CHAPTER II

COMPLEX MILLER - GOOD METHOD

II.1. Introduction

The JWKB semiclassical approximation is one of the most versatile techniques of quantum mechanics. The applicability of the method, however, could not be fully exploited because of a serious drawback which shows up at the classical turning points, i.e. points where the classical velocity of the particle vanishes. Unfortunately, classical turning points appear in most problems of physical interest. In a scattering event, the incident wave is reflected from at least one turning point, whereas for a bound state, there are at least two turning points. The JWKB wave function becomes singular at these points. In order to get a finite wave function, one has to make use of the connection formula across the turning point. Also, the correction terms of higher order in $\hbar^2$ diverge badly at the turning points. The method is suitable for potentials which vary so slowly that the momentum of the particle remains nearly constant over many wavelengths. The method obviously fails when the particle energy is low.

To overcome these difficulties, Miller and Good[1] proposed a modification of the JWKB method. The method has been developed further by a number of workers, Rosen and Yennie[2], Lu and Measure[3], Wald and Lu[4] and Berry and Mount[5]. The first step in this method is to choose a 'model equation' which is exactly solvable and also similar to the equation to be solved. The solutions of both the equations should have similar behaviour

asymptotically. It is the difference in their asymptotic phases which will be determined by a semiclassical approximation. It is no longer necessary to use any connection formula across the turning points.

The generalized Miller - Good method even with only the first order correction term is fairly accurate. This has been tested for real potentials by a number of authors[6,7,8]. In the next chapter we shall also consider a few simple cases to exhibit the accuracy and the efficacy of the method. The application of the method to a complex potential, however, needs further consideration. The role of complex trajectories in the semiclassical approach has been a subject of intensive study by Balian and Bloch[9], Knoll and Schaeffer[10], Koeling and Malfliet[11], Rowley and Marty[12], Brink and Tagikawa[13] and a number of other authors[14]. Their results are not, in general, directly applicable to the complex Miller-Good (CMG) method. In the latter case, only the difference in phases are determined by the semiclassical method, while in the former, the phase shift is determined directly. However, the role of complex trajectories in the Miller-Good method remains to be studied.

The presentation will be as follows. The method has been briefly reviewed in section II.2. In section II.3, we shall consider a generalization of the method for a complex potential, with special reference to a Woods-Saxon potential.

II.2. Miller-Good method for a Real potential

Let us assume that it is possible to write the Schrödinger radial equation for the problem as

$$\left(\frac{d^2}{dy^2} + \frac{t_1(y)}{\hbar^2} \right) G(y) = 0. \quad \ldots(2.1)$$

Consider another equation

$$\left(\frac{d^2}{ds^2} + \frac{t_2(s)}{\hbar^2} \right) u(s) = 0, \quad \ldots(2.2)$$

which permits an exact solution. We shall call equation (2.2) a 'model equation' for the problem, provided $t_1(y)$ and $t_2(s)$ are 'similar' in the following sense:

(1) They should have equal number of turning points, i.e. for every real physical y_t, which makes $t_1(y_t) = 0$, there should be a real, physical s_t giving $t_2(s_t) = 0$. It is also desirable that the two functions should have the same number of extrema, a condition which is useful when higher order corrections are taken into account.

(2) The two functions should have similar behaviour near the respective singular points. However, fairly accurate phase shifts can be obtained in some cases, even when this condition is not satisfied, particularly in cases where the singularity is in the classically inaccessible region. We shall return to this point later on.

If both these conditions are satisfied one considers a transformation T (y) so that

$$G(y) = T(y)\, u\,[\, s(y)] \qquad \ldots(2.3)$$

where s is considered to be a function of y. Substituting (2.3) into equation (2.1) and making use of the equation (2.2), we get the consistency condition

$$s'^2 t_2 - t_1 = \hbar^2 \frac{T''}{T} , \qquad \ldots (2.4)$$

and

$$\frac{T'}{T} = -\frac{1}{2} \frac{s''}{s'} , \qquad \ldots(2.5)$$

where the primes imply differentiation w.r.t. the respective arguments. A solution of (2.5) is found easily

$$T = \frac{1}{\sqrt{s'(y)}} . \qquad \ldots(2.6)$$

Substitution of (2.6) into the equation (2.4) gives

$$s'^2 t_2 - t_1 = \frac{\hbar^2}{4}\left[3 \frac{s''^2}{s'^2} - 2 \frac{s'''}{s'}\right] . \qquad \ldots (2.7)$$

We may now expand s (y) and $t_2(s)$ in powers of $\hbar^2$ and consider terms upto a given order in $\hbar^2$ to satisfy the condition (2.7). Thus the condition can be written

as follows:

(i) to the lowest order in $\hbar^2$:

$$\sqrt{t_1(y)}\, dy = \sqrt{t_2(s)}\, ds \qquad \ldots (2.8)$$

which may be integrated to obtain

$$\int_{y_t}^{y} \sqrt{t_1(y)}\, dy = \int_{s_t}^{s} \sqrt{t_2(s)}\, ds \qquad \ldots (2.9)$$

where y_t, s_t are the respective classical turning points.

