Appendix B

Iteration for Stationary Points

This appendix gives a brief summary of how one may determine the points b_x of the stationary phase, i.e., the solutions of

$$X'(b_x) = q, \tag{B.1}$$

for $q > 0$. Explicit solutions are only available in a few special cases. Typically, one therefore has to determine the solutions by some iterative procedure. In general, the roots of Eq. (B.1) will be located off the real axis, in the complex b_x-plane. Some care therefore has to be exercised, in order to secure a convergent iteration. This may be further complicated by the fact that, as q is varied (increased, say), two solutions of Eq. (B.1) may come arbitrarily close together at a rainbow point, and then separate again (going in different directions) as q is further increased.

An easy way to survey some specific $X'(b_x)$ is to plot out the curves in the relevant part of the complex b_x-plane, where $\operatorname{Im} X'(b_x) = 0$. This can be done using some contour-plotting facility. These curves will consist of solutions to Eq. (B.1), not only for $q > 0$, but also for $q < 0$. The latter are not of interest, but the solutions for $q > 0$ and $q < 0$ may be separated if one also plots out curves where $\operatorname{Re} X'(b_x) = 0$ and determine where the two sets of curves intersect.

We are only interested in solutions to Eq. (B.1) that lie in the lower half-plane (including the real axis), $\operatorname{Im} b_x \leq 0$. Of these, usually only the two or three highest-lying ones are relevant for the actual path of integration. For any given value of q, there will thus typically be two or three solutions to Eq. (B.1) that are required. These might be distinguished by some index j, which we shall suppress in the following.

In order to establish the precise relation between b_x and q, for one particular trajectory j, we have found the following procedure useful:

(1) Consider some large, but finite value of q, which we denote $q^{(N)}$.
(2) Find some expression (even approximate) for $b_x^{(N)}$, which permits explicit evaluation, or at least iteration, for large values of $q^{(N)}$. If $X(b_x)$ has singularities, $b_x^{(N)}$ will be close to these singularities.
(3) Iterate the above expression for $b_x^{(N)}$.
(4) Improve on this solution, using, for example, the Newton–Raphson method i.e., making use of $X''(b_x)$. This is usually very efficient, and an arbitrary precision may be obtained. However, this method fails where $X'(b_x)$ is singular, which is why we start with a finite value of $q^{(N)}$.

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(5) Choose a somewhat smaller q, denoted $q^{(N-1)}$. Take $b_x^{(N)}$ as a start value for the iteration, and perform steps 3 and 4.
(6) Choose a somewhat smaller q, denoted $q^{(N-2)}$. Determine the start value for iteration by extrapolation from $b_x^{(N)}$ and $b_x^{(N-1)}$. Peform step 4.

Step (6) is repeated, until one reaches a $q^{(1)}$ that is as small as the smallest value of q one is interested in. As more solutions $b_x^{(N)}, \ldots, b_x^{(N-l+1)}$ are obtained, it is convenient to determine the start point for the iteration for the next one by a second-order extrapolation from the preceding three points.

When a rainbow point is encountered, i.e., a point where $X'' = 0$, special methods are required. There are two reasons for this. Firstly, in the neighborhood of a rainbow point, $|X''|$ becomes small, and the Newton–Raphson method becomes inefficient or fails altogether. Secondly, the trajectory in the complex b_x-plane, of $b_x^{(N)}, \ldots, b_x^{(1)}$ versus $q_x^{(N)}, \ldots, q_x^{(1)}$, sharply changes direction at the rainbow point, and no reasonable start value for the iteration below the rainbow point may be obtained by a simple extrapolation from the points obtained above the rainbow point.

We here only consider rainbow points where $X''(b_x)$ has a simple zero. Because $X'(b_x)$ is analytic in some neighborhood around the rainbow point, we may write

$$X'(b_x) = X'(b_{x,\mathrm{R}}) + \tfrac{1}{2}X'''(b_{x,\mathrm{R}})(b_x - b_{x,\mathrm{R}})^2 + \cdots . \tag{B.2}$$

From this quadratic form, it follows that at the rainbow point, there are two lines along which $\operatorname{Im} X'(b_x) = 0$, intersecting at an angle of 90°. Thus, the trajectory of $b_x^{(N)}, \ldots, b_x^{(1)}$ versus $q_x^{(N)}, \ldots, q_x^{(1)}$ changes direction by $\pm 90^\circ$ at rainbow points. To a considerable extent, this observation solves the problem of extrapolating across the rainbow point in order to determine the starting point for the iteration.

We have encountered rainbow points in the complex plane, but the more typical situation is that they occur on the real axis. This would normally happen when $X'(b_x)$ is real-valued for real b_x. With increasing q, the trajectory $b_x^{(N)}, \ldots, b_x^{(1)}$ will then at a typical rainbow point approach the real axis at a right angle for $q \gtrsim q_{\mathrm{R}}$, and then run along the real axis for $q < q_{\mathrm{R}}$. It should be noted, however, that even if $X'(b_x)$ is real for real b_x, more complicated situations may arise. In order to illustrate this, suppose that $X'(b_x)$, in addition to having maxima at $b_{x,\mathrm{R}} = b_{x,\,\max}$, satisfying $X'(b_{x,\,\max}) > 0$, also has minima $b_{x,\,\min}$ satisfying $X'(b_{x,\,\min}) > 0$. Such minima would then also be rainbow points, but with the "bright side" for $q > q_{\mathrm{R}}$. As q is *decreased* beyond such a rainbow point, the points of stationary phase would depart from the real b_x-axis and go off into the complex plane (at right angles with respect to the real axis).

