QCD CALCULATIONS BY NUMERICAL INTEGRATION

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I describe a method for performing next-to-leading order QCD calculations in which all of the integrations are performed numerically. This is an alternative to the usual method in which some integrations are performed numerically and some analytically. I illustrate the method with a simple example.

In this talk, I discuss a method ¹ for calculating e^+e^- event shape observables at next-toleading order in QCD. It should be possible to extend the method to processes in which there are hadrons in the initial state, such as $e + p \rightarrow e + jets$ and $p + \bar{p} \rightarrow jets$. However, I have so far worked on the e^+e^- case as the simplest way to try out the methods.

Of course, we already have a very good method for calculating e^+e^- event shape observables at next-to-leading order. The method currently used is due to Ellis, Ross, and Terrano² and is implemented in programs by Kunszt and Nason³, Glover and Sutton⁴ and Catani and Seymour⁵. The Ellis, Ross, and Terrano method also works for QCD calculations with hadrons in the initial state. Thus it may seem that we do not need another method. Nevertheless, the method to be described is different enough from the method normally used that it could have advantages.

I have constructed a computer program that calculates e^+e^- event shape observables at next-to-leading order in QCD using this method. In Fig. 1, I display the results for the thrust distribution $d\sigma/dT$. What I have calculated is the ratio R of the coefficient of α_i^2 in the perturbative expansion of $d\sigma/dT$ to the same quantity as calculated by Kunszt and Nason³. Within the systematic errors, estimated at 1% and indicated by the horizontal lines, there is good agreement.

The main idea of the numerical integration method is simple. It is this main idea that I wish to describe here, using an easy calculation as an example.

Figure 1: Coefficient of α_s^2 in the thrust distribution compared to the results of Kunszt and Nason³.

Figure 2: Graphs to be calculated as an example. Left: The uncut graph. Right: The four cuts of this graph.

Consider the two loop diagram in ϕ^3 theory that is depicted in Fig. 2. Here the line carrying. momentum q^{μ} is the analog of the virtual γ or Z^0 line in e^+e^- annihilation. There are four possible final state cuts for this graph, as indicated in the right hand side of Fig. 2. In each cut graph, we supply a measurement function that equals the total transverse energy of particles in the final state, $\sum |\vec{k}_{T,i}|$, where $\vec{k}_T \cdot \vec{q} = 0$. This is the analog of measuring, say, the average value of one minus the thrust in e^+e^- annihilation.

In the definition of the simple example, we also include an integration over the incoming energy q^0 with fixed \vec{q} and a function $h(q^0)$ that serves to cut off large q^0 . (However, in the figures that follow, I have set $h(q^0) = 1$.)

Having defined the problem, we are now ready to calculate. We first integrate over the energies. For each final state parton, we have a factor $\delta(E^2 - \vec{k}^2) \Theta(E > 0)$. Thus, $E = |\vec{k}|$. With three final state particles, we eliminate the integral over $q⁰$ and the integrals over two loop energies. With two final state particles, we eliminate the integral over $q⁰$ and the integral over one loop energy. One integral over the energy in a virtual loop remains. We perform this integration by "closing the contour." This gives successive $E = |k|$ substitutions, one for each propagator in the loop. Thus the entire process of integrating over the energies is a succession of simple algebraic replacements.

We now have an integration over the three-momenta in the loops:

$$
\mathcal{I} = \int d^3 \vec{\ell}_4 \, d^3 \vec{\ell}_2 \, \sum_C \, g(C; \ell). \tag{1}
$$

The key feature is that we put sum over cuts C is inside the integrations. The integrands contain singularities. We must distinguish between pinch singular points and singularities that are not pinched. We deform the integration contour away from singularities that do not pinch it. Call the loop momentum on the deformed contour $\vec{\ell} + i\vec{\kappa}$. We make a definite choice for $\vec{\kappa}$ as a function of $\tilde{\ell}$. With this choice, the integral is convergent. We calculate it by Monte Carlo integration .

To calculate the integral by Monte Carlo integration, we choose points ℓ_i with a density $\rho(\ell_i)$ and compute

$$
\mathcal{I} = \int d\ell \ f(\ell) \approx \frac{1}{N} \sum_{i} \frac{f(\ell_i)}{\rho(\ell_i)}.
$$
 (2)

This will give a good approximation to the integral for a large number of points N if the quantity $|f(\ell)|/\rho(\ell)$ is never too large. Thus one must choose ρ carefully. In particular, one must let ρ be singular at the point $\vec{\ell}_2 = 0$ where the exchanged parton becomes soft.

In the left hand part of Fig. 3, I plot $\Re[f(\ell)/\rho(\ell)]$ versus $\ell_{2,x}, \ell_{2,y}$ with $\ell_{2,z} = 0$ for a particular choice of $\tilde{\ell}_4$ with $\tilde{\ell}_{4,z} = 0$ in a frame in which \vec{q} lies along the x-axis. In making this graph, I have taken a particular choice of the deformation $\vec{\kappa}$ and of the density of points ρ . We see that $\Re[f(\ell)/\rho(\ell)]$ is everywhere finite, indicating that the Monte Carlo integration will converge.

Figure 3: $\Re[f(\ell)/\rho(\ell)]$. Left: All cuts together. Right: Three particle cuts separately. The plotting program used cannot reproduce the very narrow ridge in the center of the left hand figure, so a cross section through this ridge is shown instead.

The method normally used to perform calculations like this is due to Ellis, Ross, and Terrano². Applying this method to the present example, one would perform the integrations for virtual subgraphs analytically. Then the remaining loop integrations in cut graphs with a virtual subgraph would be done numerically. For cut graphs with no virtual subgraphs, all of the integrations would be performed numerically. In the right hand part of Fig. 3, I plot $\Re[f(\ell)/\rho(\ell)]$ versus $\ell_{2,x}, \ell_{2,y}$ as before for just the three particle cuts. Note that there are singularities, which arise from collinear configurations of the final state particles. These singularities are not integrable. The resulting infinities cancel against infinities from the virtual graphs. In order to make the calculation work, one can, for instance, slice away the region near the singularities and perform the integration over the remaining region numerically. The integration from the singular region must then be done analytically using dimensional regulation so that the infinite terms can be canceled against the infinite terms from the virtual graphs.

In the present approach, we note that the contributions to $\Re[f(\ell)/\rho(\ell)]$ from the cut graphs that have virtual subgraphs have singularities at just the locations of the singularities visible in the right hand part of Fig. 3. The singularities, however, have the opposite signs. The net $\Re[f(\ell)/\rho(\ell)]$ is finite, as we have seen in the left hand figure. The point of the method described here is to take advantage of this cancellation by summing over cuts before integrating. Then the entire integral can be performed numerically. The calculation is simpler, and one has the flexibility of being able to modify the integrand if one wishes.

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