separated, and becomes the three equations

$$\begin{align*}
\left(\frac{\partial W_{rc}}{\partial r}\right)^2 + \frac{L^2}{r^2} + V(r) &= E, \\
\left(\frac{\partial W_{\theta c}}{\partial \theta}\right)^2 + \frac{L_\phi^2}{\sin^2 \theta} &= L^2, \\
\left(\frac{\partial W_{\phi c}}{\partial \phi}\right)^2 &= L_\phi^2.
\end{align*}$$

(4.4)
These three equations will be recast in terms of the classical momentum functions $p_{rc}(r, E, L)$, $p_{\theta c}(\theta, L, L_{\phi})$ and $p_{\phi c}(\phi, L_{\phi})$, where these functions and their coordinate arguments are considered complex. The momentum functions are defined thus:

$$p_{rc}(r, E, L) = \frac{\partial W_{rc}(r, E, L)}{\partial r},$$

$$p_{\theta c}(\theta, L, L_{\phi}) = \frac{\partial W_{\theta c}(\theta, L, L_{\phi})}{\partial \theta},$$

$$p_{\phi c}(\phi, L_{\phi}) = \frac{\partial W_{\phi c}(\phi, L_{\phi})}{\partial \phi}. $$

Equations (4.4) then can be written as

$$p_{rc}^2(r, E, L) + L^2/r^2 + V(r) = E, \quad (4.5)$$

$$p_{\theta c}^2(\theta, L) + L_{\phi}^2/\sin^2 \theta = L^2, \quad (4.6)$$

$$p_{\phi c}^2(\phi, L_{\phi}) = L_{\phi}^2. \quad (4.7)$$

**Action variables $J_{\theta c}$ and $J_{\phi c}$**

The above separation facilitates the definition of new momenta, $P_r$, $P_\theta$ and $P_{\phi}$, which we choose as the action variables $J_{rc}$, $J_{\theta c}$ and $J_{\phi c}$ respectively. The latter two can be defined without reference to the central potential while the former requires further study of equation (4.5). We focus on defining $J_{\theta c}$ and $J_{\phi c}$ here. The definition of $J_{rc}$ will be discussed in later chapters.

From (4.7) we have

$$p_{\theta c}(\theta, L, L_{\phi}) = [L^2 - L_{\phi}^2/\sin^2 \theta]^{1/2}. $$

$\theta_1$ and $\theta_2$ are the two turning points of the $\theta$—motion, i.e., $p_{\theta c}$ vanishes at $\theta_1$ and $\theta_2$. These two points are the branch points of $p_{\theta c}(\theta, L, L_{\phi})$ and we connect them by
a branch cut through the real axis. $p_{\theta c}$ is positive just below the cut. We define $J_\theta$ by the contour integral in the complex $\theta$ plane by

$$J_{\theta c} = \frac{1}{2\pi} \oint_{C_{\theta}} p_{\theta}(\theta, L, L_{\phi})d\theta,$$

(4.8)

where $C_{\theta}$ is a counterclockwise contour enclosing $\theta_1$ and $\theta_2$. On performing this integral by the method of residues we get [1]

$$J_{\theta c} = L - L_{\phi}.$$

(4.9)

The motion of the particle in the coordinate $\phi$ is unbounded and, unlike $p_{\theta c}, p_{\phi c}$ lacks any turning points, as is evident from eq. (4.7). We define the action variable $J_{\phi c}$ to be $L_{\phi}$.

Our definition of $J_{rc}$ will be a contour integral of $p_{rc}(r, E, L)$ in the complex $r$ plane over a suitably chosen contour. Thus,

$$J_{rc} = J_{rc}(E, L)$$

Inverting this, $E = E(J_{rc}, L) = E(J_{rc}, J_{\theta c} + J_{\phi c})$.

from (4.9) and the definition of $J_{\phi c}$. Therefore $J_{\theta c}$ and $J_{\phi c}$ occur in $E$ only in the combination $(J_{\theta c} + J_{\phi c})$ (see equation (4.9)). Hence the angular frequencies $\omega_\theta = \partial E/\partial J_\theta$ and $\omega_\phi = \partial E/\partial J_\phi$ are equal to each other for all central potentials.

**Quantum motion**

We now show, following the classical analysis, that the quantum Hamilton-Jacobi equation for a particle in a spherically symmetric potential can be separated into three one-dimensional equations, one for each of $r, \theta$ and $\phi$. The quantum action variables
$J_r, J_\theta$ and $J_\phi$, will be introduced and will be shown to be quantized. The energy of the particle, being a function of these action variables, is therefore quantized.

**Separation of the quantum Hamilton-Jacobi equation**

The generalization of the quantum Hamilton-Jacobi equation to three dimensions [1] is

$$-i\hbar \nabla^2 W + (\nabla W)^2 = E - V$$

where $W = W(r, \theta, \phi, P_r, P_\theta, P_\phi)$ is the quantum characteristic function that generates a quantum canonical transformation between the “old” coordinates-momenta set $(r, \theta, \phi, P_r, P_\theta, P_\phi)$ and the “new” set $(X_r, X_\theta, X_\phi, P_r, P_\theta, P_\phi)$. We can separate (4.10) by letting

$$W(r, \theta, \phi, P_r, P_\theta, P_\phi) = W_r(r, E, L) + W_\theta(\theta, L, l_\phi) + W_\phi(\phi, l_\phi).$$

$E$ and the separation constants $L$ and $l_\phi$ are functions of the “new” momenta $P_r, P_\theta$ and $P_\phi$ which will be defined later. Equation (4.10) then separates into three equations:

$$-i\hbar \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial W_r}{\partial r} \right) + \left( \frac{\partial W_r}{\partial r} \right)^2 + \frac{L^2}{r^2} + V(r) = E,$$

$$-i\hbar \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial W_\theta}{\partial \theta} \right) + \left( \frac{\partial W_\theta}{\partial \theta} \right)^2 + \frac{l_\phi^2}{\sin^2 \theta} = L^2,$$

$$-i\hbar \frac{\partial^2 W_\phi}{\partial \phi^2} + \left( \frac{\partial W_\phi}{\partial \phi} \right)^2 = l_\phi^2.$$
Equations (4.12) then become

\begin{align}
-\frac{i\hbar}{r^2} \frac{\partial}{\partial r} \left[ r^2 \tilde{p}_r(r, E, L) \right] + p_r^2(r, E, L) + \frac{L^2}{r^2} + V(r) &= E, \\
-\frac{i\hbar}{\sin \theta} \left[ \sin \theta p_\theta(\theta, L, l_\phi) \right] + p_\theta^2 + \frac{L_\phi^2}{\sin^2 \theta} &= L_\phi^2, \\
-\frac{i\hbar}{\partial \phi} \frac{\partial p_\phi(\phi, l_\phi)}{\partial \phi} + p_\phi^2 &= L_\phi^2.
\end{align}

The physical requirements on these momentum functions are

\begin{align}
\lim_{\hbar \to 0} \tilde{p}_r(r, E, L) &= p_{rc}(r, E, L), \\
\lim_{\hbar \to 0} p_\theta(\theta, L, l_\phi) &= p_{\theta c}(\theta, L, l_\phi), \\
p_\phi(\phi + 2\pi, l_\phi) &= p_\phi(\phi, l_\phi).
\end{align}

(4.17) and (4.18) require the quantum momentum functions \( \tilde{p}_r \) and \( p_{\theta c} \) to approach their classical counterparts in the limit of \( \hbar \) going to zero. This will be referred to as the classical limit. (4.18) requires \( p_\phi(\phi, l_\phi) \) to be unchanged under a rotation of \( 2\pi \) around the azimuthal axis. Equations (4.13) - (4.15) and boundary conditions (4.16) - (4.18) define the three momentum functions uniquely for all complex values of their coordinate arguments.

**Action variables \( J_\theta \) and \( J_\phi \)**

Using the above \( p_r, p_\theta \) and \( p_\phi \) we can define the new momenta, the action variables \( J_r, J_\theta \) and \( J_\phi \), as in the classical case. It will be shown that the the boundary conditions on the momentum functions quantize these action variables. The total energy of the system, being a function only of the the new momenta, is therefore quantized. \( J_r \) will be defined, in later chapters, as a contour integral of \( \tilde{p}_r \) in the complex \( r \) plane over a suitably chosen contour \( C \). We can define a related
momentum function \( p_r(r, E, L) \) by

\[
p_r(r, E, L) = \tilde{p}_r(r, E, L) - \frac{i\hbar}{r}.
\]

It obeys the momentum function equation (see equation 4.14)

\[
-\hbar \frac{\partial p_r(r, E, L)}{\partial r} + p_r^2(r, E, L) = E - V(r) - \frac{L^2}{r^2},
\]

\[
= p_r c^2(r, E, L),
\]

(4.19)

with \( p_r \) satisfying the same boundary condition as \( \tilde{p}_r \). Equation (4.19) is a differential equation identical to the one dimensional equation (3.5). Also, one can define \( J_r \) as an integral over \( C \) in the complex \( r \) plane of \( p_r \) instead of \( \tilde{p}_r \) provided the point \( r = 0 \) is not in the interior of \( C \). Our later discussions of \( J_r \) will be based on \( p_r \) and eq. (4.19).

The action variable \( J_\theta \) is defined as the contour integral in the complex \( \theta \) plane

\[
J_\theta = \frac{1}{2\pi i} \oint_{C_\theta} p_\theta(\theta, L^2, l_\phi) d\theta,
\]

(4.20)

where \( C_\theta \) is a closed counterclockwise contour enclosing \( \theta_1 \) and \( \theta_2 \), the two turning points, and the part of the real axis in between them. From eq. (4.14) and the boundary condition (4.17) it can be shown that \( p_\theta(\theta, L, l_\phi) \) has \( 0, 1, 2, \ldots \) poles of residue \( -i\hbar \) between \( \theta_1 \) and \( \theta_2 \). Thus, by (4.20) and the residue theorem, \( J_\theta = n_\theta \hbar \), with \( n_\theta = 0, 1, 2, \ldots \) corresponding to \( 0, 1, 2, \ldots \) enclosed poles of \( p_\theta \). It is shown in [1] that

\[
J_\theta = J_\theta(L, l_\phi) = \sqrt{[L^2 + (\hbar/2)^2]/\hbar^2 - \hbar/2 - l_\phi}.
\]

(4.21)

We next define the action variable \( J_\phi \) as \( l_\phi \). The periodic boundary condition (4.18) restricts the allowed values of \( l_\phi \) to integral multiples of \( \hbar \) only. Thus,

\[
J_\phi = n_\phi \hbar, \quad \text{with} \quad n_\phi = 0, \pm 1, \pm 2, \ldots
\]

(4.22)
Solving (4.21) for the separation constant $L$ we get

$$L^2 = [J_\theta + J_\phi + (\hbar/2)^2] - (\hbar/2)^2$$

$$= (n_\theta + n_\phi)(n_\theta + n_\phi + 1)\hbar^2 = l(l + 1)\hbar^2$$

(4.23)

where $l = n_\theta + |n_\phi|$.

Thus the allowed values of $L^2$ are quantized; for a given value of $l$ the allowed values of $l_\phi$ are $n_\phi\hbar$ with $-l \leq n_\phi \leq l$.

Using (4.24) in the momentum function equation (4.19) we obtain

$$-i\hbar \frac{\partial p_r(r, E, L)}{\partial r} + p_r^2(r, E, L) = p_re^2(r, E, L),$$

$$= E - V(r) - l(l + 1)\hbar^2/r^2.$$ (4.24)

This equation will be studied extensively for the locations of the poles of $p_r(r, E, l)$ in the complex $r$ plane with a view to defining the action variable $J_r$ as a contour integral. Such a $J_r$ should yield the bound state energies of the system when it is quantized in terms of $\hbar$. We will study the constructions of $J_r$ for the two physically important spherical potentials, Coulomb and Yukawa.
Chapter 5. Coulomb Potential - Classical Case

The Coulomb potential is of the form \(-g/r\), where \(g\), the coupling constant squared, is a measure of the attraction of the particle to the center of attraction. We study in this chapter the definition of the radial action variable \(J_{rc}\) for a particle moving in this potential. The bound state motion (negative energy) is first studied and the frequency of radial oscillations obtained using \(J_{rc}\). We then review the work of Nanayakkara [2] in extending the definition of \(J_{rc}\) to the scattering states of the particle.

Bound states and radial periodic motion

From eq. (4.6) the classical momentum function \(p_{rc}(r, E, L)\) is

\[
p_{rc}(r, E, L) = \left[ E + \frac{g}{r} - \frac{L^2}{r^2} \right]^{1/2}.
\]  (5.1)

As shown in Figure 5.1 the particle has an energy \(V_0 < E < 0\) where \(V_0\) is the minimum of the effective potential energy. The particle's radial coordinate oscillates between the two turning points \(r_1\) and \(r_2\). There is a branch cut of \(p_{rc}\) connecting its two branch points \(r_1\) and \(r_2\). We define \(p_{rc}\) to be positive just below the cut. This is equivalent to the condition

\[
p_{rc}(r, E, L) \simeq -\frac{iL}{r} \text{ around } r = 0.
\]  (5.2)
Figure 5.1: Bound state motion in Coulomb potential
The radial action variable is defined as

\[ J_{rc} = \frac{1}{2\pi} \oint_C p_{rc}(r, E, L)dr, \]  

(5.3)

where \( C \) encloses \( r_1 \) and \( r_2 \) and the branch cut between them. Condition (5.2) and the contour \( C \) make \( J_{rc} \) real and positive for physical bound motion; and furthermore, will be shown later to be consistent with the usual conventions of scattering theory.

The integral (5.3) is evaluated by distorting \( C \) into \( C_0 \) and \( C_\alpha \) and using the residue theorem. \( p_{rc} \), given by (5.1), can be written in terms of the turning points as

\[ p_{rc} = \frac{-iL}{\sqrt{r_1 r_2}} \frac{(r-r_1)^{1/2}(r-r_2)^{1/2}}{r}, \]  

(5.4)

with

\[ r_{1,2} = \frac{-g \mp \sqrt{g^2 + 4EL^2}}{2E}. \]  

(5.5)

\( p_{rc} \) has a simple pole of residue \(-iL\) at \( r = 0 \) (see eq. (5.2)). Thus, by the residue theorem,

\[ \frac{1}{2\pi} \oint_{C_0} p_{rc}(r, E, L)dr = L. \]  

(5.6)

The Laurent series for \( p_{rc}(r, E, L) \) on \( C_\alpha \) is obtained by binomial expansion:

\[ p_{rc}(r, E, L) = \frac{-iL}{\sqrt{r_1 r_2}} \left[ 1 - \frac{1}{2} (r_1 + r_2) \frac{1}{r} + \ldots \right], \]

so,

\[ \frac{1}{2\pi} \oint_{C_\alpha} p_{rc}(r, E, L)dr = \frac{-L}{2\sqrt{r_1 r_2}} (r_1 + r_2). \]  

(5.7)

Using (5.6) and (5.7), we obtain

\[ J_{rc} = -L - \frac{L}{2\sqrt{r_1 r_2}} (r_1 + r_2) \]

\[ = -L + \frac{g}{2\sqrt{-E}}. \]  

(5.8)
Solving this for $E$ in terms of $Jrc$ we get

$$E = - \frac{(g/2)^2}{(Jrc + L)^2}. \quad (5.9)$$

The angular frequency $\omega_r$ is

$$\omega_r = \frac{\partial E}{\partial Jrc} = \frac{4(-E)^{3/2}}{g}.$$  

As the semimajor axis of the particle's elliptic orbit is proportional to $1/(-E)$ we have derived Kepler's third law of planetary motion which states that the square of the planet's period is proportional to the cube of the semimajor axis.

**Definition of $Jrc$ as a contour integral for all energy**

We seek to extend the definition of the radial action variable to positive energies. For these energies the particle's classical radial motion under the Coulomb potential is unbounded. If the initial condition is such that the particle approaches the attractive center then it is deflected by the center and it recedes from it continuously. Such a scattering state has only one physical radial turning point $r_1$, the other turning point $r_2$ being negative, and therefore unphysical. The traditional definition of $Jrc$ for bound states as the integral $\frac{1}{2\pi} \oint_{prc} dr$ over one cycle of the radial motion cannot be extended to scattering states; such an integral is singular for scattering states since the orbit is unbounded and the radial momentum $pr$ is non-zero even as the particle moves far away from the scattering center. The definition of $Jrc$ as a contour integral in the complex $r$ plane does not suffer from this deficiency; the definition used for bound states lends itself to a natural extension to scattering states.

The contour integral definition of $Jrc$ requires a study of how $r_1$ and $r_2$, the branch points of $prc(r, E, L)$, move with energy. Also the nature of $prc(r, E, L)$ for all
complex $r$ for both positive and negative energies is needed. The energy is considered complex with a positive imaginary part $\epsilon E$ and is written as $\mathcal{E} = E + i \epsilon E$. $r_1$ and $r_2$ are functions of $\mathcal{E}$ and $L$ given by (5.5). We study the motion of these two turning points by varying $\mathcal{E}$, but keeping the total angular momentum $L$ fixed at a positive value.

The motion of the turning points with respect to the energy is shown in Figure 5.2. Though the physically allowed energies of the particle are greater than $V_0$, the minimum of the effective potential energy, we study $r_1$, $r_2$ and $\rho_{rc}$ as functions of $\mathcal{E}$ for all energy, to understand how their character transforms in a smooth way as $\mathcal{E}$ shifts from one region to the next. $a_1$ shows the location of $r_1$ for $E = E_a$, $a_2$ the location of $r_2$ for $E = E_a$, etc. The following is the variation of $r_1$ and $r_2$:

(i) For $E = E_a$, with $E_a < V_0$, $r_1$ is in the lower half plane and $r_2$ in the upper half plane and they are both near $r = 0$ (see Figure 5.3. The positive nature of $\epsilon E$ makes $r_1$ lie wholly in the lower half plane and $y_g$ wholly in the upper half plane for the energies considered in Figure 5.3.

(ii) As $E$ increases $r_1$ and $r_2$ loop and as $E \to V_0$ they approach each other. If $\mathcal{E} = V_0$ then $r_1 = r_2$. The non-zero $\epsilon E$ thus avoids this situation.

(iii) As $E$ increases to $E_f$, $r_1$ and $r_2$ are near the positive part of the real $r$ axis, with $r_1$ a little below and $r_2$ a little above the real axis. $r_1$ remains close to the positive part of the real axis as $E$ is increased further and approaches $r = 0^+$.