The method may be clarified by a brief discussion of a moderately complicated example. Consider a combination of forms discussed in Chapter 12,

$$X(b_x) = \frac{\chi_0}{1 + \exp[(b_x - c)/\beta]} + 2\eta \log\sqrt{b_x^2 + a^2}, \tag{B.3}$$

which leads to

$$\begin{aligned} X'(b_x) &= \frac{-\chi_0 \exp[(b_x - c)/\beta]}{\beta\{1 + \exp[(b_x - c)/\beta]\}^2} + 2\eta \frac{b_x}{b_x^2 + a^2} \\ &\equiv X'_{\mathrm{N}}(b_x) + X'_{\mathrm{C}}(b_x). \end{aligned} \tag{B.4}$$

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For some large $q^{(N)}$, the corresponding solutions to Eq. (B.1) will be close to singularities of Eq. (B.4), which are:

(i) Double poles at $b_x = c \pm (2n+1)i\pi\beta, \quad n = 0, 1, \ldots$
(ii) Double poles at $b_x = -c \pm (2n+1)i\pi\beta, \quad n = 0, 1, \ldots$
(iii) Simple poles at $b_x = \pm ia.$

There will thus, for large values of q, be two solutions in the neighborhood of each double pole, and one solution near each simple pole. Suitable expressions for the iteration discussed under points (2) and (3) above are obtained by retaining the leading terms in Eq. (B.4).

In order to determine approximately the solutions close to the double poles (i), we write Eq. (B.1) as a quadratic equation for $\exp[(b_x - c)/\beta]$,

$$\left[\exp[(b_x - c)/\beta] + 1\right]^2 + \frac{\chi_0}{\beta\left[q - X'_{\mathrm{C}}(b_x)\right]} \exp[(b_x - c)/\beta] = 0. \tag{B.5}$$

The solutions are conveniently expressed in terms of the small quantity

$$\lambda \equiv \frac{\chi_0}{2\beta\left[q - X'_{\mathrm{C}}(b_x)\right]}, \tag{B.6}$$

as

$$b_x = c - i\pi\beta + \beta \log\left[1 + \lambda + \sqrt{2\lambda + \lambda^2}\right]. \tag{B.7}$$

It should be noted that the logarithm and the square root are both multivalued, and that in Eq. (B.7) an explicit choice of branches has been made. The branch of the logarithm has been chosen such as to select the double pole that is closest to (but below) the real axis. The two branches of the square root reflect the fact that these singularities are *double* poles. There will thus be two roots of Eq. (B.5) that for $q \to \infty$ meet at these double poles; the sign in front of the square root is chosen to select the trajectory of stationary points that is closer to the real axis. The above equation is well-suited for the iteration of point (3), starting at $b_x = c - i\pi\beta$, since λ only has a weak b_x-dependence. It is not necessary to iterate Eq. (B.7) to a very high precision, since the Newton–Raphson iteration [point (4)] is more efficient. The final iteration should therefore be performed as discussed under point (4) above, i.e., using the approximation

$$b_x^{\mathrm{new}} = b_x^{\mathrm{old}} - \left[X'(b_x^{\mathrm{old}}) - q\right] / X''(b_x^{\mathrm{old}}). \tag{B.8}$$

When the phase shift function is analytic, it is less obvious where to start the iteration. If the phase shift function is "sufficiently simple," a guess based on the plot of lines where $\mathrm{Im}\, X'(b_x) = 0$ will often suffice to get started. (One has to guess not only $b_x^{(N)}$, but also $q_x^{(N)}$.) By "sufficiently simple" we mean that $X'(b_x)$ and $X''(b_x)$ should be reasonably smooth and that $|X''(b_x)|$ should not be too small in the region of complex b_x where the stationary points are searched for. If, however, $X''(b_x)$ at the guessed point is very different from its value at the stationary point, the Newton–Raphson iteration [point (4)] will usually not converge. In such cases, the following method is useful: Choose a line, starting on the real axis and going parallel to the imaginary axis out into the complex plane. This line should be chosen such that it will intersect the desired trajectory of stationary points.

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Choose next a small interval, Δb_x, and investigate successive segments of the line, from $n\Delta b_x$ to $(n+1)\Delta b_x$ until a segment is found that satisfies the conditions

$$\big(\operatorname{Im} X'[n\Delta b_x]\big)\big(\operatorname{Im} X'[(n+1)\Delta b_x]\big) < 0, \tag{B.9}$$

and

$$\operatorname{Re} X'[n\Delta b_x] > 0. \tag{B.10}$$

The trajectory of stationary points will thus intersect this interval. If Δb_x is reduced, $\Delta b_x \to \Delta b_x/10$, and this procedure is repeated a couple of times, a sufficiently precise start point may be obtained as the point $\tilde{b}_x^{(N)}$ which by interpolation between $n\Delta b_x$ and $(n+1)\Delta b_x$ makes $\operatorname{Im} X'[\tilde{b}_x^{(N)}]$ vanish. The corresponding value of q is given by $\operatorname{Re} X'[\tilde{b}_x^{(N)}]$.

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