(ii) The condition (2.7), upto terms of order $\hbar^2$ becomes

$$\int_{y_t}^{y} p_1\, dy + \frac{\hbar^2}{8} \int_{y_t}^{y} \left(3\, \frac{p_1'^2}{p_1^3} - 2\, \frac{p_1''}{p_1^2} \right) dy$$

$$= \int_{s_t}^{s} p_2\, ds + \frac{\hbar^2}{8} \int_{s_t}^{s} \left(3\, \frac{p_2'^2}{p_2^3} - 2\, \frac{p_2''}{p_2^2} \right) ds \,, \qquad \ldots (2.10)$$

with $t_1(y) = p_1^2$, $t_2(s) = p_2^2$. $\qquad \ldots (2.11)$

The integrals in (2.10) appear to be divergent at the lower limit, i.e. at the turning points. Of course, the divergence may be eliminated in some cases by following the method of Bertocchi et al[14], which consists in converting the integrals in (2.10) into contour integrals

in the s (or y) planes. The choice of the contour is as follows. One takes a contour from $\infty - i\epsilon$ to $\infty + i\epsilon$, going round the turning point in a clockwise direction. On integrating by parts and using the result

$$\oint u\,d\omega = \lim_{\epsilon \to 0} \left[u\omega\right]_{\infty - i\epsilon}^{\infty + i\epsilon} - \int_{\infty - i\epsilon}^{\infty + i\epsilon} \omega\, du$$

$$= - \oint \omega\, du \qquad \ldots (2.12)$$

repeatedly, we can eliminate the p_i from the denominator. Going back to the original contour, we obtain, upto terms of order $\hbar^2$,

$$\int_{y_t}^{y} \sqrt{t_1(y)}\, dy + \frac{\hbar^2}{12} \int_{y_t}^{y} \mathcal{Q}\left[t_1\right] \sqrt{t_1(y)}\, dy$$

$$= \int_{S_t}^{S} \sqrt{t_2(s)}\, ds + \frac{\hbar^2}{12} \int_{S_t}^{S} \mathcal{Q}\left[t_2\right] \sqrt{t_2(s)}\, ds\,, \qquad \ldots (2.13)$$

where

$$\mathcal{Q}\left[t_i\right] = \frac{t_i'''' }{t_i'^2} - 4\,\frac{t_i''' \, t_i''}{t_i'^3} + 3\,\frac{t_i''^3}{t_i'^4}\,, \qquad \ldots (2.14)$$

the primes indicating the number of times the functions are differentiated w.r.t. their respective arguments. While the relation (2.14) does not have p_i in the denominator, the problem is solved only if p_i' does not

have any zero within the range of integration. If p_i does have an extremum, one may still try to evaluate the integral, excluding the singularity[4]. It may be emphasized that the singularity appears only because one is considering only upto a given order of $\hbar^2$. If it were possible to consider all terms of all orders, the singularity will cancel out.

(iii) Upto terms of order $\hbar^4$, one may write

$$\int_{y_t}^{y} \sqrt{t_1(y)}\, dy + \frac{\hbar^2}{12}\int_{y_t}^{y} \mathcal{Q}\left[t_1\right]\sqrt{t_1(y)}\, dy - \frac{\hbar^4}{1440}\int_{y_t}^{y} G\left[t_1\right]\sqrt{t_1(y)}\, dy$$

$$= \int_{S_t}^{S} \sqrt{t_2(s)}\, ds + \frac{\hbar^2}{12}\int_{S_t}^{S} \mathcal{Q}\left[t_2\right]\sqrt{t_2(s)}\, ds - \frac{\hbar^4}{1440}\int_{S_t}^{S} G\left[t_2\right]\sqrt{t_2(s)}\, ds \qquad \ldots (2.15)$$

where

$\mathcal{Q}\left[t_i\right]$ is given by equation (2.14) and

$$G\left[t_i\right] = \frac{5\, t_i^{\mathrm{VII}}}{t_i'^{3}} - \frac{44\, t_i^{\mathrm{VI}} t_i^{\mathrm{II}} + 76\, t_i^{\mathrm{V}} t_i''' + 47\, t_i^{\mathrm{IV}\,2}}{t_i'^{4}}$$

$$+ \frac{222\, t_i^{\mathrm{V}} t_i''^{2} + 680\, t_i'''' t_i''' t_i'' + 140\, t_i'''^{3}}{t_i'^{5}}$$

$$- \frac{1540\, t_i'''^{2} t_i''^{2} + 810\, t_i'''' t_i''^{3}}{t_i'^{6}}$$

$$+ \frac{2205\, t_i''' t_i''^{4}}{t_i'^{7}} - \frac{735\, t_i''^{6}}{t_i'^{8}}, \qquad \ldots (2.16)$$

with

$$t_1^{\overline{VII}} = \frac{d^7 t_1}{dy^7} \quad \text{etc.}$$

... (2.17)