(iv) $\text{Re}(r_2)$ increases with increasing $E$ and as $E$ changes sign from negative to positive, $r_2$ moves along a counterclockwise curve in the upper half plane, approaching the negative real axis ($f_2 \to h_2$) in Figure 5.4. The radius of this curve is inversely proportional to $\sqrt{\epsilon E}$. 
Energies of the particle

Figure 5.2: Variation of the turning points $r_1$ & $r_2$ with energy
Figure 5.3: Contour $C$ for evaluating $J_{rc}$ for Coulomb potential
With $E$ positive and increasing, $\text{Re}(r_2)$ approaches $r = 0$. The branch cut of $p_{rc}(r, \mathcal{E}, L)$ is drawn connecting $r_1$ and $r_2$ as shown in the Figure (5.3). It is a straight line for $E = E_a$ and is varied continuously as a simple curve connecting the moving turning points. The sense of the contour $C$, which encloses $r_1$ and $r_2$ and the cut, is counterclockwise for all $\mathcal{E}$. The condition (5.2) at the origin is maintained for all $\mathcal{E}$ so that when the particle is in the bound state region $V_0 < E < 0$, $\text{Re}(p_{rc})$ is negative just above the branch cut and positive just below the cut. As the particle's radial coordinate oscillates, its radial momentum is positive during the first half of the cycle and is negative during the second half. The nature of $p_{rc}(r, \mathcal{E}, L)$ just above and below the cut and the orientation of the contour $C$, over which the integral $\int p_{rc}dr$ is performed in the definition of $J_{rc}$, reflects this. When the energy becomes positive $p_{rc}(r, \mathcal{E}, L)$ is positive in the physically allowed region of $r > \text{Re}(r_2)$, with $r$ real. It represents the radial momentum of a particle going away from the attractive center.

We define $J_{rc}$ for all $\mathcal{E}$ by

$$J_{rc} = \frac{1}{2\pi} \int_C p_{rc}(r, \mathcal{E}, L)dr.$$  

(5.10)

This definition of the radial action variable coincides with our previous definition (5.3) for the physical, bound state case of $V_0 < E < 0$. It analytically extends this definition to all other values of $E$. As in (5.3) the integral is evaluated in each case by distorting $C$ into $C_0$ and $C_{\alpha}$ and using the residue theorem. As before, the integral over $C_0$ gives $-L$ and that over $C_{\alpha}$ gives $g/2\sqrt{-E}$ yielding (5.8) again.

The variation of the radial action variable with energy is shown in Figure 5.4. With this definition of the radial action variable $J_{rc}$ is a real monotonically increasing function of $E$ for $E < 0$, correctly giving the frequency for the allowed periodic
motion. For positive energy $J_{rc}$ is positive imaginary, with $Im(J_{rc})$ monotonically decreasing with $E$; the frequency becomes purely imaginary. These unbound orbits for positive energy have a periodicity in time if time were imaginary. $J_{rc}$ for the bound state is a constant of the motion which is a measure of one complete cycle of the motion. This $J_{rc}$ is a successful construction of such a measure of the entire motion for scattering states of positive energy.

**Modified definition of $J_{rc}$**

While definition (5.10) correctly serves as an analytic continuation of $J_{rc}$ to all $E$ a modified but equivalent definition of $J_{rc}$ is presented in this section [2]. As will be seen in the next chapter this modified definition will be useful in the context of
quantum mechanics while (5.10) itself cannot be extended into quantum mechanics.

The integrand in (5.10) has two poles, one at \( r = 0 \) and the other at \( r = \infty \) and they both make their contributions to \( J_{\text{rc}} \), the former through the contour \( C_0 \) and the latter through \( C_\alpha \). If we changed this integrand in such a way that its pole at \( r = \infty \) is "moved" to a point \( r = 1/\epsilon_r \), with \( \epsilon_r \) positive imaginary and, after the evaluation of \( J_{\text{rc}} \) as a contour integral, we take the limit of \( \epsilon_r \to 0 \), then we recover the definition of \( J_{\text{rc}} \) above. Such a modification is shown here.

The modified definition of \( J_{\text{rc}} \) is

\[
J_{\text{rc}}(\epsilon_r) = \lim_{\epsilon_r \to 0} J_{\text{rc}}(\epsilon_r)
\]

with a positive imaginary \( \epsilon_r \), and the contour \( C \) defined as in Figure 5.5. The evaluation of this integral is done by distorting \( C \) into the contours \( C_0, C_\epsilon \) and \( C_\alpha \) (see Figure (5.5)). The denominator in the integrand makes the integral over \( C_0 \) vanish. The denominator also produces a second order pole of the integrand at \( r = 1/\epsilon_r \). The contribution from \( C_0 \) does not change. The integral over \( C_\epsilon \) yields

\[
\frac{g - 2L^2 \epsilon_r}{2\sqrt{V_{\text{eff}}(r = 1/\epsilon_r) - \mathcal{E}}},
\]

where \( V_{\text{eff}}(r) = -g/r + L^2/r^2 \) is the effective potential. Thus,

\[
J_{\text{rc}} = -L + \frac{g - 2L^2 \epsilon_r}{2\sqrt{V_{\text{eff}}(r = 1/\epsilon_r) - \mathcal{E}}},
\]

In the limit of \( \epsilon_r \) vanishing this becomes (5.10) again, showing thereby that this definition of \( J_{\text{rc}} \) which requires a modification of the integrand is equivalent to the one in the previous section.
Figure 5.5: Contours for the modified $J_{rc}$
CHAPTER 6. SEMICLASSICAL STUDY - COULOMB POTENTIAL

The definition of the quantum radial action variable $J_r$ requires a study of the locations of the poles of $p_r$ in the complex $r$ plane. This study is carried out here using a semiclassical method. Results of a numerical study based on the semiclassical method are presented.

$J_r$ for bound states and energy eigenvalues

From eq. (4.19) the radial momentum function equation for a particle moving in the Coulomb potential is

$$-i\hbar \frac{\partial p_r(r, E, l)}{\partial r} + p_r^2(r, E, l) = p_{rc}^2(r, E, l),$$

$$= E + g/r - l(l+1)\hbar^2/r^2, \quad (6.1)$$

with the boundary condition

$$\lim_{\hbar \to 0} p_r(r, E, l) = p_{rc}(r, E, l). \quad (6.2)$$

We define the quantum radial action variable $J_r$ by

$$J_r = \frac{1}{2\pi} \oint_{C} p_r(r, E, l)dr, \quad (6.3)$$

where $C$ is the same contour as the one used in evaluating $J_{rc}$, i.e., a counterclockwise contour in the complex $r$ plane enclosing $r_1$ and $r_2$ and the region in between.
Figure 6.1: The poles of $p_r$ in the complex $r$ plane
them, as shown in Figure 6.1. This problem is identical to a one dimensional bound state problem studied in section 3.2. $C$ encloses $n_r$ poles of $p_r(r, E, l)$ of residue $-i\hbar$ on the real axis between $r_1$ and $r_2$, hence, by the residue theorem, $J_r = n_r \hbar$. The integral in (6.3) can be performed, as in the evaluation of $J_{rc}$, by distorting $C$ into $C_0$ and $C_\infty$. To obtain the series expansion for $p_r$ on $C_0$, we note that it must have a simple pole at $r = 0$ since $p_{rc}$, its classical counterpart which it approaches in the classical limit, is of the form $-i\sqrt{l(l+1)\hbar^2/r + \cdots}$ there. Thus the momentum function equation (6.1) would be satisfied only if $p_r$ is of the form

$$p_r = \frac{a_{-1}}{r} + a_0 + a_1 r + \cdots.$$  \hspace{1cm} (6.4)

On the same contour $C_0$, the series form for $p_{rc}$ is

$$p_{rc} = \frac{A_{-1}}{r} + A_0 + A_1 r + \cdots,$$  \hspace{1cm} (6.5)

where

$$A_{-1} = -i\sqrt{l(l+1)\hbar^2}, \ldots.$$  

Substituting (6.4) and (6.5) in (6.1), we get

$$a_{-1}^2 + i\hbar a_{-1} - A_{-1}^2 = 0,$$

thus $a_{-1} = -i(l+1)\hbar$ or $i\hbar$. The latter results in a series for $p_r$ that does not satisfy the classical boundary condition (6.2) and, therefore, must be rejected. The contribution from $C_0$ to the integral (6.3) is therefore $l+1$. A similar method yields the contribution from $C_\infty$ which is $g/2\sqrt{-E}$. The square root is positive for negative energy. Therefore,

$$J_r = -(l+1)\hbar + g/2\sqrt{-E} = n_r \hbar,$$  \hspace{1cm} (6.6)
with \( n_r = 0, 1, 2, \ldots \). Solving this for \( E \) we get the energy eigenvalues of the system:

\[
E = -\frac{(\sigma/2)^2}{(n_r + l + 1)^2 \hbar^2}.
\]  

(6.7)

Here \( n_r \) is the radial quantum number and \( n = n_r + l + 1 \) is the principal quantum number.

The boundary condition (6.2) was crucial in obtaining these eigenvalues. It is shown in [1] that this requirement is equivalent to the normalizability condition on the radial wave function of the particle. It is also shown there that for these discrete energies the only poles of the integrand in eq. (6.3) in the complex \( r \) plane are the ones on the real axis between \( r_1 \) and \( r_2 \) and the two fixed poles at \( r = 0 \) and \( r = \infty \).

The condition of normalizability is relaxed in the study of wave functions for positive energy states. Similarly, in the rest of this chapter, where we consider states of both negative and positive energy, the boundary condition (6.2) is relaxed. A study of the nature of \( p_r \) reveals that, for non-negative energy eigenvalues, in addition to the above poles there is a family of infinite poles. Before we can define \( J_r \) as a contour integral in the complex \( r \) plane for such energies we need to know the location and motion of these infinite poles of \( p_r \); this will be the subject of the next part of this chapter.

**Semiclassical method for the study of the poles of \( p_r \)**

The quantum momentum function equation (6.1) is a Riccati equation which can be converted to the Schrödinger equation

\[
h^2 u'' + p_r^2 \psi u = 0,
\]  

(6.8)
by the transformation

\[ p_r = -i\hbar u'/u, \quad (6.9) \]

where prime denotes differentiation with respect to \( r \) (see [1]). The poles of \( p_r \) in the complex \( r \) plane (to be referred to as 'poles') are then the zeroes of the radial wave function \( u(r, E, l) \) (to be referred to as the 'zeroes').

**Boundary condition on \( u(r, E, l) \)**

The boundary condition (6.2) on the momentum function \( p_r \) is relaxed since we consider, besides energy eigenvalues, energies of the particle which are either unphysical or positive. This amounts to removing normalizability as a requirement on the wave function \( u(r, E, l) \). Equation (6.8) is linear and has a regular singular point at \( r = 0 \), because \( p_r^2 \) around that point is of the form \( -l(l+1)\hbar^2/r^2 \). The two linearly independent solutions of \( u \) have the character of \( r^{l+1} \) and \( r^{-l} \). The physical interpretation of \( u/r \) as the probability amplitude for the particle to be found between \( r \) and \( r + dr \) rules out the solution of the second form, for energy eigenvalues. Thus \( u \sim r^{l+1} \) around \( r = 0 \) for bound states. We continue to maintain this condition on \( u \) for all energies of the particle. Thus, for all energy \( E \),

\[
\lim_{r \to 0} u(r, E, l) = \begin{cases} 0 & \text{for } l \neq 0, \\ \text{a constant} & \text{for } l = 0. \end{cases} \quad (6.10)
\]

If the energy is a negative eigenvalue then \( u \to 0 \) as \( r \to +\infty \) and is normalizable, as we will see later. From eq. (6.9), the character of \( p_r \) at \( r = 0 \) on a negative energy eigenvalue, viz, a simple pole of residue \(-i\hbar(l + 1)\), is maintained for all energies.
Approximate solution of Schrödinger equation - Stokes phenomenon

The WKB approximation for a solution of (6.8) is of the form

$$u \simeq (1/\sqrt{p_{rc}})[Ae^{iW_{rc}/\hbar} + Be^{-iW_{rc}/\hbar}], \quad (6.11)$$

where $A$ and $B$ are constants and

$$W_{rc}(r, E, l) = \int_{r_0}^{r} p_{rc}(r, E, l) dr, \quad (6.12)$$

$r_0$ being a turning point, viz, $p_{rc}(r_0, E, l) = 0$. Such a solution is good in regions which are far from the turning points and the singularities of $p_{rc}$ (see [5]). The constants $A$ and $B$ have to be chosen differently in different regions of the complex plane for the following reason. $u$ is single valued throughout the finite complex $r$ plane but the right hand side of (6.11) is not, since $W_{rc}$, being the integral of $p_{rc}$ (a discontinuous function) is discontinuous. It has a branch cut starting at the turning point $r_0$ and going to $r = \infty$. We describe here a method due to Furry [6] that selects $A$ and $B$ in the different regions such that the approximate solution is relatively smooth.

We need to know the nature of $W_{rc}$ around the turning point $r_0$ before we can choose the appropriate constants $A$ and $B$. Since $p_{rc}^2 = E - V(r) = V'(r_0)(r - r_0) + \ldots$, with $V(r)$ the effective potential, the functional form of $p_{rc}$ very near $r_0$ is

$$p_{rc} \simeq \frac{1}{2}[-V'(r_0)]^{1/2}(r - r_0)^{1/2}.$$

Thus, by (6.12), $W_{rc}$ near $r_0$ is of the form

$$W_{rc} \simeq \frac{2}{3}[-V'(r_0)]^{1/2}(r - r_0)^{3/2}. \quad (6.13)$$
It follows from (6.13) that the phase of $W_{rc}$ around $r = 0$ changes by $180^\circ$ as that of $\Delta r = r - r_0$ changes by $120^\circ$. There are three directions, making angles of $120^\circ$ with each other, along which we can move from $r_0$ in the complex $r$ plane in such way that the expression in (6.13) is purely imaginary. Once we have started out in any one of these directions we can choose the increments $dr$ such that $p_{rc}dr$ is imaginary, and thus define a locus along which $W_{rc}$ is purely imaginary. Such a locus is called a 'Stoke's line' and is, in general, a curved line (see Figure 6.2). One of the two exponentials in (6.11) dominates the other along a Stokes line. Complementing these Stokes lines are three 'anti-Stokes lines' which start out at angles of $60^\circ$ with respect to the Stokes lines and along which $W_{rc}$ is purely real. In Figure 6.2 these anti-Stokes lines are marked 1, 2 and 3. The branch cut for $W_{rc}$ is chosen along the anti-Stokes
line 1 and 4 represents the other side of the branch cut. \( W_{rc} \) is negative along 1 (the definition of \( p_{rc} \) fixes this character), negative imaginary along \( S_1 \), positive along 2, positive imaginary along \( S_2 \), negative along 3, negative imaginary along \( S_3 \) and positive along 4. In a solution of the form (6.11) both \( \exp(\pm iW_{rc}) \) have unit magnitude along an anti-Stokes line. We represent the approximate solution along the anti-Stokes line 1 by \( u_1 \approx (1/\sqrt{p_{rc}})[A_1 e^{iW_{rc}/\hbar} + B_1 e^{-iW_{rc}/\hbar}] \). As we rotate from a point on 1 counterclockwise the magnitude of \( \exp(iW_{rc}) \) grows till we reach the Stokes line \( S_1 \) on which this exponential completely dominates in strength the other exponential \( \exp(-iW_{rc}) \). Now, if the approximate solution on the anti-Stokes line 2 were assumed to be \( u_2 \approx (1/\sqrt{p_{rc}})[A_2 e^{iW_{rc}/\hbar} + B_2 e^{-iW_{rc}/\hbar}] \), and extend this solution clockwise onto the Stokes line \( S_1 \), it must agree with the first solution \( u_1 \) within the limits of the approximation. This would force the two coefficients of the dominant exponential, viz, \( A_1 \) and \( A_2 \), to be identical while allowing for a discontinuity in the coefficients of the subdominant exponential \( B_1 \) and \( B_2 \). This is referred to as the Stokes phenomenon. Thus,

\[
A_2 = A_1, \quad B_2 = B_1 + \gamma A_1,
\]

where \( \gamma \) is called the 'Stokes constant'. That the constants \( (A_2, B_2) \) are linear functions of \( (A_1, B_1) \) follows from the linearity of the Schröedinger equation (6.8) whose solutions admit of superposition. A similar set of relations hold between \((A_2, B_2)\) and \((A_3, B_3)\) on the one hand and \((A_4, B_4)\) and \((A_3, B_3)\) on the other, with the subscripts on the constants denoting the respective anti-Stokes lines on which the constants are used in the representation of the approximate solution. Finally, we need to impose the continuity of the approximate solution on the branch cut. These requirements completely determine the four sets of constants \( (A_j, B_j) \) if any one of
them is known. All the Stokes constants $\gamma$ can be shown to be $i$ [6] and the connection formulas relating the different $(A_j, B_j)$ are

\[
\begin{align*}
A_2 &= A_1 & A_3 &= A_2 + iB_2 & A_4 &= A_3, \\
B_2 &= B_1 + iA_1 & B_3 &= B_2 & B_4 &= B_3 + iA_3.
\end{align*}
\]

(6.14)

In summary, there are, surrounding every turning point, three regions, with the Stokes lines separating adjacent regions and an anti-Stokes line in the middle of each region. Within each region we represent the wave function $u$ by an expression of the form (6.11) with suitably chosen constants $A$ and $B$ to satisfy the boundary conditions on $u$ in that region. The connection formulas (6.14) then provide the constants to be chosen in the other two regions. If in a region the solution has non-zero coefficients $(A_j, B_j)$, there is the possibility that the two exponentials cancel each other and that $u(r, E, l)$ has zeroes, and so $p_r$ poles, in that region. Setting the right hand side of (6.11) to zero we obtain an equation for the zeroes $r_n$ of $u$ in the region where the solution is valid:

\[
W_{rc}(r_n, E, l) = \left[ (1/2i) \ln(-B/A) + n\pi \right] \hbar
\]

(6.15)

This furnishes us with a means to search semiclassically for the poles in the complex $r$ plane. We undertake such a search for the poles of $p_r$ for a particle moving in the Coulomb potential; it is done analytically within the approximation of the semiclassical method above. In the last section of this chapter we examine the results of a numerical study based on the this method. A similar method is used to search for the poles in the case of the Yukawa potential.
Figure 6.3: Stokes lines (broken lines) from turning points $r_1$ and $r_2$ for $E < V_0$

Poles for $E < V_0$

Figure 6.3 shows the different regions around the two turning points $r_1$ and $r_2$ for energy $E < V_0$. The regions around $r_1$ are numbered 2, 3, 4 and 5 as shown. The primed numbers similarly denote the regions around $r_2$. We have followed a scheme in numbering these lines that show how the different regions around a turning point transform as we increase the particle's energy. There are two turning points here instead of one; so one has to define two $W_{rc}$s, one corresponding to $r_1$ and the other to $r_2$. In the definition (6.12) the turning point used for defining $W_{rc1}$ is $r_1$ and that for $W_{rc2}$ is $r_2$. The approximation for $u$ around $r_1$ is expressed in terms of $W_{rc1}$ and that around $r_2$ in terms of $W_{rc2}$. The constant coefficients to be used in the solution around $r_2$ are not independent of the ones used in the solution around $r_1$; there is the
region common to 2 and $5'$ (or 5 and $2'$) and the $u$ expressed in terms of $W_{rc1}$ should match the one expressed in terms of $W_{rc2}$. From the requirement (5.2) on $prc$, as $r \to \infty$, $prc \to k = \sqrt{E}$, which by our definition of $prc$, is positive imaginary for negative energy. Thus for large $r$, $prc dr$ is positive or negative imaginary depending on whether $dr$ is positive or negative. The Stokes lines are thus asymptotically horizontal in the complex $r$ plane for negative energy. Similarly the anti-Stokes lines are vertical.

We first obtain the solution in region 2 consistent with the boundary condition (6.10). Close to the point $r = 0$ both the $W_{rc2}$s are proportional to $\ln r$ whose character is positive imaginary on the Stokes line from $r_1$ that goes into $r = 0$. Thus $\exp(-iW_{rc1}/\hbar)$ is singular at $r = 0$ and its coefficient $B_2$ must be zero. $A_2$ is arbitrary. Using these constants $A_2$ and $B_2$ we can determine $(A_3, B_3),$ $(A_4, B_4)$ and $(A_5, B_5)$ using the connection formulas (6.14). These constants are

$$A_3 = A_2, \quad A_4 = A_2, \quad A_5 = 0,$$

$$B_3 = 0, \quad B_4 = iA_2, \quad B_5 = iA_2.$$ (6.16)

Thus only region 4 around $r_1$ has an approximate solution $u$ containing both the exponentials $\exp(\pm iW_{rc1}/\hbar)$; Using eq. (6.16) in (6.15) we obtain the poles $r_n$ in this region:

$$W_{rc}(r_n, E, l) = (n - 1/4)\pi\hbar,$$ (6.17)

with $n = 1, 2, 3, \ldots$. Since all the poles are located at points where $W_{rc}$ is real it follows that the anti-Stokes line that points south of $r_1$ is the locus of infinitely many poles. Next, we obtain the solution in region $2'$, which overlaps with 5. The two
different representations of \( u \) here are

\[ u_{2t} \simeq (1/\sqrt{p_{rc}})[A_{2t} e^{iW_{rc2}/\hbar} + B_{2t} e^{-iW_{rc2}/\hbar}] \] (6.18)

and

\[ u_5 \simeq (1/\sqrt{p_{rc}})[A_5 e^{iW_{rc1}/\hbar} + B_5 e^{-iW_{rc1}/\hbar}], \] (6.19)

which, from (6.16) is

\[ u_5 \simeq iA_2 (1/\sqrt{p_{rc}}) e^{-iW_{rc1}/\hbar}. \] (6.20)

In Figure 6.4

\[ \int_{C_1} p_{rc} \, dr = \int_{C_2} p_{rc} \, dr + \int_{C_3} p_{rc} \, dr \]
Thus, from the definition (5.10) of the classical radial action $J_{rc}$, the two $W_{rc}$s are related by

$$W_{rc1} = \pi J_{rc} + W_{rc2}$$

Equating $u_5$ and $u_{2'}$ from (6.18) and (6.20), we get

$$A_{2'} = 0 \quad B_{2'} = -i\alpha A_2, \quad (6.21)$$

where

$$\alpha = \exp(-i\pi J_{rc}/\hbar).$$

The rest of the primed constants $A$ and $B$ can be obtained using the connection formulas (6.14):

$$A_{3'} = \alpha A_2, \quad A_{4'} = \alpha A_2, \quad A_{5'} = \alpha A_2,$$
Crossini

\[ E \text{ just below } V_0 \]

\[ E \text{ just above } V_0 \]

Figure 6.6: Stokes and anti-Stokes lines for \( E \approx V_0 \)

\[ B_{3'} = -i \alpha A_2, \quad B_{4'} = 0, \quad B_{5'} = 0. \] \hspace{1cm} (6.22)

We see that region 3', with \( u \) having two exponentials, has infinitely many poles located on the anti-Stokes line going north of \( r_2 \), a result we could have predicted by symmetry. The resulting picture of poles in the complex \( r \) plane for \( E < V_0 \) is shown in Figure 6.5. Anti-Stokes lines 4 and 3' go to \( r = \infty \). The limit point of the poles located on these anti-Stokes lines is thus \( r = \infty \).

**Poles for \( V_0 < E < 0 \)**

As seen in chapter 5 \( r_1 \) and \( r_2 \) move onto the positive real axis of the \( r \) plane and remain there for \( V_0 < E < 0 \) corresponding to the region of classical physical bound states. The Stokes and anti-Stokes lines from these two turning points are
shown in Figure 6.7. Figure 6.6 shows the geometry of these lines for energies close to \( V_0 \); the first of these is for \( E \) slightly less than \( V_0 \) and the second for \( E \) slightly greater than \( V_0 \). The two turning points are near each other for these energies. The transition to the the physically allowed region of \( E > V_0 \) from the unphysical \( E < V_0 \) region is characterized by the crossing of two Stokes lines, one each from \( r_1 \) and \( r_2 \) as shown in the figure; these lines rotate counterclockwise closing region 5' and opening region 1 while simultaneously closing region 5 and opening region 1'. One significant change after this transition is that the set of poles that were south of \( r_1 \) (in region 4) which used to follow the motion of \( r_1 \) now move to region 2' and follow \( r_2 \).

We first construct the semiclassical wave function \( u \) in region 2; here \( B_2 \), the coefficient of the dominant exponential has to vanish to satisfy the boundary condition
Table 6.1: Coefficients $A$ and $B$ of exp($\pm iW/h$)

<table>
<thead>
<tr>
<th>Energy Range</th>
<th>$A_1$</th>
<th>$B_1$</th>
<th>$A_2$</th>
<th>$B_2$</th>
<th>$A_3$</th>
<th>$B_3$</th>
<th>$A_4$</th>
<th>$B_4$</th>
<th>$A_5$</th>
<th>$B_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E &lt; V_0$</td>
<td>1</td>
<td>$-i$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>$i$</td>
<td>0</td>
<td>$i$</td>
</tr>
<tr>
<td>$V_0 &lt; E &lt; 0$</td>
<td>$1$</td>
<td>$-i$</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>$i$</td>
<td>0</td>
<td>$i$</td>
</tr>
<tr>
<td>$E &gt; 0$</td>
<td>$A_1'$</td>
<td>$B_1'$</td>
<td>$A_2'$</td>
<td>$B_2'$</td>
<td>$A_3'$</td>
<td>$B_3'$</td>
<td>$A_4'$</td>
<td>$B_4'$</td>
<td>$A_5'$</td>
<td>$B_5'$</td>
</tr>
<tr>
<td>$E &lt; V_0$</td>
<td>$-1/\alpha$</td>
<td>$-i\alpha$</td>
<td>$-i\alpha$</td>
<td>$\alpha$</td>
<td>$\alpha$</td>
<td>0</td>
<td>$\alpha$</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$V_0 &lt; E &lt; 0$</td>
<td>$-1/\alpha$</td>
<td>$-i\alpha$</td>
<td>$-i\alpha$</td>
<td>$\alpha$</td>
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<td>0</td>
<td>$\alpha$</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E &gt; 0$</td>
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<td>$\alpha$</td>
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<td>$\alpha$</td>
<td>0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$\alpha = \exp(-i\pi J_{rc}/h) \quad \beta = \alpha + 1/\alpha$

(6.10) on $u$ at $r = 0$ which lies in this region. The coefficient $A_2$ of the subdominant solution is arbitrary. The other three sets of constant coefficients of $u$ around $r_1$ are obtained from the connection formulas. The wave function is then extended to regions around $r_2$ by matching $u$ in the overlapping regions 4 and 1'. All the coefficients are listed in Table 6.1. Having determined the semiclassical wave function all over the $r$ plane we now examine the different regions for the presence of poles. A region where $u$ is proportional to the single exponential $\exp(iW_{rc1}/h)$ or $\exp(-iW_{rc1}/h)$ has no poles that move as the energy varies, unlike regions where $u$ has two exponentials.

**Poles in between $r_1$ and $r_2$**

In region 1

$$u_1 \simeq (1/\sqrt{prc})[e^{iW_{rc1}/h} - ie^{-iW_{rc1}/h}]$$

$$\sim (1/\sqrt{prc}) \sin(W_{rc1}/h - \pi/4), \quad (6.23)$$
which is the form of the solution, up to a constant, in between the turning points \( r_1 \) and \( r_2 \). The poles occur on the real axis when \( W_{rc1} = (n + 1/4)\pi\hbar \), with \( n \) an integer. If \( E \approx V_0 \), \( W_{rc1} \approx 0 \) for all \( r \) in between \( r_1 \) and \( r_2 \) and there are no poles on the real axis. As the energy increases the absolute value of \( W_{rc1} \) also increases and more and more poles appear between \( r_1 \) and \( r_2 \). We call these 'poles in the well'.

**Poles in the southern half plane**

In region 2' the wave function is of the form (see Table 6.1)

\[
\psi_{2'} = \frac{1}{\sqrt{\pi p_c}}[(1/\alpha)e^{iW_{rc2}/\hbar} + i\beta e^{-iW_{rc2}/\hbar}]
\]

\[
\sim (1/\sqrt{\pi p_c})[e^{iW_{rc2}/\hbar} + i(1 + \exp(-2i\pi J_{rc}/\hbar))e^{-iW_{rc2}/\hbar}], \quad (6.24)
\]

where \( \beta = \alpha + 1/\alpha \). We can deduce the following results from this form of the solution:

1. The part of the real axis \( r > r_2 \) is a boundary of the region where the above form of the solution is valid. For the range of energy under consideration \( J_{rc} \) is real and positive. For those energies for which \( J_{rc} = (n_r + 1/2)\hbar \), for integer \( n_r \) the coefficient of the dominant exponential in \( u \) vanishes, leaving the wave function a subdominant exponential for \( r > r_2 \); a normalizable wave function results for these special energies. These energies are the energy eigenvalues in the WKB approximation.

2. From (6.15) and (6.24) the \( j \)th pole \( r_j \) of \( p_r \) in this region is given by

\[
W_{rc2}(r_j, E, l) = [(1/2i) \ln [1 + \exp(-2i\pi J_{rc}/\hbar)] + (j + 1/4)\pi] \hbar \quad (6.25)
\]
We can write

$$W_{rc}(r,E,l) \approx [kr + O(\ln r)], \quad (6.26)$$

for $|r|$ large, with $E = k^2$. We define $k = i\kappa$ with $\kappa > 0$ and define

$$T(E) = \rho_T(E) e^{-i\phi_T(E)} = 1 + \exp(-2i\rho_{rc}(E,l)/\hbar). \quad (6.27)$$

For large $j$, from (6.25), (6.26), and (6.27)

$$r_j = x_j + iy_j \approx [-(1/2\kappa) \ln(\rho_T)] + (i/\kappa)(\phi_T/2 - (j + 1/4)\pi)]\hbar. \quad (6.28)$$

In this approximation, therefore, all the poles are located along a vertical line south of $r_2$, with a spacing of $\pi\hbar/\kappa$ between successive poles. As the energy increases, $\kappa = \sqrt{-E}$ decreases and the inter-pole distance increases.
(3) We can use equation (6.28) to study the motion of poles with energy. For $J_{re}(E + i\epsilon_E) = J + i\epsilon J$ with $J = Re(J_{re})$ and $Im(J_{re}) = \epsilon J > 0$ the distance in the complex $T$ plane between $T(E)$ and 1 is $|T(E) - 1| = \exp(2\pi\epsilon J/h) > 1$ (see Figure 6.8). As the energy increases from $V_0$, following definition (6.27), $T(E)$ moves clockwise around the point $T_0 = 1$ because $\phi_T$ increases (see eq. (6.8)). As $\phi_T \to \pi$, $\rho_T$ attains its minimum value $\approx 2\epsilon J/h$ and $x_j$, which is proportional to $-\ln(\rho_T)$ is maximum. As $\phi_T$ increases further $\rho_T$ increases and $x_j$ decreases. Thus as the phase $\phi_T$ passes through $\pi$ ($B \to C \to D$ in the figure) the pole goes out east and then comes back west. Such an eastward excursion of the pole followed by a westward return repeats cyclically for $\phi_T = \pi, 3\pi, 5\pi, \ldots$. If $\epsilon_E = 0$ then $\epsilon J = 0$ and $\operatorname{Min}(\rho_T) = 0$; the poles would move east all the way to $r = \infty$. This vanishing of $T$ results in $u$ being proportional to a single decaying exponential for $r \to \infty$ on the real $r$ axis, from (6.24), corresponding to an energy eigenvalue. $y_j$ depends on $E$ through both $\kappa$ and $\phi_T$. The dependence on $\phi_T$ is significant as $T(E)$ moves from $B$ to $D$ in Figure 6.8. On the curve $BCD$, $\theta_J = 2\pi J/h \approx \pi$, thus $J(E)$ and hence $\kappa(E)$ is nearly a constant for $T(E)$ on $BCD$. However for this short range of energy $\phi_T(E)$ varies through $\pi$, resulting in the advance of $y_j$ through approximately $\pi/\kappa_C$. As the energy passes by an eigenvalue the pole moves up towards the $x$ axis by about $\pi/\kappa_C$. For the parts $A \to B$ and $D \to F$ in figure 6.9 $\phi_T$ advances by $\pi$ tending to increase $y_j$; $\kappa$ decreases for this variation of $E$ tending to decrease $y_j$. Of these two counter influences determining the variation of $y_j$ it can be shown that the latter is more significant. During the advance of $E$ in carrying $T(E)$ from $A$ to $F$, there is a net upward movement of $y_j$, i.e., the pole comes closer to the $x$ axis. The resulting motion of such a “southern pole” corresponding to $j = 3$ for three cycles of $\phi_T$ is
Figure 6.9: Movement of a southern pole with energy

shown in Figure 6.9. These poles eventually become poles in the well, entering the
region between \( r_1 \) and \( r_2 \).

Poles in the northern half plane

The WKB form of the wave function in region \( 3' \) is of the form

\[
\psi' \sim (1/\sqrt{prc})(e^{i\sqrt{2/\hbar}} - i(1 + \exp(2i\pi J_{rc}/\hbar)e^{-i\sqrt{2/\hbar}}].
\]  

(6.29)

Defining

\[
T'(E) = \rho T'(E) e^{i\phi T'(E)} = 1 + \exp(2i/\pi J_{rc}(E, l)/\hbar)
\]

\[
= 1 + \exp(-2i\varepsilon J/E)/\hbar) \exp(2i\pi J(E)/\hbar).
\]

(6.30)

\( T' \) varies with \( E \) as shown in Figure 6.10. It moves counterclockwise with increasing
energy around the point \( T_0' = 1 \). This \( T' \) path does not encircle the point \( T' = 0 \),
since \( \exp(-2\epsilon_j/\hbar) < 1 \). The location of the \( j \)th pole is given by

\[
 r_j = x_j + iy_j \approx \left[ -(1/2\kappa) \left\{ \ln(\rho_T^j) + (i/\kappa)(j - 1/4)\pi - \phi_{T^j}/2 \right\} \right] \hbar. \tag{6.31}
\]

These poles are thus located on a vertical line going north of \( r_2 \). The variation of \( x_j \) is similar to the case of southern poles. The variation of \( y_j \) is however different; the phase \( \phi_{T^j} \) does not monotonically increase. It is bounded by the angle \( OB^j \) and \( OD^j \) make with the \( x \) axis; and \( \phi_{T^j} \) oscillates between \( \angle D'OOC' \) and \( \angle B'OOC' \). \( \kappa \) decreases, and therefore \( y_j \), which is proportional to \( 1/\kappa \) increases, with increasing negative energy. These "northern poles" do not approach the real axis unlike the southern poles. This lack of symmetry between the poles in the southern and northern half planes arises because of the positive nature of \( \epsilon_j \) which, in turn, results from
Figure 6.11: Movement of a northern pole with energy

our choice of a positive \( \epsilon_D \). The variation of a northern pole with energy is shown in Figure 6.11. Figure 6.12 shows the locations of poles as the energy increases from one negative eigenvalue to the next.

**Poles for \( E > 0 \)**

As \( E \) becomes positive the turning point \( r_2 \) moves to the negative real axis of the \( r \) plane while \( r_1 \) continues to be on the positive real axis. The pictures of Stokes and anti-Stokes lines during this transition are shown in Figure 6.13. As in the transition around \( E = V_0 \), Stokes lines from the two turning points cross over around \( E = 0 \), pushing regions 1 and 1' out while forming the new regions 5 and 5'. The important change is in the character of \( p_{rC} \) which, for large \( r \), is approximately \( \sqrt{E} \) and is,
by our definition of the classical momentum function, positive for positive $E$. The Stokes lines, corresponding to the direction of $dr$ that yields imaginary $p_r c d r$, point north and south in the $r$ plane asymptotically for negative energy; and the anti-Stokes lines point east and west, i.e., they are oriented perpendicular to the Stokes lines asymptotically. After the transition from negative to positive energy the anti-Stokes line 4 assumes the role of $2'$ in that it now is in the center of the region that contains the poles which were located south of $r_2$ for negative energy. Following the counterclockwise rotation through $90^\circ$ of the anti-Stokes line 4 the southern poles also rotate by $\pi/2$ and now move to the real axis. Similarly the northern poles follow the anti-Stokes line $3'$ and move to the negative real axis. This motion of all the poles as the energy changes from negative energy to positive energy after passing through the negative eigenvalues is shown in Figure 6.15. The Stokes and anti-Stokes lines
Figure 6.13: Stokes and anti-Stokes lines for $E \approx 0$

for positive energy are shown in Figure 6.14

From Table 6.1 the two regions of pole locations are 4 and $3'$. Using the coefficients $A$ and $B$ from this table we write the wave functions in these two regions:

$$u_4 \sim \frac{1}{\sqrt{prc}} \sin \left\{ \frac{W_{rc1}}{\hbar} - \frac{\pi}{4} \right\},$$
$$u_{3'} \sim \frac{1}{\sqrt{prc}} \cos \left\{ \frac{W_{rc1}}{\hbar} - \frac{\pi}{4} \right\}.$$

The zeroes $r_j$ thus lie to the right of $r_1$ on the real axis for $W_{rc1}(r_j) = (n + 1/4)\pi \hbar$ and to the left of $r_2$ on the real axis for $W_{rc2}(r_j) = (n + 1/4)\pi \hbar$, as predicted.
Figure 6.14: Stokes and anti-Stokes lines for $E > 0$

Figure 6.15: Motion of the southern and northern poles with increasing energy
Semiclassical numerical study of the motion of poles with energy

We present here the results of a semiclassical numerical study of the determination of the poles as a function of energy. The equations \( u_2^j(r_j) = 0 \) and \( u_3^j(r_j) = 0 \) are solved numerically by the Newton-Raphson method. For convenience we have set \( \hbar = 1 \). The energies used in the calculation are shown in the complex \( E \) plane. As seen before, the maxima of \( \text{Re}(r_j(E)) \), where \( r_j \) is the \( j \)th southern pole, is approximately proportional to \( \ln \epsilon_j \). We can thus restrict the rapid variation of the location of a pole around the energy eigenvalues by controlling the magnitude of \( \epsilon_j \).