It may be useful to indicate how the consistency condition leads to the determination of the phase shift, relevant for the equation (2.1). Suppose the asymptotic behaviour of the functions G(y) and u(s) are written as:

$$G(y) \xrightarrow[y \to \infty]{} \text{Sin}\,(y + f_1(y) + \sigma) \qquad \ldots(2.18)$$

and

$$u(s) \xrightarrow[S \to \infty]{} \text{Sin}\,(s + f_2(s) + \delta). \qquad \ldots(2.19)$$

Since, by assumption the two solutions have similar behaviours at infinity, one may write

$$\sigma = \delta + \lim_{\substack{y \to \infty \\ S \to \infty}} (s - y + f_2(s) - f_1(y))$$

...(2.20)

The right-hand side can be determined from the consistency condition upto a given order of $\hbar^2$. Some applications of this method will be considered in subsequent chapters.

II.3. Generalization for complex potentials

The Miller-Good method outlined in the last section cannot be generalized for complex potentials in a straightforward manner. The difficulty stems mostly from the fact that the turning points are in general complex and also too many in number. With a Woods-Saxon potential, which is commonly used in the optical model treatment of heavy ion collisions, the situation is even worse, there being an infinite number of turning points due to the complex poles of the Woods-Saxon function. One has to decide if all or only some of them will contribute and also to find out how to combine these contributions in calculating the phase shifts.

The first attempt to study the complex potential was rather casual. Instead of writing for the wave vector

$$K(r) = \left[K^2 - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2} (V_R + i V_I) \right]^{\frac{1}{2}}, \qquad \ldots(2.21)$$

one expands and keeps terms upto first order in V_I. The resulting JWKB expression for the phase shifts involves integration over the real path from the classical turning points, determined entirely by the real potential, the imaginary part contributing only a damping factor to

each of the partial waves. The approximation seems to be reliable for a small absorption. However, as the energy increases, more and more inelastic channels open up, making this treatment completely unsuitable. It was, therefore, necessary to look for an alternative way of studying complex potentials in the semiclassical approach.

Koeling and Malfliet[11] studied this problem and suggested a generalization of the semiclassical method which includes contributions from all possible complex trajectories. Knoll and Schaeffer[10] have studied the problem analytically and showed that it is not necessary to consider all the complex trajectories. Although the results of Knoll and Schaeffer are not directly applicable to the Miller-Good method, it will be useful to recall some of their results. The relative importance of the contributions for single reflections from different turning points and of possible multiple reflections can be estimated following their analysis. Their prescriptions cannot be given in simple mathematical expressions and may even be difficult to use in some cases. In the case of one dimensional problems, one has to study the topology of Stokes lines around the turning points and in cases of higher dimensions one has to consider the topology of saddles, their positions and heights. But in cases of interest to us, i.e. heavy ion scattering, the topological structure will remain almost unchanged in the range of laboratory energies and for any standard model for the optical potential.

It has been shown that in most of the cases only a few of the complex trajectories make dominant contributions.

We consider a specific example to emphasize the point. Let us consider $^{16}O - ^{16}O$ scattering in which the nuclear potential is given by a Woods-Saxon function

$$V_N = \frac{-(V + iW)}{1 + \exp\left(\frac{r - R}{a}\right)}, \qquad \ldots(2.22)$$

with $V = 50$ Mev, and $W = 20$ Mev, $R = 6.05$ fm and $a = 0.6$ fm. If we consider only the real part of the potential including the centrifugal term, the potential has a pocket for some low values of L, but it decreases monotonically for a large L. One, therefore, gets one real turning point r_1 at high energies, but three real turning points $r_1 > r_3 > r_2$ at lower energies. The transition energy between the two cases is given by[15] (for $a \ll R$)

$$E_0 \simeq \tfrac{1}{2} V_c + V \left[(R - 2a)^2 + 2a^2 \right] / 8aR \qquad \ldots(2.23)$$

which for the values chosen is given by $E_0 \simeq 55$ Mev. If we now include the absorptive part, the real turning point r_1 moves into the complex plane, but two other complex turning points r_2, r_3 also appear. While for larger L values, only the complex trajectory from r_1 contributes, at lower L

values, contributions from both r_1 and r_2 will have to be considered. This is the case even at lower energies. This shows clearly that one cannot simply continue the formula for real trajectories into the complex plane to account for the absorptive part of the potential. However, there is some simplification if the absorption is fairly strong. The turning point r_2 is usually well within the potential so that the reflected wave from r_2 is heavily damped. This leaves the contribution from the outer turning point as the dominant one. Knoll and Schaeffer assert that for a fairly good approximation one needs consider only the outer turning point r_1, if the absorptive potential is strong. In chapter IV of this thesis we shall consider heavy ion scattering in which the prescription of Knoll and Schaeffer will be useful.

The observation of Knoll and Schaeffer makes it easy to generalize the Miller-Good method for a realistic heavy ion scattering. We need to locate the outer turning point r_1 and evaluate the integrals occuring in the expressions (2.13) along a complex trajectory. The contour is then distorted without crossing any singularity of $t_1(y)$ as shown in Fig.2.1. The method is applied to various problems in the following chapters. The simplicity of this prescription makes it possible to obtain $\hbar^2$ correction term also by a simple calculation. It should be emphasized that neglect of the contribution from r_2 introduces an error and this may make any higher order calculation meaningless.

Fig. 2.1. The distorted contour for path intigration.

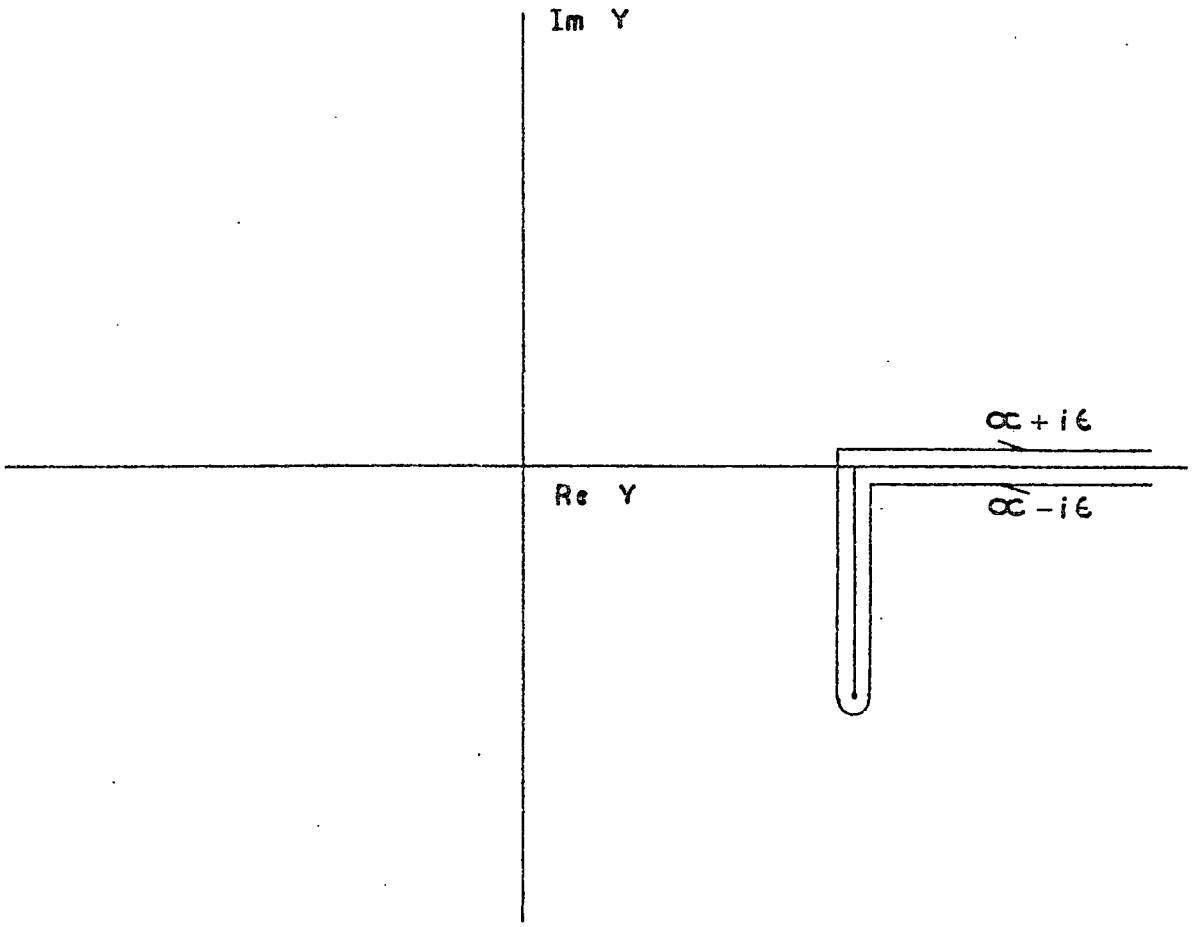

FIG. 2.1 .

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