Figures 6.16 and 6.17 show the motion of the three topmost southern poles with energy computed numerically. These figures correspond to successively smaller values of constant \( \epsilon_j \) (this makes the imaginary part of energy, which is proportional to \( \epsilon_j \), also smaller for successive computations). The numbers 1, 2, 3, ... in the figure indicate the positions of the poles for \( E = E_1 + i\epsilon E, E_2 + i\epsilon E, E_3 + i\epsilon E, \ldots \) respectively. As predicted the poles go out farther east, as the energy nears an eigenvalue, the smaller \( \epsilon_j \) is at an energy eigenvalue. The sensitivity of the maximas of \( \text{Re}(r_j) \) to \( \epsilon_j \) is logarithmic as is evident from the figures. Also the increase in \( \text{Im}(r_j) \) as the energy passes by an eigenvalue is the same for every pole; the WKB analysis predicts this increase to be \( \pi/\sqrt{-E_n} \), where \( E_n \) is the \( n \)th energy eigenvalue, which matches the computed increase in \( \text{Im}(r_j) \). The \( n \)th southern pole enters the region of the real axis between \( r_1 \) and \( r_2 \) as the system’s energy equals that of the \( n \)th excited state. All the southern poles are on the positive real axis for positive energies. Figure 6.18 shows the first ten southern poles computed for negative energies.

Figures 6.19 and 6.19 show the movement of the northern poles with energy, computed by an identical method. As predicted, these poles perform right-left oscilla-
tions with energy for negative energies, with \( \text{Re}(r_j) \) displaying the same logarithmic sensitivity to \( \epsilon E \) as the southern poles for energies near an eigenvalue. As \( E \) becomes positive, the northern poles move counterclockwise and reach the negative real axis. This can be understood by following the rotation of anti-Stokes line 3' in Figure 6.13 as \( E \) changes sign from negative to positive values. The northern poles have this anti-Stokes line as their asymptote, since \( W_{rc2} \) is real on this line; and from equation (6.29) these poles are located where \( W_{rc2}(r_j) \approx (j - 1/4) \) for large \( j \). That the line 3' rotates counterclockwise around \( E = 0 \) follows from the character of \( W_{rc2} \) far from the origin: \( W_{rc2} \approx kr \) there. The phase of \( E \) decreases from \( \pi \) to 0 as the sign of \( E \) becomes positive; the phase of \( k = \sqrt{E} \) decreases from \( \pi/2 \) to 0. The phase of \( W_{rc2} \approx kr \) on the anti-Stokes line 3' is \( \pi \) and has to retain this character even during the rapid change of phase of \( k \) around \( E = 0 \). This is achieved by the counterclockwise rotation of \( r \), the position of a point on the anti-Stokes line, increasing its phase by \( \pi/2 \), so that the phase of \( kr \) remains \( \pi \) for points on the anti-Stokes line.

We will see in Chapter 7 that the exact positions of these poles and their characteristic variations with energy, as determined by numerically integrating Schrödinger equation, are represented quite accurately by the numerical method based on the WKB approximation of the wave function in the complex \( r \) plane presented in this chapter.
Figure 6.16: First three southern poles of $p_r$ computed using the WKB approximation for the Coulomb wavefunction.
Figure 6.17: First three southern poles of $p_r$ computed using the WKB approximation for the Coulomb wavefunction with smaller $\epsilon E$.
Figure 6.18: Ten southern poles of $p_r$ in the complex $r$ plane computed using the WKB approximation for the Coulomb wavefunction
Figure 6.19: First northern pole of $p_r$ computed using the WKB approximation for the Coulomb wavefunction
Figure 6.20: First northern pole of $p_T$ computed using the WKB approximation for the Coulomb wave function with smaller $\epsilon E$.
Figure 6.21: Ten northern poles of $p_r$ in the complex $r$ plane computed using the WKB approximation for the Coulomb wavefunction.
CHAPTER 7. EXACT STUDY OF THE POLES OF MOMENTUM FUNCTION - COULOMB POTENTIAL

We describe in this chapter a numerical method used to find the poles of the quantum momentum function $p_r(r, \mathcal{E}, L)$ of a particle moving in the Coulomb potential as a function of energy. The results of the computation of the poles is presented along with their comparison with the predictions of the semiclassical analysis of Chapter 6.

**Computation of the poles of $p_r(r, \mathcal{E}, L)$**

From the semiclassical analysis of the locations of the poles of $p_r(r, \mathcal{E}, L)$ for a particle moving in a Coulomb potential we know that for $E = E_{\text{high}} \gg 0$ the zeroes of $u(r, \mathcal{E}, L)$ are located to the right of $r_1$ and to the left of $r_2$ on the real axis in the complex $r$ plane. We first find the approximate location of these zeroes $r_j$ by solving equations (6.25) numerically. We then numerically integrate the Schrödinger equation (6.8) from the initial point $r_0 = (\epsilon r_0, 0)$, with initial conditions $u(r_0, E_{\text{high}}, l) = \epsilon r_0^{l+1}, u'(r_0, E_{\text{high}}, l) = (l+1)\epsilon r_0^l$, with $\epsilon r_0 << 1$, to the point $r = r_j$. These initial conditions are consistent with (6.10). Having obtained $u(r_j, E_{\text{high}}, l)$ and $u'(r_j, E_{\text{high}}, l)$ we search for the zero closest to $r_j(E_{\text{high}}, l)$. The integration is performed by a 4th order Runge-Kutta method and the search for a zero is carried out using the Newton-Raphson method. Once we have the zero
$r_j(E_{\text{high}}, l)$ the energy is incremented by $-\Delta E$ and the search for $r_j, E_{\text{high}} - \Delta E, l)$ done as before. This procedure is repeated for an energy range that extends up to $E = E_{\text{low}} < 0$.

Results of numerical computation of poles and their comparison with semiclassical results

Figures (7.1) and (7.2) show the first three northern poles computed as functions of energy. Figure (7.3) is similar; the energies used for this computation had a constant imaginary part unlike the previous two figures where the imaginary part of energy was varied to keep $\epsilon_j$ constant. If the energy were purely real those poles not on the real axis move all the way to $r = \infty$ for energy eigenvalues. By our choice of a complex energy we have avoided this situation; these figures show the sensitivity of $\text{Re}(r_j)$ to $\epsilon_j$. The variation of these poles with energy is very similar to that predicted by the WKB analysis of Chapter 6. The numbers $n$ in the figures represent the location of the poles when $E = E_n$. The maxima of $\text{Re}(r_j)$ are attained on energy eigenvalues. The $n$th southern pole enters the region between $r_1$ and $r_2$ for $E = E_n$. Thus every pole comes on to the real axis for some negative energy. As the energy is increased the number of poles in the well increases by one when $E$ passes by an eigenvalue. For positive $E$ all the southern poles are on the real axis.

Figure (7.4) shows the motion of the second southern pole with energy for successively increasing total angular momentum $l$. As $l$ increases, from equation (6.7), $|E(nr, l)|$ decreases, and the WKB expression (6.28) predicts the maxima of $\text{Re}(r_j)$ to be inversely proportional to $\sqrt{|E(nr, l)|}$. This explains the greater eastward motion of the poles around eigenvalues for higher $l$. 
Figure (7.5) represents the computed locations of the northern poles. These are again consistent with the corresponding pictures of chapter 6 based on the WKB analysis. The passage of $E$ from negative to positive values brings these northern poles onto the negative real axis to the left of $r_2$, by moving them in an arc in the $r$ plane.

**Effectiveness of the WKB method**

All the features observed in the motion of the poles of $p_r(r, \mathcal{E}, L)$ with $\mathcal{E}$ can be explained using the semiclassical expressions of Chapter 6. Instead of finding an exact expression for the wave function for all energies of the system we can make use of the approximate wave function to locate the poles; the location of the poles of the quantum momentum function and their variation with energy is accurately predicted by the WKB analysis, as our comparison of the precisely computed pole locations with the corresponding ones obtained by the semiclassical analysis reveals. Our study of the momentum function for the Yukawa potential will parallel this analysis.
Figure 7.1: First three southern poles of \( p_\ell \) obtained by numerical integration of the Schrödinger equation for the Coulomb potential
Figure 7.2: First three southern poles of $p_T$ obtained by numerical integration of the Schrödinger equation for the Coulomb potential

Figure 7.3: First three southern poles of $p_T$ with constant $\epsilon_E$
Figure 7.4: Second southern pole of $p_r$ for three successively higher values of angular momentum
Figure 7.5: Northern poles of $p_r$ obtained through numerical integration of the Schrödinger equation for the Coulomb potential.
CHAPTER 8. DEFINITION OF $J_r$ FOR COULOMB POTENTIAL

The definition of the analytically extended quantum radial action variable has to meet the following requirements:

(i) $J_r$ must be a continuous function of energy, smoothly interpolating between physical bound states.

(ii) Its definition should have the same form for states of all energy, negative and positive.

(iii) The definition should agree with the contour integral definition of $J_r$ for bound states.

(iv) The form of the definition in the quantum case should correspond to the definition in the classical case.

We provide in this chapter such a definition of $J_r$ for a particle moving in the Coulomb potential. Our definition (6.3) of $J_r$ for quantum bound states is an integral of the form $(1/2\pi) \int p_r dr$ over a contour in the complex $r$ plane that enclosed the dynamical poles in the potential well. The integral has contributions from two fixed poles of the integrand, one at $r = 0$ and the other at $r = \infty$. We have seen in Chapters 6 and 7 that, for non-negative energy eigenvalues and for positive energies, there is an additional family of infinite poles whose limit point is $r = \infty$; thus the point $r = \infty$ cannot play the role of an isolated pole of the integrand for non-energy eigenvalues.
and for positive energy. We now describe a contour integral definition of $J_r$, due to Nanayakkara [2], that overcomes this problem. It involves a modification of the integrand on the lines of the one introduced in the definition of the classical radial action variable in chapter 5.

**Definition of $J_r$ by modifying the integrand**

The definition of $J_r$ for all energy is

$$J_r = \lim_{\epsilon_r \to 0} J_r(\epsilon_r)$$

with a positive imaginary $\epsilon_r$, and the clockwise contour $C'$, defined in Figure (8.1), encloses the points $r = 0$ and $r = 1/\epsilon_r$. The dynamical poles of $p_r$ (whose location is a function of energy) are in the exterior of $C'$ for all energies. We now show that the integrand in (8.1) has two fixed poles, one at $r = 0$ and another at $r = 1/\epsilon_r$. Thus the integral around $C'$ is done by distorting the contour into $C_0$ and $C_\infty$. Around $r = 0$ the integrand $\sim -(i/2\pi)(l + 1)\hbar/r$ as the denominator $(1 - \epsilon_r r)^2$ is $\approx 1$ and $p_r \sim -i(l+1)\hbar/r$, from (6.4). The contribution to $J_r$ from $C_0$ is, therefore, $-(l+1)\hbar$. Next, the denominator in the integrand has a second order zero at $r = 1/\epsilon_r$. This results in a second order pole for the integrand at that point if $p_r(r = 1/\epsilon_r, \mathcal{E}, l)$ is non-zero and finite. We obtain a semiclassical expression for $p_r$ at $r = 1/\epsilon_r$ and show that it indeed has such a character.
Figure 8.1: Contour $C'$ for the definition of $J_r$ for all energies
Semiclassical expression for $p_r$ near $r = 1/\epsilon_r$

For $E < 0$ the WKB wave function $u$ in the region containing $r = 1/\epsilon_r$ is of the form

$$u \approx (1/\sqrt{pr_c})[\exp(iW/\hbar) + G\exp(-iW/\hbar)],$$

where $G$ is a constant and $W$ is $W_{r\text{cl}}$ if $E < V_0$ and $W_{r\text{c2}}$ if $V_0 < E < 0$ (region 4 in Figure (6.3) and Table 6.1). The form of $W$ for large $r$ is

$$W = \int_{r_0}^{r} [E + g/r - (l + 1/2)^2\hbar^2/r^2]^{1/2} dr$$

$$= \int_{r_0}^{r} [k + (g/2k)/r + \ldots] dr$$

$$\approx c + kr + (g/2k)\ln(r) + O(1/r^2),$$

where $r_0$ is an appropriate turning point, $k = i\kappa = \sqrt{E}$ with $\kappa > 0$ for $E < 0$ and $c$ a constant. Since $\epsilon_r = i|\epsilon_r|$, $\exp(iW/\hbar)$ at the point $r = 1/\epsilon_r$ is proportional to $[1/|\epsilon_r|]g/2\hbar\kappa|\epsilon_r|$. This is large compared to $[|\epsilon_r|]g/2\hbar\kappa|\epsilon_r|$ to which the other exponential $\exp(-iW/\hbar)$ is proportional to. Thus around $r = 1/\epsilon_r$, for $E < 0$,

$$u \approx (1/\sqrt{pr_c}) \exp(iW/\hbar). \quad (8.2)$$

For $E > 0$, the point $1/\epsilon_r$ lies in a region where $u$ has the form $(1/\sqrt{pr_c}) \exp(iW/\hbar)$ (region 4 in Figure (6.3), region 2' in Figure (6.7 and region 3 in Figure (6.14); see Table 6.1)). Using (8.2) and the connection $p_r = -i\hbar u'/u$ between $u$ and $p_r$ we obtain

$$p_r \approx pr_c + O(1/r^2) \text{ and } p'_r = p'_{r c} + O(1/r^3). \quad (8.3)$$

for all energy $E$. Noting that $p'_{r c} \sim O(1/r^2)$ and that $p'_r$ is equal to $p'_{r c}$ to the leading order in $r$ we see that the contribution, to the zeroth order in $\epsilon_r$ of $C_\epsilon$ to $J_r$ is identical
Figure 8.2: Poles of $p_r$ for eigenvalue $E = E_2$

to that in the corresponding classical case, viz, $g/2\sqrt{-E}$. This is the contribution of $C_\infty$ in eq. (5.12) to $J_r$ when the energy of the system is a negative eigenvalue. $J_r$ is again given by eq. (6.6) as a function of $E$ and $l$ for all energies of the system.

**Definition of $J_r$ by modifying the integrand**

If the energy of the system is a negative eigenvalue (with $\epsilon_E = 0$) then the only poles of the integrand in (8.1) exterior to $C'$ will be the poles in the well, equal in number to the excitation $n_r$ of the system; the northern and southern poles recede to $r = \infty$ (see Figure (8.2)). The contour $C'$ can then be distorted into $C$ and
$C_\infty$ for evaluating the integral in (8.1). The denominator in the integrand, being a quadratic, and the numerator, to the leading order in $r$, a constant on $C_\infty$, means the integral over $C_\infty$ vanishes. The contribution from $C$, to the leading order in $\epsilon r$, is $n_r \hbar$. Definition (8.1) thus correctly reduces to our previous definition (6.3) of $J_r$ on negative energy eigenvalues. It also analytically extends the definition of the quantum radial action variable to all physically allowed energies of the system while also interpolating between physically allowed bound states.

**Significance of quantum Coulomb radial action variable**

Analogous to the classical radial excitation families which consist of orbits having the same angular momentum but different values of the radial action variable and energy, we can classify quantum states of a particle by their common angular momentum. The $J_r$ of such states with a common angular momentum is a function of energy; its energy dependence for Coulomb states is shown in Figure (8.3). For negative energies the physical bound states are characterized by integral $J_r$ only; this is unlike in the classical case where any real $J_{rc} > 0$ corresponded to a bound orbit. This quantization of $J_r$ thus quantizes the physical negative energies of the particle. The variation of $J_r$ with energy is shown in Figure (8.4). The quantum radial action variable, so defined by the same contour integral for all energies, while bringing out the significance of the physical bound states, also interpolates between these states smoothly by assuming noninteger values for the unphysical negative energy states. Such a definition, valid for all energies of the particle (including positive energy), is useful in the study of quantum resonances which, though unbound, are special positive energy states. The Coulomb potential does not admit resonances because it does
not have a potential well of finite width; a study of resonances thus has to await the construction of $J_r$ for a potential of the Yukawa type which does have resonances. This will be the focus of the next four chapters.
Figure 8.4: Variation of $J_T$ with energy for Coulomb potential
CHAPTER 9. CLASSICAL ACTION VARIABLE - YUKAWA POTENTIAL

The Yukawa potential is a model potential for the strong interaction between hadrons. It is attractive and dominant at short distances, providing strong binding. It is of the form \(-\frac{g}{r}\exp(-r/R)\) where \(g\), as in the Coulomb case, represents the square of the coupling constant and \(R\) is the range of the force. The mediation of a force between two particles by a massive particle of mass \(\mu\) produces a force of range \(\propto 1/\mu\). In the limit of zero \(\mu\) a potential of infinite range, like the Coulomb potential, results. A plot of the effective Yukawa potential, that includes the angular momentum barrier \(L^2/r^2\), is shown in figure 9.1. We consider Yukawian potentials with \(g\) and \(R\) such that

\[
L^2/g < 0.42R. \tag{9.1}
\]

It can be shown that this results in both a potential well and a potential hill for non-zero \(L\); the former is essential for the existence of bound states. It has a minimum strength of \(V_0\), which is the depth of the well, at \(r = r_0\) shown in figure 9.1. For a given radial distance \(r\) from the attractive center, the strength of the effective Yukawa potential is weaker than the corresponding Coulomb potential due to the presence of \(\exp(-r/R)\). There is, therefore, a potential well of finite width; the effective potential cuts off to zero rapidly after attaining a maximum \(V_h\) at \(r_h\).
Figure 9.1: Effective Yukawa potential as a function of real $r$. 
In this chapter we define the radial action variable for a classical bound state of the Yukawa potential and extend it analytically to all energies of the system, negative and positive.

**Location of classical turning points**

We first locate the classical turning points to define the classical momentum function \( p_{rc}(r, \mathcal{E}, L) \) as a suitable branch of \( \sqrt{\mathcal{E} - V_{\text{eff}}(r)} \) in the complex \( r \) plane. Unlike in the case of the Coulomb potential, the Yukawa potential has an infinite number of turning points with branch cuts of \( p_{rc}(r, \mathcal{E}, L) \) originating from each one of them. The classical momentum function is

\[
p_{rc}(r, \mathcal{E}, L) = \left[ \mathcal{E} + (g/r) \exp(-r/R) - L^2/r^2 \right]^{1/2}.
\]  

(9.2)

The turning points \( r_j \), which are functions of \( \mathcal{E}, L \) and \( g \), are obtained from

\[
p_{rc}(r_j, \mathcal{E}, L) = 0
\]

\[
\Rightarrow \mathcal{E} r_j^2 + g \exp(-r_j/R) r_j - L^2 = 0.
\]  

(9.3)

Equation (9.3), being transcendental, can be solved only approximately or numerically. We try an approximate solution first and then compare the answer with a numerical solution.

**Case (i):** \( E << -g^2/4L^2 \) and \( |r_j| << L^2/g \)

We rewrite eq. (9.3) as

\[
r_j = (-g/2\mathcal{E}) \exp(-r_j/R) \pm \sqrt[g \exp(-r_j/R)/2\mathcal{E}]^2 + L^2/\mathcal{E}.
\]  

(9.4)
For $|r_j| \ll L^2/g$, which from eq. (9.1), is $< R$, the exponential is approximately 1, so

$$r_j \simeq (-g/2\mathcal{E}) \pm \sqrt{[g/2\mathcal{E}]^2 + L^2/\mathcal{E}}, \quad (9.5)$$

which is identical in form to the corresponding Coulomb equation (5.5). For $E \ll -g^2/4L^2$ ($\equiv$ potential energy minimum $V_0$ in the Coulomb case), the first term in the square root can be ignored. Then $r_j$ has a real part that increases, and an imaginary part that increases in magnitude, as the negative $E$ increases. We conclude that there are two turning points $r_1$ and $r_2$ around $r = 0$ which move with energy like their Coulomb counterparts; this motion is shown in Figure 9.2a.

**Case (ii): $E \approx -g^2/4L^2$ and $r_j \approx r_0 \approx 2L^2/g$**

Now, an equation of the form (9.4) still holds locally around $r = r_0$, with $g$ replaced by $g' = g \exp(-r_0/R)$. This defining relation for turning points, being Coulombic in nature, moves the turning points $r_1$ and $r_2$ along paths shown in Figure 9.2b, similar to those of the corresponding Coulomb turning points. Alternately, the potential energy is quadratic in $(r - r_0)$ at the bottom of the potential well locally and for such a quadratic potential, the equation $E - V_{eff}(r) = 0$ has two roots of the form $r_{1,2} = r_0 \pm \Delta_0$, with $\Delta_0$ positive imaginary if $E < V_{eff}(r_0)$ and positive if $E > V_{eff}(r_0)$. As the energy enters the physically allowed region of $E > V_0$, $r_1$ moves to the left of $r_0$ and $r_2$ to the right of $r_0$ on the real axis, as shown in Figure 9.2c. We see from this figure that for any higher energy, $r_1$ is on the real axis and approaches $r = 0$ as $E \to \infty$. $r_2$ moves eastward along the real axis till it comes close to $r_h$ for $E \simeq V_h$, the potential hill peak. Figure 9.3 shows the computed motion of $r_1$ and $r_2$ with energy for $l = 1$, $g = 55$, $R = 1$; here, $V_0 = -702$. 
Figure 9.2: Motion of $r_1$ and $r_2$ with energy
Case (iii): $E \approx E_h$ and $r_j \approx r_h$

For energies $0 < E < E_h$, there are two turning points, $r_2$ and $r_3$, one on each side of $r_h$. This is shown in Figure 9.2d. Approximating the potential by a quadratic in $(r - r_0)$ around $r = r_h$ yields two turning points near $r_h$ of the form $r_{2,3} = r_h \pm \Delta_h$ with $\Delta_h$ positive for $E < E_h$ and negative imaginary if $E > E_h$. Thus $r_2$ moves into the upper half and $r_3$ into the lower half of the complex $r$ plane for $E > E_h$. This is shown in Figure 9.4a.

Case (iv): $E_h < E < E_w$ and $|r_j| \approx r_h$

For this range of energy $r_2$ moves along a counterclockwise arc in the upper half plane; $r_3$, its complex conjugate moves in the lower half plane (see Figure 9.4b). The
two approach each other near \( r = r_w \) for \( E \approx E_w \) where there is the second minimum of the potential energy. The quadratic approximation for \( V_{\text{eff}}(r) \) at \( r = r_w \) again shows that for \( E > E_w \), \( r_2 \) is to the right and \( r_3 \) to the left of \( r_w \). The motion of \( r_2 \) and \( r_3 \) for the energy range \( E > E_h \) is shown in Figure 9.4c. It is clear that for energies higher than \( V_w \), \( r_2 \) and \( r_3 \) will be on the negative real axis, with \( r_2 \to 0 \) and \( r_3 \to -\infty \) as \( E \to \infty \). Figure 9.5 shows the computed motion of \( r_2 \) and \( r_3 \) with energy for the range \( E = 2V_0 \to E \geq V_w \). The motion of \( r_3 \) for the energy range \( E < V_0 \to E \approx 0 \) requires a study of the region \( \Re(r) < 0 \).

Case (v): \( \Re(r) < 0 \)

For \( \Re(r/R) << 0 \) we can ignore the last term in eq. (9.3) and write

\[
\mathcal{E} r_n + g \exp(-r_n/R) \approx 0.
\]  

Writing \( r_n = r_nR + i r_nI \) and \( \mathcal{E} = |\mathcal{E}| \exp(i \theta \mathcal{E}) \) and substituting these in eq. (9.6) we get

\[
|\mathcal{E}| \cos(\theta \mathcal{E}) r_nR - |\mathcal{E}| \sin(\theta \mathcal{E}) r_nI \approx -g \exp(-r_nR/R) \cos(r_nI/R),
\]

\[
|\mathcal{E}| \sin(\theta \mathcal{E}) r_nR + |\mathcal{E}| \cos(\theta \mathcal{E}) r_nI \approx g \exp(-r_nR/R) \sin(r_nI/R).
\]

These two equations can be rewritten as

\[
r_nR \approx \frac{-g \exp(-r_nR/R)}{|\mathcal{E}|} \cos[r_nI/R + \theta \mathcal{E}],
\]

\[
r_nI \approx \frac{-g \exp(-r_nI/R)}{|\mathcal{E}|} \cos[r_nI/R + \theta \mathcal{E}],
\]

or, \( \frac{r_nI}{r_nR} \approx -\tan[r_nI/R + \theta \mathcal{E}] \).

If \( |r_nI/r_nR| >> 1 \), then from eq. (9.11),

\[
r_nI/R + \theta \mathcal{E} \approx (n + 1/2) \pi, \quad n = 0, \pm 1, \pm 2, \ldots
\]
Figure 9.4: Motion of $r_2$ and $r_3$ with energy
Figure 9.5: Computed motion of \( r_2 \) and \( r_3 \) with energy for the range \( E = 2V_0 \) to \( E \geq V_w \) with \( R = 1 \)

From eq. (9.11) and (9.12),

\[
\exp(-r_nR/R) \simeq (-1)^n \frac{|E|}{g} r_n I
\]  \hspace{1cm} (9.13)

For \( r_n I > 0 \), from eqs. (9.12) and (9.10) we have,

\[
r_n I/R \simeq (2n + 1/2) \pi - \theta \xi, \quad n = 1, 2, 3, \ldots
\]  \hspace{1cm} (9.14)

\[
r_{nR}/R \simeq -\ln \left( \frac{|E|R}{g} \right) \left( (2n + 1/2) \pi - \theta \xi \right)
\]  \hspace{1cm} (9.15)

and for \( r_n I < 0 \),

\[
r_n I/R \simeq (2n + 3/2) \pi - \theta \xi, \quad n = -1, -2, -3, \ldots
\]  \hspace{1cm} (9.16)

\[
r_{nR}/R \simeq -\ln \left( \frac{|E|R}{g} \right) \left( (2n + 3/2) \pi - \theta \xi \right)
\]  \hspace{1cm} (9.17)

Thus, the imaginary parts of these "western turning points" is relatively insensitive to the energy; their real parts depend on the energy logarithmically. As the energy
Figure 9.6: Motion of the western turning points with energy

increases, these turning points move east for $E < 0$ and move west for $E > 0$. The phase of the energy, $\theta_E$ decreases from $\pi$ to 0 as $E$ changes sign from $-$ to $+$; thus the western turning points move northwards by $\pi R$ around $\mathcal{E} = 0$. These predicted motions of the western turning points are shown in Figure 9.6. The turning points in the second quadrant are denoted by $r_{Tn}$ and those in the third by $r_{Bn}$, for “top” and “bottom” respectively. The exactly computed turning points are shown in Figure 9.7. The results agree with the above conclusions except for the first four turning points in the south.
Figure 9.7: Computed motion of the western turning points with energy for the range $E = 2V_0$ to $E \geq V_w$ with $R = 1$
Case (vi): Western turning points for $E \approx 0$

To understand the motion of the first three western turning points $r_{B1}$, $r_{B2}$ and $r_{B3}$ around $E \approx 0$ in Figure 9.7, we construct the following model. The zeroes $r_{0n}$ of the potential energy $V_{eff}(r)$ are given by

$$ g r_{0n} \exp(-r_{0n}/R) - L^2 = 0 $$  \hspace{1cm} (9.18)

An approximate solution of (9.18) is

$$ r_{0n} \approx [\ln(g/L^2) + \ln(2n\pi)] + i(2n + 1/2)\pi \quad n = 0, 1, 2, \ldots $$

and their complex conjugates. They are in the first and the fourth quadrants; Figure 9.8a shows their locations. We recast Equation (9.3) into the form

$$ \exp(-\delta_n) = \frac{1 - (E r_{0n}^2/L^2) \{1 + \delta_n R/r_{0n}\}^2}{1 + \delta_n R/r_{0n}} $$  \hspace{1cm} (9.19)

where $\delta_n = (r_n - r_{0n})/R$, $r_{0n}$ being the zero of the effective potential nearest to the turning point $r_n$. Assuming that the turning points are very nearly equal to the zeroes of $V_{eff}$ for $E \approx 0$, i.e., $|\delta_n/r_{0n}| \ll 1$, we can write, using eq. (9.19),

$$ \exp(-\delta_n) \approx 1 - \frac{E r_{0n}^2}{L^2} \delta_n \approx -\ln \left[1 - \frac{E r_{0n}^2}{L^2}\right]. $$  \hspace{1cm} (9.20)

If $|E r_{0n}^2/L^2| \ll 1$, which is true for turning points for low $n$ and $E \approx 0$, we can expand the logarithm in (9.20) yielding,

$$ \delta_n \approx [E r_{0n}^2/L^2] + \frac{1}{2}[E r_{0n}^2/L^2]^2. $$  \hspace{1cm} (9.21)

Figures 9.8b through 9.8g illustrate the use of eq. (9.21) to obtain the dependence on $E$ of the turning points $r_{Bn}$ near the real axis. By using the phases of $r_{0n}$ and
Figure 9.8: Motion of the western turning points with energy for $E \approx 0$
We can find the phase of $E' = E r_0^2 / L^2$; and from the phase of $E'$, we get the phase of $\delta_n$. Since $(r_n - r_{0n})$ is proportional to $\delta_n$, the turning point $r_n$ goes around the zero of $V_{eff}(r)$ clockwise. In Figure (9.7) we see $r_{B1}$, $r_{B2}$ and $r_{B3}$ display this behavior; the points in this figure indicate the locations of $r_{0n}$ in the fourth quadrant.

Using eq. (9.19) we can also explain the motion of $r_{B4}$ which moves in an arc rapidly for $E \approx 0$. A self consistent solution of eq. (9.19) is obtained by

$$1 - \left( E r_{0N}^2 / L^2 \right) \left( 1 + \frac{\delta N R}{r_{0N}} \right)^2 \approx 0$$

(9.22)

for some $n = N$; it leads to

$$\delta N = \frac{1}{R} \left[ -r_{0N} + L/\sqrt{E} \right].$$

(9.23)

It makes this particular turning point $r_{BN} = r_{0N}$ move in an arc counterclockwise through an angle $\pi/2$ as $\theta_E$ changes through $\pi$, and moving it onto the real axis to the right of $r_h$ where it becomes the turning point $r_3$. Which of the western turning points moves in an arc and reaches the real axis to become $r_3$ for positive $E$ thus depends on the magnitude of $\epsilon_E$; the smaller $\epsilon_E$ is, the lower is the western turning point that transforms itself into $r_3$, since $|\epsilon| \text{ in eq. (9.22)}$ is $\approx \epsilon_E$.

Definitions of the classical momentum function $p_{rc}(r, E, L)$ and $J_{rc}$

We choose branch cuts for $p_{rc}(r, E, L)$ for different energies as shown in Figures 9.9 through 9.11. One cut connects the turning points $r_1$ and $r_2$. The cuts from the western turning points go west to $r = \infty$. We choose + sign for $p_{rc}$ just below the cut connecting $r_1$ and $r_2$ for energies $V_0 < E < 0$ that correspond to classical bound
Figure 9.9: Branch cuts of $p_{rC}(r, \mathcal{E}, L)$ and the contour $C$ for $E < E_h$. 

- For $E < V_0$, $\xi = V_0 + i \varepsilon_E$.
- For $V_0 < E < 0$, $\xi = i \varepsilon_E$. 

where $r_1, r_2, r_3$ are the contour points, and $T_1, T_2, T_3$ are the branch cut points.
Figure 9.10: Branch cuts of $p_{rc}(r, \varepsilon, L)$ and the contour $C$ for $0 < E < E_w$.
Figure 9.11: Branch cuts of $p_{rC}(r, \mathcal{E}, L)$ and the contour $C$ for $E > E_w$
states. For all energies the counterclockwise contour $C$ encloses the turning points $r_1$ and $r_2$ and the cut joining them. We define $J_{rc}$, the classical action variable, by

$$J_{rc} = \frac{1}{2\pi} \oint_C p_{rc}(r, \mathcal{E}, L) \, dr.$$  

(9.24)

The evaluation of the integral in eq. (9.24) can be done using the perturbation theory developed in [7]. Writing the square of the classical momentum function as

$$p_{rc}^2 = -\frac{L^2}{r_1r_2} \frac{(r-r_1)(r-r_2)}{r^2} f^2(r)$$

(9.25)

with

$$f^2(r) = 1 + \sum_{n=1}^{\infty} v_n r^n,$$

(9.26)

we can show (see Appendix B) that

$$v_n \sim \left(\frac{r_2}{R}\right)^{n+1}.$$  

(9.27)

Using

$$f(r) = 1 + \sum_{n=1}^{\infty} t_n r^n,$$

(9.28)

squaring it to get the expansion for $f^2(r)$ and comparing that expansion with the one in eq. (9.27), we get

$$t_n = \frac{1}{2} [v_n - \sum_{j=1}^{n-1} t_j t_{n-j}],$$  

(9.29)

$$\sim \left(\frac{r_2}{R}\right)^{n+1}.$$  

(9.30)

Thus, $p_{rc}(r, \mathcal{E}, L)$ for the Yukawa potential has the same form as the one for the Coulomb potential (see eq. 5.4) in the zeroth order in $(r_2/R)$. From equations (9.24)
and (9.25) we can write $J_{rc}$ as a series:

$$J_{rc} = J_{rc}(\text{Coulomb}) + \sum_{n=1}^{\infty} P(r_1, r_2, n+1) t_n,$$

(9.31)

where

$$P(r_1, r_2, n) = \sum_{j=0}^{n} b_j b_{n-j} n! n^{n-j},$$

(9.32)

$b_j$ being the coefficients in the binomial expansion

$$[1 - x]^n = \sum_{j=0}^{\infty} b_j x^j.$$

(9.33)

In the limit of $R \to \infty$ (which turns the Yukawa potential into the infinite range Coulomb potential), all the $t_n$ (from eq. (9.30)) vanish and we recover the expression (5.8) for $J_{rc}$.

**Alternate definition of $J_{rc}$**

A classical Lagrangian of the form

$$\mathcal{L} = \frac{1}{4} \left[ \frac{\dot{r}^2}{(1 - \epsilon_r r)^4} + r^2 \dot{\theta}^2 + r^2 \sin^2 \theta \dot{\phi}^2 \right] - V(r),$$

(9.34)

with $\epsilon_r$ a positive number, reduces to the correct Lagrangian for a particle moving in a central potential $V(r)$ in the limit of $\epsilon_r \to 0$. The Lagrange equations of motion separates in the $r$, $\theta$ and $\phi$ coordinates and the equation of motion for $r$ is

$$\frac{d}{dt} \left[ \frac{1}{2} \frac{\dot{r}}{(1 - \epsilon_r r)^4} \right] = - \frac{V'(r)}{r} + \frac{2L^2}{r^3}.$$

(9.35)

Here $(1 - \epsilon_r r)^{-4}$ appears as the "effective mass" of the particle. The $\theta$ and $\phi$ equations of motion do not contain $\epsilon_r$. The Hamiltonian that corresponds to the
Lagrangian (9.34) is

\[ H = (1 - \epsilon_r r)^4 \mathcal{P}_{rc}^2 + \frac{p_{\theta c}^2}{r^2} + \frac{p_{\phi c}^2}{r^2 \sin^2 \theta} + V(r) \]  

(9.36)

Since \( H \) does not explicitly depend on time it is a constant, \( \mathcal{E} \), of the motion. Also the total angular momentum \( L \) is a constant of the motion. The classical momentum function \( \mathcal{P}_{rc} \) of such a particle at the radial coordinate \( r \) is

\[ \mathcal{P}_{rc}(r, \mathcal{E}, L) = \frac{\sqrt{\mathcal{E} - V(r) - L^2/r^2}}{(1 - \epsilon_r r)^2}. \]  

(9.37)

The classical turning points of the motion are independent of \( \epsilon_r \); thus they continue to be at the locations given in Figures 9.9 through 9.11. We define \( \mathcal{J}(\mathcal{E}, L, \epsilon_r) \) by

\[ \mathcal{J}_{rc}(\mathcal{E}, L, \epsilon_r) = \frac{1}{2\pi} \oint_{C'} \mathcal{P}_{rc}(r, \mathcal{E}, L) \, dr, \]  

(9.38)

where the counterclockwise contour \( C' \) encloses the turning points \( r_1 \) and \( r_2 \) and the point \( r = 1/\epsilon_r \), as shown in Figure 9.12, and the action variable is defined by

\[ \mathcal{J}_{rc} = \lim_{\epsilon_r \to 0} \mathcal{J}(\mathcal{E}, L, \epsilon_r). \]  

(9.39)

The integral over \( C' \) can be performed by distorting the contour \( C' \) into two contours \( C \) and \( C_\epsilon \). The integral over the former yields

\[ \frac{1}{2\pi} \oint_{C} \sqrt{\mathcal{E} - V(r)} \, dr + O(\epsilon_r), \]  

(9.40)

since the denominator in eq. (9.37) can be expanded, using the binomial theorem, in positive powers of \( \epsilon_r \). The integral over \( C_\epsilon \) is done using Cauchy's integral formula:

\[ \frac{1}{2\pi} \oint_{C} \frac{\sqrt{\mathcal{E} - V(r)}}{(1 - \epsilon_r r)^2} \, dr = \frac{i}{\epsilon_r^2} \left[ g \epsilon_r^2 (1 + \frac{1}{\epsilon_r R}) \exp(-1/\epsilon_r R) - 2L^2 \epsilon_r^2 \right]. \]  

(9.41)
Figure 9.12: Contour $C'$ for the definition of $J_{RC}$

$\tilde{J}(\mathcal{E}, L, \varepsilon_r)$, which is the sum of the integrals in (9.40) and (9.41), thus becomes $J_{RC}$ defined in eq. (9.24) in the limit of $\varepsilon_r \to 0$.

The usefulness of this alternate definition of $J_{RC}$ by a contour integral over $C'$ rather than $C$ will be evident when we consider the corresponding quantum problem. The interior of $C'$ has an infinite number of poles of the quantum momentum function $\mathcal{P}_r(r, \mathcal{E}, L)$ that vanish into the point $r = 1/\varepsilon_r$ on negative energy eigenvalues and an analytic continuation of $J_r$ for energies other than negative eigenvalues requires that we use a modified Hamiltonian of the type (9.36). We have demonstrated here that such a modification of the Hamiltonian leads to a definition of $J_{RC}$ that parallels the corresponding quantum definition.
Features of the Yukawa $J_{rc}$

We saw in chapter 5 the energy dependence of $J_{rc}$ for the Coulomb potential; the Coulomb turning point $r_2$ moves all the way to $r = \infty$ as $\mathcal{E}$ approaches 0 resulting in $J_{rc} \to \infty$ in this limit. The period of the bound radial Coulomb motion, as a consequence, grows indefinitely. For the Yukawa potential, on the other hand, the action variable $J_{rc}$ is finite as $\mathcal{E} \to 0$; there is a bound $r_h$ for the turning point $r_2$. This makes the integral in eq. (9.24) finite for $\mathcal{E} = 0$. A consequence of this, as we will see in chapter 11, is that the quantum bound states for the Yukawa potential, unlike for the Coulomb potential, are finite in number.
CHAPTER 10. SEMICLASSICAL STUDY - YUKAWA POTENTIAL

We study in this chapter the energy dependence of the locations of the poles of the quantum momentum function for the Yukawa potential using the WKB wave functions. We find that the structure of these poles bears similarity to those found in the case of the Coulomb potential. It also displays features that are distinctly different; instead of one family of infinite poles there are infinitely many such families, a result of the presence in the potential of the exponential which is periodic in the imaginary part of its argument. The short range nature of the potential which has a well of finite width curtails the total number of bound states to a finite number, unlike the Coulomb potential. The semiclassical method, due to its reliance on the turning points, which are infinitely many in this case, also poses problems that are peculiar to the Yukawa potential.

Nature of $W_{rc}(r, \varepsilon, L)$ west of the western turning points

From our study of the Yukawa potential we know that there are an infinite number of western turning points, in addition to the Coulomb like turning points $r_1$ and $r_2$. There are Stokes and anti-Stokes lines radiating outwards from these turning points, dividing the complex $r$ plane into regions in each of which one uses a WKB wave function which has the form of two exponentials $\exp(\pm iW_{rc}/\hbar)$; the
coefficients of the exponentials in each region are chosen so that the WKB solutions on the two sides of the boundary separating the two regions are relatively smooth, allowing for a discontinuity only in the subdominant exponential on the boundary (which is a Stokes line). A particularly simple insight into the nature of the Stokes and anti-Stokes lines originating at the western turning points is available. Consider a point $r$ west of the western turning points at which there is a Stokes line. To know the direction along which the Stokes line proceeds from this point $r$, we approximate the classical momentum function by

$$p_{rc}(r, \mathcal{E}, L) \simeq \sqrt{\frac{g}{r}} \exp\left(-\frac{r}{R}\right);$$

this is justified since the exponential has a real part $\exp\left(-\frac{Re(r)}{R}\right)$ that dominates the other two terms in $p_{rc}(r, \mathcal{E}, L)$. The phase of $p_{rc}(r, \mathcal{E}, L)$ is $-1/2(Im(r)/R + \theta_r)$, where $\theta_r$ is the phase of $r$. Since $|\theta_r| < |Im(r)|$ for $|r/R| < 1$ (very far west,) the phase of $p_{rc}(r, \mathcal{E}, L)$ is $\simeq -Im(r)/2R$. Thus for $Im(r) = (2n + 1)\pi R$, $n$ being an integer, $p_{rc}$ is imaginary and the line element $dr$ along the Stokes line must be real. This shows that there are Stokes lines, west of the turning points, going west, with vertical spacing of $2\pi R$, with $Im(r) = (2n + 1)\pi R$. Similarly there are anti-Stokes lines going west in the western half plane with $Im(r) = 2n\pi R$. This is true for all energies, positive and negative. We choose the branch cuts of $p_{rc}(r, \mathcal{E}, L)$ originating at the western turning points to lie along these anti-Stokes lines. In the right half plane, on the other hand, the pattern of Stokes and anti-Stokes lines depends on the sign of the energy. For $Re(r)$ large and positive, $p_{rc} \simeq \sqrt{E}$; therefore, $W_{rc}$, which is the integral of $p_{rc}(r, \mathcal{E}, L)$ is imaginary along paths going east of the western turning points for negative energy, hence the Stokes lines go east of the western turning points for $E < 0$; similarly the anti-Stokes lines go north and south. For $E > 0$, this
situation reverses; Stokes lines go north and south and anti-Stokes lines go east. We now study the different regions for the presence of poles by mapping the Stokes and anti-Stokes lines around each turning point and constructing the WKB wave function in each region.

**Poles for $E < V_0$**

Figure 10.1 shows the division of the $r$ plane into different regions with the Stokes lines (represented by the dashed lines) forming the boundaries of regions within which we can use a WKB wave function $u(r, \mathcal{E}, L)$ with a particular set of coefficients of $\exp(\pm iW_{rc}/\hbar)$. The nature of $W$ along a Stokes line ($\pm i$ like) is also shown ($W$ here refers to the the $W$ defined with respect to the turning point at which that particular Stokes line starts). The constant coefficients $A, B$ in the different regions surrounding a turning point are related by the connection formulas (6.14). Since the pattern of Stokes and anti-Stokes lines around the turning points $r_1$ and $r_2$ is identical to the corresponding picture in the Coulomb case (see figure 10.1), the coefficients $A_2, B_2, A_3, B_3, A_4, B_4, A_5, B_5$ and $A_{2'}, B_{2'}, A_{3'}, B_{3'}, A_{4'}, B_{4'}$ are the same as the ones listed in table 6.1, with $J_{rc}$ for the Coulomb potential replaced by the one for the Yukawa potential. The difference from the Coulomb case is that region $3'$ does not extend all the way to $\infty$ north but is bounded by the Stokes line going east from $r_{T1}$, the first western turning point on top of the real axis. This is because the the WKB solution $u(r, \mathcal{E}, L)$ in the region $3'$ surrounding the turning point $r_2$, expressed in terms of $\exp(\pm iW_{rc2}/\hbar)$ has to match the $u(r, \mathcal{E}, L)$ written in terms of $\exp(\pm iW_{T1}/\hbar)$ in the region 2 around $r_{T1}$; this matching is done in the region labeled "strip 2", which is part of both these regions. The subscripts on the $W$s here
Figure 10.1: Stokes and anti-Stokes lines for $E < V_0$
denote the turning points with respect to which these extended classical characteristic functions are defined, e.g., \( W_{T_1} \) is \( \int_{r_{T_1}} p_{rc}(r, \mathcal{E}, l) \, dr \) (see eq. (6.12)). Similar strips numbered 2, 3, 4, \ldots occupy the entire region to the east of the top western turning points, each strip numbered \( n + 1 \) representing the region where the wave function expressed in terms of \( W_{T_n} \) has to match the wave function expressed in terms of \( W_{T_{n-1}} \). This matching of the different WKB representations of \( u(r, \mathcal{E}, L) \) restricts us to use the \( W_{T_1} \) form of \( u \) in strip 3 instead of the \( W_{rc2} \) form, though both forms coincide in strip 2. Similar restrictions apply in the southern half plane.

The WKB solution \( u \) is first obtained in region \( 5' \) by imposing the boundary condition (6.10). This solution is extended to regions \( 2', 3' \) and \( 4' \) around \( r_2 \) using the connection formulas (6.14). The solution in region 2 around \( r_{T_1} \) is then obtained by matching it with the solution in region 3' near \( r_2 \). The connection formulas are again used to obtain the solution all around \( r_{T_1} \). One continues this procedure of extending the solution from regions surrounding a top turning point to the regions surrounding the next higher turning point. The solution in the southern half plane is similarly obtained. Table 10.1 shows the coefficients \( (A, B) \) of \( \exp(\pm iW/\hbar) \) for the regions around \( r_2 \) and \( r_{T_1} \). We identify regions where \( u \) has the form of two exponentials in order to locate the zeroes of \( u \). As in the Coulomb case region \( 3' \) (strip 2) has zeroes north of \( r_2 \). Similarly strip 3 has zeroes since region 3 near \( r_{T_1} \) has a \( u \) of the double exponential form. Every strip has zeroes, by extension. The spacing between these zeroes is of the order of \( \pi \hbar/\sqrt{|E|} \), which follows from an equation of the form (6.28). From this near constant spacing between the zeroes we can deduce that every strip has only finitely many zeroes, as these zeroes are near the anti-Stokes lines which run perpendicular to the strips and there is only a finite
Table 10.1: Coefficients $A$ and $B$ of $\exp(\pm i W/\hbar)$ for $E < V_0$

<table>
<thead>
<tr>
<th>$A_2$</th>
<th>$B_2$</th>
<th>$A_3$</th>
<th>$B_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$A_4$</td>
<td>$B_4$</td>
<td>$A_5$</td>
<td>$B_5$</td>
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</tr>
<tr>
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<td>$B_2'$</td>
<td>$A_3'$</td>
<td>$B_3'$</td>
</tr>
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<td>$-i\alpha$</td>
<td>$\alpha$</td>
<td>$-i\alpha$</td>
</tr>
<tr>
<td>$A_4'$</td>
<td>$B_4'$</td>
<td>$A_5'$</td>
<td>$B_5'$</td>
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<tr>
<td>$\alpha$</td>
<td>0</td>
<td>$\alpha$</td>
<td>0</td>
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</tbody>
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$\alpha = \exp(-i\pi J_{rc}/\hbar)$ \hspace{1cm} $\beta = \alpha + 1/\alpha$

$I_{2T_1} = \int_{r_2^{T_1}}^{r_1} prc(r, \epsilon, L) \, dr = W_{rc2}(r = r_{T_1})$

$\gamma_{2T_1} \exp \{ i W_{rc2}(r = r_{T_1}) / \hbar \}$

The length of the anti-Stokes line in any strip. The zeroes in the northern plane east of the western turning points is thus infinitely many, there being an infinite number of strips. These zeroes are very similar to the northern zeroes one encounters in the case of the Coulomb potential. A similar set of southern zeroes are present south of $r_1$. The other region around $r_{T_1}$ that has zeroes is region 4; The zeroes in this region have the anti-Stokes line west of $r_{T_1}$ as their asymptote. These are infinitely many; the spacing between them decreases exponentially as one goes west, since, from eq. (6.15),

$W_{T_1}(r_{n+1}) - W_{T_1}(r_n) = \pi \hbar$,
There is a similar train of zeroes west of every western turning point. These "western zeroes" of $u(r, E, L)$ or "western poles" of $p_r(r, E, L)$ grouped into infinitely many trains, with each train containing an infinite number of zeroes, are a new feature of the Yukawa potential. As the energy increases, these western zeroes move east along with the western turning points. This eastern motion with energy increase becomes less pronounced as one follows the motion of farther zeroes. The northern and southern zeroes have a motion similar to their Coulomb counterparts; they steadily get farther apart with energy increase. The pattern of the zeroes is shown in Figure 10.2.

**Poles for** $V_0 < E < 0$

As $E$ increases beyond $V_0$ the turning points $r_1$ and $r_2$ come onto the real axis. The plot of Stokes and anti-Stokes lines is shown in figure 10.3. The WKB coefficients $(A, B)$ for regions around $r_2$, $r_{T1}$ and $r_{B1}$ can be found as before. We obtain $u(r, E, L)$ by matching the WKB wave functions expressed in terms of $W_{rc}^s$ corresponding to neighboring turning points, following the sequence

$$r_1 \rightarrow r_2 \rightarrow r_{T1} \rightarrow r_{T2},$$  

$$r_1 \rightarrow r_2 \rightarrow r_{B1} \rightarrow r_{B2}.$$

The pattern of the lines around $r_2$ is similar to the one in the Coulomb case. The solution in every strip contains an exponential of the form $\exp(-iW/h)$ whose coefficient is proportional to $\cos(\pi J_{rc}/\hbar)$. This exponential is the dominant of the two exponentials in the solution on the Stokes lines east of the western turning points.
Figure 10.2: Poles of $p_r$ for $E < V_0$
Figure 10.3: Stokes and anti-Stokes lines for $V_0 < E < 0$
Table 10.2: Coefficients $A$ and $B$ of $\exp(\pm iW/\hbar)$ for $V_0 < E < 0$

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<td>$\alpha \gamma_2 T_1 + \beta/\gamma_2 T_1$</td>
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<th>$B_1 T_2$</th>
<th>$\gamma_2 T_1 \gamma_1 T_1 T_2^0 - i(1/(\gamma_2 T_1 \gamma_1 T_1 T_2) + \gamma_1 T_1 T_2/\gamma_2 T_1)$</th>
<th>$B_2 T_2$</th>
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<td>$\alpha \gamma_2 T_1 + \beta/\gamma_2 T_1$</td>
<td>$i\alpha/\gamma_2 T_1$</td>
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<th>$B_3 T_2$</th>
<th>$\gamma_2 T_1 \gamma_1 T_1 T_2^0 + (1/(\gamma_2 T_1 \gamma_1 T_1 T_2) + \gamma_1 T_1 T_2/\gamma_2 T_1)$</th>
<th>$B_4 T_2$</th>
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<td>$\alpha \gamma_2 T_1 + \beta/\gamma_2 T_1$</td>
<td>$i\alpha/\gamma_2 T_1$</td>
<td>$\alpha \gamma_2 T_1 + \beta/\gamma_2 T_1$</td>
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</table>

$\alpha = \exp(-i\pi J_R c/\hbar)$

$\beta = \alpha + 1/\alpha$

\[
I_{2T1} = \int_{\gamma_2 T_1} T_1 p_c(r, \varepsilon, L) \, dr = W_{rc2}(r = r_{T1})
\]

\[
I_{T1T2} = \int_{\gamma_1 T_1} T_2 p_c(r, \varepsilon, L) \, dr = W_{rcT1}(r = r_{T2})
\]

\[
\gamma_{2T1} = \exp\{iW_{rc2}(r = r_{T1})/\hbar\}
\]

\[
\gamma_{T1T2} = \exp\{iW_{rcT1}(r = r_{T2})/\hbar\}
\]
The energy eigenstates in the semiclassical approximation are characterized by this dominant exponential vanishing, for \( J_{rc}(\mathcal{E}, l) = (n + 1/2)\hbar \) for integral \( n \). For such energies \( \mathcal{E} = E_n + i\epsilon E \) the northern and southern poles go out east and move back west, with their eastern most location during this looping motion proportional to \( \ln(\epsilon_f) \). This is identical to the behavior of the Coulomb zeroes near energy eigenvalues. The southern zeroes move north steadily and at each energy eigenvalue the topmost southern zero enters the potential well, increasing by 1 the number of zeroes in between \( r_1 \) and \( r_2 \). The northern poles move north steadily. The important difference in the motion of the northern and southern poles with energy between the Coulomb and Yukawa potentials is the following. Since \( J_{rc} \) can increase without bound as one approaches \( \mathcal{E} = 0 \) in the Coulomb case the relation \( J_{rc} = (n + 1/2)\hbar \) is satisfied for infinitely many energies, thus the Coulomb potential admits of an infinite number of bound states. The Yukawa potential, on the other hand, sets an upper bound to \( J_{rc} \) by restricting the turning point \( r_2 \) to a finite value (see figure 9.1), resulting in a finite number of bound states. A finite number of zeroes enter the potential well for negative energies. The western zeroes move east as in the case of \( E < V_0 \). Unlike the northern and southern poles they display no sensitivity to eigenvalues. It can be shown, by using the WKB wave function in region 4 around \( r_{B2} \) that the train of zeroes west of that turning point never recede to \( r = \infty \); it is a result of the integral \( J_{2B1} \) not being real for any \( \mathcal{E} \). The pattern of zeroes for \( V_0 < E < 0 \) is shown in Figure 10.4.
Figure 10.4: Poles of $p_r$ for $V_0 < E < 0$
Poles for $E \approx 0$

The pattern of Stokes and anti-Stokes lines for $E \approx 0$ is shown in Figure 10.5. The turning point $r_{B4}$ breaks out of the sequence of southwestern turning points and arcs counterclockwise onto the real axis for positive energy to become $r_3$. As seen in Chapter 9, which of the southwestern turning points becomes $r_3$ depends on the magnitude of $\epsilon_E$. The southern zeroes, that have not entered the potential well follow the motion of $r_3$ and come onto the real axis. The poles and their motion for $E \approx 0$ is shown in Figure 10.4. The western zeroes move down while the western turning points move up by $\pi R$ as the energy changes sign from negative to positive.

Poles for $0 < E < V_0$

Figure 10.7 shows the Stokes and anti-Stokes lines for energies in the range $0 < E < E_h$. The semiclassical approach of Furry fails for this range for the following reason. There is a Stokes line connecting $r_2$ and $r_3$. $W_{rc2}$ is $+i$ like along the line from $r_2$ to $r_3$ while $W_{rc3}$ is $-i$ like along the line from $r_3$ to $r_2$. If $u$ in region marked I in Figure 10.7 is written as

$$ u_1 = \frac{1}{\sqrt{p_{rc}}} \left[ A_1 \exp(iW_{rc2}/\hbar) + B_1 \exp(-iW_{rc2}/\hbar) \right]. \quad (10.1) $$

We can also express $u_1$ in terms of $W_{rc3}$ as

$$ u_1 = \frac{1}{\sqrt{p_{rc}}} \left[ A'_1 \exp(iW_{rc3}/\hbar) + B'_1 \exp(-iW_{rc3}/\hbar) \right]. \quad (10.2) $$
Figure 10.5: Stokes and anti-Stokes lines for $E \approx 0$
Figure 10.6: Poles of $p_r$ for $E \approx 0$
Expressing $W_{rc2}$ in terms of $W_{rc3}$ we obtain the constant coefficients $A'_I, B'_I$ in terms of $A_I, B_I$:

$$A'_I = A_I \gamma_{23}, \quad B'_I = B_I / \gamma_{23} \quad (10.3)$$

where

$$\gamma_{23} = \exp(i \int_{r_2}^{r_3} \frac{pr_c}{\hbar} dr/h).$$

We can similarly write the wave function in the region marked II using the two $W$s:

$$u_{II} = (1/\sqrt{pr_c}) \left[ A_{II} \exp(iW_{rc2}/\hbar) + B_{II} \exp(-iW_{rc2}/\hbar) \right],$$

$$u_{II} = (1/\sqrt{pr_c}) \left[ A'_{II} \exp(iW_{rc3}/\hbar) + B'_{II} \exp(-iW_{rc3}/\hbar) \right], \quad (10.4)$$

with

$$A'_{II} = A_{II} \gamma_{23}, \quad B'_{II} = B_{II} / \gamma_{23}. \quad (10.5)$$

Using the connection formulas (6.14) to relate the coefficients of region II with those in region I, we can show that for all the $A$s and the $B$s to be not identically zero, $\gamma_{23} \equiv 0$, which is impossible. Thus the semiclassical method is not applicable in this case.

**Poles for $V_h < E < V_w$**

For the energy range $V_h < E < V_w$ the turning points $r_2$ and $r_3$ are complex and are complex conjugates of each other as shown in Figure 10.8. The regions where $u$ has the form of two exponentials is to the right of $r_1$ which is now filled with the southern zeroes, north of $r_2$, south of $r_3$ and west of every western turning point. All these regions contain poles as shown in Figure 10.9. The northern poles get closer to the western poles for this energy range.
Figure 10.7: Stokes and anti-Stokes lines for $0 < E < V_0$
Figure 10.8: Stokes and anti-Stokes lines for $V_b < E < V_w$
Figure 10.9: Poles of $p_r$ for $V_h < E < V_w$
Poles for $E > V_w$

For $E \approx V_w$ the turning points $r_2$ and $r_3$ are very close to each other; For $E > V_w$ these two turning points become real as shown in Figure 10.10. The wave function $u$ is oscillatory inside the western unphysical potential well. The poles from the first northwestern train fill up this well just as the southern poles fill up the physical potential well. The poles east of $r_1$ get closer as the energy increases. The poles for $E > V_w$ are shown in Figure 10.11.
Figure 10.10: Stokes and anti-Stokes lines for $E > V_\omega$
Figure 10.11: Poles of $p_r$ for $E > V_w$
CHAPTER 11. EXACT STUDY OF THE POLES OF MOMENTUM FUNCTION - YUKAWA POTENTIAL

We present in this chapter the results of numerical computations of the motion of the poles of $p_r$ for the Yukawa potential. The technique is similar to the one used for the Coulomb potential. To locate a western pole we integrate, from $r = 0$ to the western turning point at the eastern extremity of the pole train and start our Newton-Raphson search for the zeroes of $u$ west of that turning point.

Discussion of the numerical results

We denote the northern and southern poles by a single index, positive for northern poles and negative for southern poles. The western poles are denoted by $r_{ij}$ with $i$ a positive integer denoting the western pole train of which it is a part (positive integer if the pole is in the upper half of the plane and negative if in the lower half) and $j$ indicating the rank of the pole within the train starting with 1 for the pole which is eastern most for negative energy.

Figures 11.1 and 11.2 show the motion of the first two southern poles with energy for $l = 1$, $g = 23$. This system has two negative energy eigenvalues and no resonances in the scattering region. The four computations were done with four successively smaller values of $\epsilon_E$. The poles move farther out east if $\epsilon_E$, and therefore
\( \epsilon_j \), is smaller which is consistent with the prediction, based on the WKB approximation, of the logarithmic dependence on \( \epsilon_j \) of the real parts of the \( j \)th southern pole \( r_j \). In Figure 11.2, the figure corresponding to \( \epsilon_E = 2 \times 10^{-5} \), shows the large displacement of the first pole around the first energy eigenvalue with very little change in energy.

Figure 11.3 shows the first five southern poles move with energy with \( \epsilon_E = 0.1 \). The first pole, comes onto the real axis after an eastern excursion around the ground state energy. Poles \( r_{-2} \) through \( r_{-5} \) shown in the figure move in an arc around \( E \approx 0 \) and come onto the positive real axis. This behavior is unlike the motion of the southern poles for the Coulomb potential all of which reach the positive real axis for a negative energy.

Figures 11.4 through 11.6 show poles for three systems, each with \( g = 55 \) and \( l \) of 1, 2 and 3 (we have set \( \hbar = 1 \) in the computation). The \( l = 1 \) system has 4 negative energy eigenvalues, the \( l = 2 \) system 3 eigenvalues and the \( l = 3 \) system one eigenvalue and a resonance state. The one with \( l = 2 \) has the first three southern poles landing on the real axis but the fourth pole moves west around \( E \approx 0 \) and joins the western poles. It is observed that if a system has \( n \) bound states, then the first \( (n - 1) \) southern poles reach the positive real axis for positive energy while a finite number of southern poles immediately below the first \( (n - 1) \) join the train of western poles. The remaining ones of this group (infinitely many) arc around and come onto the positive real axis. The third of these systems is very interesting. It has the first southern pole come onto the positive real axis while the rest of the southern poles have an arcing eastward movement around the energy of resonance (determined by a phase shift analysis). This excursion of these southern poles for a positive energy
$l = 1$
$g = 23$

Figure 11.1: First two southern poles of $p_l(r, \xi, l)$ for $V_0 < E < V_w$ and $l = 1, \ g = 23$
Figure 11.2: First two southern poles of $p_r(r, \mathcal{E}, l)$ for $V_0 < E < V_W$ and $l = 1$, $g = 23$
Figure 11.3: First five southern poles of $p_r(r, \mathcal{E}, l)$ for $V_0 < E < V_w$ and $l = 1$, $g = 23$.
is very similar to their behavior around negative energy eigenvalues. The second one, after displaying negative eigenvalue like behavior of rapid motion around the resonant energy, moves west. This behavior of those southern poles that move west instead of coming onto the real axis requires further study. The WKB method, with limited regions of validity of the solutions, is not particularly suited to the study of the behavior of poles for $E \approx 0$.

Figure 11.7 shows the motion of northern and northwestern poles with energy for an $l = 1$, $g = 20$ system which has two bound states. The northern poles are sensitive to energy eigenvalues, like their southern counterparts, performing rapid motion with energy around energy eigenvalues. All except the first northern pole join the western train of poles for positive energy. The northwestern poles are insensitive to energy eigenvalues and move west for increasing negative energy. Around $E \approx 0$ they start a south and westward motion and come down vertically by about $\pi R$; the western turning points, for the same energy increment, move up vertically by $\pi R$. The vertical spacing between the turning points is $2\pi R$. Thus the poles which follow the eastward motion of a turning point for negative energy switch to following the motion of the turning point one below for positive energy while moving westward. The first northwestern train of poles (two poles $r_{11}$ and $r_{12}$ are shown in the figure) come down to the negative real axis. They fill the western potential well very much like the southern poles filled the physical eastern potential well.

Summary of the motion of poles with energy

(i) A system described by a Yukawa potential that admits $n$ bound states has $n - 1$ southern poles coming onto the region of the physical potential well. As the
Figure 11.4: First four southern poles of \( p_r(r, \mathcal{E}, l) \) for \( V_0 < E < V_w \) and \( l = 1, \ g = 55 \), with four bound states
Figure 11.5: First five southern poles of $p_r(r, \epsilon, l)$ for $V_0 < E < V_w$ and $l = 2, \, g = 55$ with three bound states
Figure 11.6: First three southern poles of $p_r(r, E, l)$ for $V_0 < E < V_w$ and $l = 3$, $g = 55$ with one bound state and a resonant state.
Figure 11.7: Northern and northwestern poles of $p_T(r, E, l)$ for $V_0 < E < V_w$ and $l = 1, \quad g = 20$ with two bound states
energy approaches an eigenvalue these southern poles move rapidly east and then west as the energy passes by the eigenvalue.

(ii) A finite number of the southern poles of rank \( n \) and higher move west for positive energy and join the southwestern train of poles.

(iii) The remainder of the southern poles move in an arc around \( E \approx 0 \) and come onto the positive real axis.

(iv) The northern poles perform rapid eastward motion for energies near negative energy eigenvalues. A finite number of them come into the unphysical western potential well. The rest of the northern poles join the trains of western poles.

(v) The western poles move east with increasing negative energy and move west with increasing positive energy. For energies near \( E = 0 \) they move down vertically by \( \pi R \). The first train of northwestern poles fill the unphysical well for \( E > V_w \).

The major difference between the set of western poles and the northern-southern poles is the vanishing of the latter into \( r = \infty \) for negative energy eigenvalues. This difference will guide our attempt at analytically extending the quantum action variable to scattering states.
CHAPTER 12. QUANTUM ACTION VARIABLE - YUKAWA POTENTIAL

The point \( r = \infty \) in the complex \( r \) plane has three distinct roles in the context of the quantum motion in the presence of the Yukawa potential. It is the limit point of the set of western turning points. It is the limit point of the northern and southern poles which also vanish into it on energy eigenvalues. It is also the limit point of every western train of poles. The analytic continuation of \( J_r \) as a contour integral for energies other than the negative eigenvalues requires that we take away from \( r = \infty \) one of the latter two roles. We describe in this Chapter such a definition of \( J_r \). We also demonstrate that this method is sufficiently general to be applicable to potentials that cut off faster than \( 1/r \).

\( J_r \) on negative energy eigenvalues

The Yukawa potential, as seen in Chapter 11, admits of a finite number of energy eigenvalues. For \( \mathcal{E} = E_n \), the energy of the \( n \)th excited state, there are \( n \) poles of \( P_r \) in between \( r_1 \) and \( r_2 \) on the real axis (see figure 12.1). There are no other poles in the plane east of the western turning points. We define \( J_r \) for such an energy eigenstate by

\[
J_r = \frac{1}{2\pi} \oint_C P_r(r, E_n, l) \, dr,
\]

(12.1)
Figure 12.1: Poles of $p_r$ for the energy eigenvalue $E = E_3$

where the counterclockwise contour $C$ encloses the real axis in between $r_1$ and $r_2$. The requirement on any analytic extension of $J_r$ is that it reduce to (12.1) for $E = E_n$. We now provide such a definition of $J_r$ for all energies $E$.

**Modifying the Hamiltonian using $\epsilon_r$**

We use the quantum Hamiltonian

$$\hat{H} = (1 - \epsilon_r \hat{r})^4 \left[ \hat{p}_r^2 + \frac{\hat{L}_r^2}{r^2} \right] + V(\hat{r})$$

(12.2)

corresponding to the classical Hamiltonian (9.36) used in the context of $J_{rc}$. The correct quantum version of the Hamiltonian must be symmetrized in $\hat{r}$ and $\hat{P}_r$ to make it Hermitian. We use the unsymmetrized version of it by treating $\epsilon_r$ as a small constant; this makes the non-Hermitian part of the Hamiltonian to be of order
\( \epsilon r \). \( J_r \) is defined by evaluating a contour integral \( \tilde{J}_r(\mathcal{E}, l, \epsilon r) \) and then taking the limit of \( \epsilon r \to 0 \). We use the coordinate representation. The Schrödinger equation, 
\[ \tilde{H}\psi = \mathcal{E}\psi, \]
with \( \tilde{H} \) defined by (12.2), separates in the \( r, \theta \) and \( \phi \) coordinates as in the case of the usual central force Hamiltonian (4.1). The Schrödinger equation for the radial wave function \( \mathcal{U}(r, \mathcal{E}, l, \epsilon r) \) corresponding to this modified Hamiltonian is
\[ \hbar^2 \mathcal{U}'' + \frac{[\mathcal{E} - V_{\text{eff}}(r)\]}{(1 - \epsilon r r)^4} \mathcal{U} = 0, \] (12.3)
In the limit of \( \epsilon r \to 0 \) this equation is the usual Schrödinger equation and
\[ \mathcal{U}(r, \mathcal{E}, l, \epsilon r) \to u(r, \mathcal{E}, l). \]

The classical momentum function \( \mathcal{P}_{rc}(r, \mathcal{E}, l, \epsilon r) \), corresponding to the modified Hamiltonian, is defined by
\[ \mathcal{P}_{rc}(r, \mathcal{E}, l, \epsilon r) = \frac{\sqrt{\mathcal{E} - V_{\text{eff}}(r)}}{(1 - \epsilon r r)^2} = \frac{p_{rc}(r, \mathcal{E}, l)}{(1 - \epsilon r r)^2}, \] (12.4)
with the branch of the square root defined as in the case of \( p_{rc} \) in Chapter 10. \( \mathcal{P}_{rc} \) has a second order pole at \( r = 1/\epsilon r \). The modification by the introduction of \( \epsilon r \) into the Hamiltonian has not introduced any new classical turning points; the turning points of \( \mathcal{P}_{rc}(r, \mathcal{E}, l, \epsilon r) \) are also the turning points of \( p_{rc}(r, \mathcal{E}, l) \) and vice versa.

The quantum momentum function equation for \( \mathcal{P}(r, \mathcal{E}, l, \epsilon r) \) corresponding to the Hamiltonian (12.2) is
\[ -i\hbar \frac{\partial \mathcal{P}(r, \mathcal{E}, l, \epsilon r)}{\partial r} + \mathcal{P}^2(r, \mathcal{E}, l, \epsilon r) = \frac{[\mathcal{E} - V(r) - l(l + 1)\hbar^2/r^2]}{(1 - \epsilon r r)^4}. \] (12.5)

We now present an analysis of the locations of the poles of this \( \mathcal{P}_r(r, \mathcal{E}, l, \epsilon r) \) for negative energies in the range \( V_0 < E < 0 \); the extension to other energies is straightforward.
The point $r = 1/\epsilon_r$ is located in region 2' around the turning point $r_2$. To see how the above modification of $\mathcal{H}$ affects the Stokes and anti-Stokes lines pattern, consider a point in the eastern half plane for $\text{Re}(r) >> 0$. Here $\sqrt{E - V_{\text{eff}}(r)} \simeq \sqrt{E} = k$ and $\mathcal{P}_{rc} \simeq k/(1 - \epsilon_r r)^2$. Therefore

$$\mathcal{W}_{rc2}(r) = \int_{r_2}^{r} \mathcal{P}_r(r, E, l, \epsilon_r) \, dr \simeq c - \frac{1}{\epsilon_r^2} \frac{k}{r - 1/\epsilon_r},$$

(12.6)

where $c$ is a constant. The terminus of every anti-Stokes line (and therefore of the limit point of the associated set of infinite poles, if any) is a point at which $\mathcal{W}_{rc2} \to \infty$. From eq. (12.6), which is valid in the eastern half plane, $\mathcal{W}_{rc2} \to c$ as $r \to \infty$ and $\to \infty$ as $r \to 1/\epsilon_r$. Therefore the point $r = \infty$ does not have the character to be the limit point of the poles of $\mathcal{P}_r$ but the point $r = 1/\epsilon_r$ does. Thus those anti-Stokes lines that were east of the western turning points for the unmodified case treated in Chapter 10 and found their way into $r = \infty$ now go into $r = 1/\epsilon_r$. This is also true of the Stokes lines in the eastern half plane. The picture of Stokes and anti-Stokes lines for the case of this modified Hamiltonian is shown in Figure 12.2. The limit point of the northern and southern zeroes is the terminus of these anti-Stokes lines in the eastern half plane; therefore the limit point of these zeroes is $r = 1/\epsilon_r$ and not $r = \infty$. Furthermore, if the energy of the system is an energy eigenvalue, then, by eq. (6.15), the pole at $r_j$ belonging to the family of northern-southern poles, should have an infinite $\mathcal{W}_{rc2}(r_j)$, i.e., $r_j = 1/\epsilon_r$ for all $j$. For energy eigenvalues $E = E_n$, therefore, the northern and southern poles have moved to $r = 1/\epsilon_r$. The modification introduced has little effect in the region west of the western turning points, where the exponential in $\mathcal{P}_{rc}$ overwhelms the $r^2$ term introduced into the denominator of $\mathcal{P}_{rc}$. Thus the pattern of Stokes and anti-Stokes lines west of the western turning points and the western trains of poles changes little.
Figure 12.2: Stokes (broken lines) and anti-Stokes lines for $V_0 < E < 0$

In particular the limit point of the western poles continues to be $r = \infty$. The limit points of the two sets of poles, the northern and southern on the one hand and the western on the other, are thus different, which is unlike the cases we have studied without $\varepsilon_r$. The locations of the poles of $\mathcal{P}_r(E, l, \varepsilon_r)$ in the $r$ and $s = 1/r$ planes for energies in the range $V_0 < E < 0$ are shown in Figure 12.3.
Figure 12.3: Poles of $P_r(r, \varepsilon, l, \varepsilon_r)$ for $V_0 < E < 0$
Exploration of the singularity at \( r = 1/\varepsilon_r \)

The point \( r = 1/\varepsilon_r \) is an irregular singular point of the second order linear differential equation (12.3), as the right hand side has the term \((r - 1/\varepsilon_r)^4\) in its denominator. A solution of such a differential equation may have a branch point at an irregular singularity. The presence of a branch cut in \( U(r, \varepsilon, l, \varepsilon_r) \) may give rise to a branch cut of \( P_r(r, \varepsilon, l, \varepsilon_r) \). A branch cut would prevent us from using Cauchy’s integral theorem in evaluating integrals of \( P_r \) over contours that intersect the cut. We have explored the possible presence of a branch cut of \( U \) originating at the introduced singularity by two methods. The first is by numerically integrating the modified Schrödinger equation (12.3) in the complex \( r \) plane around the irregular singularity to a point \( r_A \) along paths that are mirror images of each other in the real \( r \) axis, shown in Figure 12.4. \( \tilde{U} \) and \( \tilde{U}' \) are real at \( r = 0 \), according to the initial conditions (6.10). The line elements and \( P_r^2(r, \varepsilon, l, \varepsilon_r) \) at corresponding points along the two paths are complex conjugates of each other, thus \( U \) and \( U' \) at \( r_A \) obtained by integration along these paths will be complex conjugates of each other; they are equal to each if the imaginary parts of these two functions vanish at \( r_A \). Integration showed the imaginary parts of these functions to be very small in comparison to their real parts; also changing the path of integration resulted in a change in the imaginary parts of \( U \) and \( U' \) while their real parts were stable. The second method is by an approximate local solution of (12.3). Both methods indicate the absence of such a cut. We describe here the approximate solution.

From eq. (12.3), \( U \) can be approximated by \( \tilde{U}(r, \varepsilon, l, \varepsilon_r) \) for \( Re(r) >> r_2 \), where

\[
\tilde{U}'' + \frac{\varepsilon}{\hbar^2 \varepsilon_r^4} \frac{\tilde{U}}{(r - 1/\varepsilon_r)^4} = 0,
\]

(12.7)
Figure 12.4: Integration paths for the modified Schrödinger equation

ignoring the effective potential in comparison to $E$. We similarly define $\tilde{\mathcal{P}}_r$ as the solution of

$$-i\hbar \frac{\partial \tilde{\mathcal{P}}_r(r, E, l, \epsilon_r)}{\partial r} + \tilde{\mathcal{P}}_r^2(r, E, l, \epsilon_r) = \tilde{\mathcal{P}}_{rc}^2(r, E, L, \epsilon_{rc}), \quad (12.8)$$

with $\tilde{\mathcal{P}}_{rc}(r, E, l, \epsilon_r) = \frac{\sqrt{E}}{\hbar^2 \epsilon_r^4}$. \quad (12.9)

This equation has two independent solutions of the form

$$\tilde{\mathcal{U}}_1 = (r - 1/\epsilon_r) \sin \left( \frac{\gamma}{r - 1/\epsilon_r} \right),$$

$$\tilde{\mathcal{U}}_2 = (r - 1/\epsilon_r) \cos \left( \frac{\gamma}{r - 1/\epsilon_r} \right), \quad (12.10)$$

where

$$\gamma = \frac{\sqrt{E}}{\hbar \epsilon_r^3}. \quad (12.11)$$
Figure 12.5: Zeroes of $\mathcal{U}(r, \mathcal{E}, l, \epsilon_r)$ in the neighborhood of $1/\epsilon_r$.

These solutions have no branch cut at $r = 1/\epsilon_r$ and the accuracy of the approximation of eq. (12.3) by eq. (12.7) increases as one chooses a smaller and smaller $\epsilon_r$. These solutions, and their linear combinations, have an infinite number of zeroes in any neighborhood of $r = 1/\epsilon_r$. It can be shown that these zeroes accumulate around $r = 1/\epsilon_r$ vertically if $E < 0$ and along the real axis for $E > 0$. Figure (12.5) shows the picture of these zeroes for both cases. This structure of the northern and southern poles of $\mathcal{P}_r$ with $r = 1/\epsilon_r$ as their limit point, revealed by $\mathcal{U}_1$ and $\mathcal{U}_2$ above is the same as the one we obtained in the previous section using the WKB approximations for $\mathcal{U}(r, \mathcal{E}, l, \epsilon_r)$.

An alternate set of linearly independent solutions of eq. (12.7) is

$$\mathcal{U}_{1'} = (r - 1/\epsilon_r) \exp \left( \frac{i \gamma}{r - 1/\epsilon_r} \right),$$

(12.12)
\[ \tilde{U}_{2f} = (r - 1/\epsilon_r) \exp \left( \frac{-i \gamma}{r - 1/\epsilon_r} \right). \]

This set of solutions is illustrative of the character of \( U \) for energy eigenvalues. Since \( \gamma = i|\gamma| \) (from eq. (12.11) and the definition of \( \sqrt{E} \)), \( \tilde{U}_{2f} \), for negative energies, is

\[ (r - 1/\epsilon_r) \exp \left( \frac{|\gamma|}{r - 1/\epsilon_r} \right) \to 0 \]

as \( r \to (1/\epsilon_r)_- \). \( \tilde{U}_{1f} \to \infty \), in the same limit and, unlike \( \tilde{U}_{2f} \), is not normalizable in the interval \( r \in (0, 1/\epsilon_r) \). The energy eigenvalues are therefore those \( \mathcal{E} \) for which \( \tilde{U}_{1f} \) component is absent in the wave function and the eigenfunctions \( \tilde{U}_n \) for \( r_2 << r < 1/\epsilon_r \) are

\[ \tilde{U}_n = (r - 1/\epsilon_r) \exp \left( \frac{i \gamma_n}{r - 1/\epsilon_r} \right), \quad (12.13) \]

with \( \gamma_n = \sqrt{E_n}/\hbar \epsilon_r^2 \). These eigenfunctions \( \tilde{U}_n \) have no zeroes in the neighborhood of \( r = 1/\epsilon_r \), which supports our conclusion in the previous section based on the WKB analysis that the zeroes move into \( r = 1/\epsilon_r \) for energy eigenvalues.

The momentum functions \( \tilde{P}_r(r, E_n, l, \epsilon_r) \) for the energy eigenvalues (using \( \mathcal{P}_r = -i\hbar \tilde{U}'/\tilde{U} \)) are

\[ \tilde{P}_r(r, E_n, \epsilon_r) = \frac{\gamma_n \hbar}{(r - 1/\epsilon_r)^2} - \frac{i \hbar}{r - 1/\epsilon_r}. \quad (12.14) \]

This shows that \( \tilde{P}_r \) for energy eigenvalues has a second order pole at \( r = 1/\epsilon_r \) just as \( \mathcal{P}_{rc} \) does. The residue of \( \tilde{P}_r \) at this pole is \(-i\hbar\). That this is also the residue of \( \mathcal{P}_r \) at \( r = 1/\epsilon_r \) can be shown by the expansion of \( \mathcal{P}_r \) in a Laurent series centered at \( r = 1/\epsilon_r \). \( \tilde{U}_{2f} \), the WKB wave function, for energy eigenvalues, is

\[ \tilde{U}_{2f} \sim \frac{1}{\sqrt{\mathcal{P}_{rc}}} \exp(i \mathcal{W}_{rc} \hbar), \]
which is correct up to the first order in $\hbar$. The corresponding momentum function, correct to order $\hbar$, is

$$\mathcal{P}_r^{WKB} = \mathcal{P}_{rc} + \hbar \frac{-iV'_{eff}(r)}{4\mathcal{P}_{rc}^{3/2}}. \quad (12.15)$$

The second term in the above is $\propto \mathcal{P}_{rc}^{-3/2} \sim (r - 1/\epsilon_r)^3$ and is finite at $r = 1/\epsilon_r$. Thus $\mathcal{P}_r$ has the same singularity at $r = 1/\epsilon_r$ as $\mathcal{P}_{rc}$. We now use the Laurent expansion

$$\mathcal{P}_r(r, E_n, l, \epsilon_r) = \frac{a_{-2}}{(r - 1/\epsilon_r)^2} + \frac{a_{-1}}{(r - 1/\epsilon_r)} + \ldots \quad (12.16)$$

in eq. (12.5), with

$$\mathcal{P}_{rc}(r, E_n, l, \epsilon_r) = \frac{A_{-2}}{(r - 1/\epsilon_r)^2} + \frac{A_{-1}}{(r - 1/\epsilon_r)} + \ldots. \quad (12.17)$$

Equating coefficients of every power of $(r - 1/\epsilon_r)$ to zero in this equation we get

$$a_{-2}^2 = A_{-2}^2 \Rightarrow a_{-2} = +A_{-2}, \quad \text{sign from eq. (12.15)),}$$

$$a_{-1} = \frac{2A_{-2}A_{-1} - 2ih a_{-2}}{2a_{-2}} = A_{-1} - ih. \quad (12.18)$$

To obtain $A_{-1}$ we expand $\sqrt{E - V_{eff}(r)}$ in eq. (12.4) in a Taylor series around $r = 1/\epsilon_r$:

$$\mathcal{P}_{rc} = \frac{1}{\epsilon^2(r - 1/\epsilon_r)^2} \left[ \sqrt{E - V^{(\epsilon)}_{eff}} - \frac{V_{eff}^{(\epsilon)}}{2\sqrt{E - V^{(\epsilon)}_{eff}}} (r - 1/\epsilon_r) + \ldots \right] (12.19)$$

where the superscript $\epsilon$ in $V$ and $V'$ refers to the functions evaluated at $r = 1/\epsilon_r$. For any potential that cuts off faster than the Coulomb potential the leading term in $V_{eff}(r)$ is $\propto 1/r^2$ (which could be the angular momentum barrier alone or the
barrier and a part of the potential that is also $\propto 1/r^2$ for $Re(r) >> R$ (or a distance within which the potential is influential). Therefore, for all such potentials including the Yukawa potential, $V_{\text{eff}}' \propto 1/r^3$ for large $Re(r)$ and

$$V_{\text{eff}}'(r) = V_{\text{eff}}'(r = 1/\epsilon_r) \sim O(\epsilon_r^3).$$

$A_{-1}$, which is the coefficient of $(r - 1/\epsilon_r)^{-1}$ in eq. (12.19), is $\propto V_{\text{eff}}'/\epsilon_r^2$ and therefore

$$A_{-1} \sim O(\epsilon_r). \quad (12.20)$$

Using (12.20) in (12.18) we get

$$a_{-1} = -i\hbar + O(\epsilon_r). \quad (12.21)$$

We will use this result in the contour integral definition of $J_r$.

**Definition of $J_r$**

The poles of $P_r$ are shown in Figure 12.6. These poles are also represented in the $s = 1/r$ plane shown in the same figure. We define the contours in the $r$ and $s$ planes and establish the correspondence between them as follows:

(i) The contour $C_e$ in the $r$ plane encloses the poles on the positive real axis and the northern and southern poles for all energies. The corresponding contour in the $s$ plane is $C_{es}$.

(ii) $C_0$ encircles the pole at $r = 0$. $C_{0s}$ is the corresponding contour in the $s$ plane.

(iii) $C_{ws}$ is a contour in the $s$ plane that encloses all the western poles. It passes between $s = 0$, which is the limit point of all the western poles, and $s = \epsilon_r$, which is
the limit point of the northern and southern poles. $C_w$ is its image in the $r$ plane.

(iv) $C_e$ encloses the point $r = 1/e$ in the $r$ plane. $C_{es}$ is its image in the $s$ plane. As the limit point of the northern and southern poles is a point in the finite $r$ plane, viz, $1/e_r$, it is always possible, for all energy, to have the contour $C_e$ enclose the set of northern and southern poles as also the poles on the positive real axis.

(v) $C$ encloses the poles on the real axis for $V_0 < E < 0$. $C_s$ is its image in the $s$ plane.

The poles can be grouped into similar distinct sets for any potential that cuts off for $r \to \infty$ along the real $r$ axis. The characteristic feature of a potential is the number and distribution of poles inside the contour $C_{ws}$ in the $s$ plane. For energy eigenvalues the northern and southern poles disappear into $s = \epsilon_r$.

We first define $J_r(E, l, \epsilon_r)$ by

$$J_r(E, l, \epsilon_r) = \frac{1}{2\pi} \oint_{C_e} P_r(r, E, l, \epsilon_r) \, dr - \hbar. \quad (12.22)$$

We study its character on energy eigenvalues. For $E = E_n$, we can distort $C_e$ into $C$ and $C_e$ to evaluate the integral in (12.22). Since $P_{rc}(r, E, l, \epsilon_r)$ has no poles at any point in the finite $r$ plane except at $r = 1/e_r$ and $r = 0$ every pole of $P_r(r, E, l, \epsilon_r)$ in the finite $r$ plane excluding $r = 1/e_r$ and $r = 0$ is a simple pole of residue $-i\hbar$. (see Appendix A). Similarly every pole of $p_r(r, E, l)$ in the finite $r$ plane excluding $r = 0$ is simple and has residue $-i\hbar$. Thus

$$\frac{1}{2\pi} \oint_{C} P_r(r, E_n, l, \epsilon_r) \, dr = \frac{1}{2\pi} \oint_{C} p_r(r, E_n, l) \, dr = n_r \hbar, \quad (12.23)$$

since $C$ encloses the same number of poles, $n_r$, of both $P_r(r, E_n, l, \epsilon_r)$ and $p_r(r, E_n, l)$, each of residue $-i\hbar$. Next,

$$\frac{1}{2\pi} \oint_{C_e} P_r(r, E_n, l, \epsilon_r) \, dr = ia_{-1}, \quad \text{by the residue theorem},$$
Figure 12.6: Contours used in the definition of $J_r(\varepsilon, l, \epsilon_r)$
from eq. (12.21), for any central potential that cuts off faster than the Coulomb potential. Using eqs. (12.23) and (12.24) in eq. (12.22) we get

\[ \hat{J}_r(E_n, l) = \frac{1}{2\pi} \int_{C_0} f \rho_r(r, E_n, l) \, dr + \frac{1}{2\pi} \int_{C_0} f \rho_r(r, E_n, l) - \hbar \]

In the limit of \( \epsilon_r \to 0 \), therefore, \( \hat{J}_r(E_n, l, \epsilon_r) \to J_r(l, E_n, l) \) for any central potential weaker than the Coulomb potential. Our definition of \( J_r \) for any such potential for any energy \( \mathcal{E} \) is

\[ J_r(\mathcal{E}, l) = \lim_{\epsilon_r \to 0} \hat{J}_r(E_n, l, \epsilon_r). \]
The radial action variable $J_{r}(E,l)$, extended analytically to both bound and scattering states of a system, provides a link between quantum bound states and resonances. We have demonstrated that the radial action variable can be defined classically and quantum mechanically, for all physically allowed states of a system described by the Yukawa potential. These definitions preserve the algebraic form of the action variable for all energies. Unlike the simpler Coulomb potential, the Yukawa potential has an infinite number of classical turning points in the western half of the complex $r$ plane, with a branch cut of the classical momentum function originating from each of them. The motion of these turning points with energy was examined both analytically and numerically. $J_{r_{c}}$ was defined as a contour integral in the complex $r$ plane with the contour enclosing the two classical turning points $r_{1}$ and $r_{2}$, which correspond to the limits of the physical bound state motion, and the branch cut between them; this definition is then extended to all energies.

The quantum radial action variable, $J_{r}(E,l)$, defined as a contour integral in the complex $r$ plane of the quantum momentum function, is quantized in units of $\hbar$ for bound states. The analytic extension of $J_{r}$ to scattering states required a study of the motion of the poles of the quantum momentum function with energy. The energy dependence of these poles was first studied by a semiclassical method and the
results confirmed by a numerical method. These studies revealed the presence of a
train of poles west of each western turning point that do not vanish into \( r = \infty \) on
energy eigenvalues. They also showed the presence of a second set of infinite poles in
the eastern half of the complex \( r \) plane that recede to \( r = \infty \) on energy eigenvalues.
The Yukawa potential thus produces two classes of infinitely many poles of \( p_r \), one
that recedes to \( r = \infty \) on energy eigenvalues (the 'northern-southern' poles), and
the other that is insensitive to energy eigenvalues. Both these sets have the same
limit point, viz, \( r = \infty \), into which the first set disappears for physical bound state
energies.

This study of the Yukawa potential reveals resemblances to the problem of the
Coulomb potential with regard to the motion of the poles with energy. The important
difference is the presence of the infinite trains of western poles which are insensitive
to energy eigenvalues, unlike the northern-southern sequence of poles (which are also
present in the Coulomb potential case). Any potential, which results in more than
two classical turning points, has, in general, such poles. That these different sets
of poles have a common limit point into which the northern-southern poles merge
poses a problem to the analytic extension of \( J_r \) to scattering states. The analytic
extension requires the enclosure of the set of northern-southern poles by a contour
in the complex \( r \) plane while excluding the set of western trains of poles, so that we
obtain, for energy eigenvalues, \( J_r = n_r \hbar \). This requires "moving" the limit point of
the northern-southern poles from \( r = \infty \) to a finite point \( r = 1/\epsilon_r \); the northern-
southern poles being thus confined to the finite complex \( r \) plane can be surrounded
by a contour. After the evaluation of \( J_r \) as an integral over that contour we make \( \epsilon_r \)
vanishingly small.
The separation of the limit points of the two sets of poles was achieved by considering a modified Yukawa Hamiltonian that describes, in its classical version, a particle whose effective mass increases as it approaches the point \( r = 1/\epsilon_r \). The corresponding Schrödinger equation has an irregular singularity at \( r = 1/\epsilon_r \) leading to a possible branch point for the wave function. We have examined the nature of the wave function in the neighborhood of the irregular singularity by constructing a local solution and by numerical integration around the singularity. These methods indicate the absence of a branch cut for the wave function, though this result requires further investigation.

The evaluation of \( J_{\epsilon R}(E, l) \) for the Yukawa potential as a perturbative series in \( 1/R \), where \( R \) is the range of the potential, has been demonstrated. A similar evaluation of \( J_{\epsilon R} \) and \( J_{\epsilon R} \) as functions of energy, for a system whose Hamiltonian involves \( \epsilon_r \) in the manner indicated above requires further study, though we have successfully demonstrated that it provides a means to analytically extend \( J_{\epsilon} \) to all energies. We have used the Yukawa potential as a prototype. The method developed here to analytically extend \( J_{\epsilon} \) for this potential can be applied to other central potentials that cut off faster than the Coulomb potential. The Coulomb potential, viewed as the long range limit of the Yukawa potential, can also be brought within the fold of this definition of \( J_{\epsilon} \); one first evaluates \( J_{\epsilon} \) for the Yukawa potential with a range \( R \) and then takes the limit of \( R \to \infty \). Particle resonances, understood as composite quantum mechanical states of strongly interacting particles, can be explored by studying the action variable of such states through suitably modeled potentials. One can form families of states of common angular momentum but different action variables, thus providing a new scheme for classifying composite systems.
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APPENDIX

Appendix A: Poles of $p_r$

Let $p_c(x, E)$ be analytic at a point $x_0$. Assume $p(x, E)$ has a pole of order $n$ at $x_0$ with $n \geq 1$. Then

$$p_c(x, E) = A_0 + A_1(x - x_0) + \ldots$$

and

$$p(x, E) = \frac{a_{-n}}{(x - x_0)^n} + \frac{a_{-(n-1)}}{(x - x_0)(n-1)} + \ldots$$

Substituting these expansions for $p_c(x, E)$ and $p(x, E)$ in eq. (3.5) we see that the coefficients of $(x - x_0)^{2n}$ can be matched on both sides only if

$$2n = n + 1 \quad \Rightarrow \quad n = 1,$$

$$i\hbar a_{-1} + a_{-1}^2 = 0$$

$$\Rightarrow \quad a_{-1} = -i\hbar$$

Thus the quantum momentum function, if it is singular at $x_0$, can only have a simple pole of residue $-i\hbar$ at $x_0$ where the classical momentum function is analytic.
Appendix B: Perturbative expansion of $p_{rc}(r, \mathcal{E}, L)$

From eqs. (9.25) and (9.26) we have

$$\frac{L^2}{r_1 r_2} (r - r_1)(r - r_2) \left[ 1 + \sum_{n=1}^{\infty} v_n r^n \right] = E r^2 + g r \exp(-r/R) - L^2.$$  

We equate coefficients of $r^n$ on both sides of this equation and obtain $v_n$.

Case (i): $L = 0$

Here we have a closed form expression for $v_n$:

$$v_n = -\frac{\exp(-n \lambda_2)}{r_{2c}^n} \sum_{j=n+1}^{\infty} \frac{(-\lambda_2)^j}{j!},$$

where $\lambda_2 = \frac{r_2}{R}$ and $|\lambda_2| < 1$ for $E < E_h$, from Figure (9.2). Thus $v_n \sim O(\lambda_2^{n+1})$.

Case (ii): $L \not= 0$

We can solve for $v_1$ and $v_2$ by equating coefficients of $r$ and $r^2$; to the leading order in $\lambda_{1,2} = \frac{r_{1,2}}{R}$. We get

$$v_1 \sim -\frac{r_{2c} + r_{1c}}{r_{2c} - r_{1c}} \left[ \frac{\lambda_2^2}{r_{1c}^2} + \frac{\lambda_2^2}{r_{2c}^2} \right].$$

Similarly, $v_2 \sim O(\lambda_{2,3}^3)$. For $n \geq 3$, we get, by equating the coefficient of $r^n$,

$$v_{n-2} - (r_1 + r_2) v_{n-1} + r_1 r_2 v_n = -\frac{gr_1 r_2}{L^2} \frac{1}{(n-1)!} \left( \frac{-1}{R} \right)^{n-1}. $$

The asymptotic solution of this difference equation is

$$v_n \sim -\frac{r_1 r_2 g}{L^2} \frac{1}{(n+1)!} \left( \frac{-1}{R} \right)^{n+1} \sim O(\lambda_{1,2})^{n+1}.$$
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