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Evaluation of Proton–Proton Elastic Scattering with Quark Hard Cores Using Glauber and Monte Carlo Methods*

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This paper shows how Monte Carlo methods can be used to evaluate multidimensional integrals that occur in Glauber scattering theory. A detailed discussion of the various Monte Carlo methods is given. The methods are used to obtain the proton–proton elastic scattering differential cross section, where the proton is composed of three quarks with hard cores. It is found that including a quark hard core has no effect on the differential cross section for a fixed rms quark distance.

I. INTRODUCTION

The Glauber approximation [1] for the high-energy scattering of composite systems has had a wide range of application in the last 15 years. It has been applied to problems in molecular, atomic, nuclear, and particle physics with a great deal of success. Inelastic [2] as well as elastic scattering phenomena have been investigated using this approximation. The multiple scattering nature of the approximation allows the total scattering amplitude to be written as a series of terms which depend on the number of constituent-particle scatters that were effective during the system–system collision. Thus, at small angles or small momentum transfers, the scattering amplitude is determined by single and double scattering processes, while at increasingly larger angles higher-order scattering processes begin to dominate. The total elastic scattering amplitude can be calculated provided one can specify how the constituent particles scatter as free particles and how they are

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bound, i.e., specifying the particle–particle scattering amplitudes and the system wavefunctions.

To evaluate the total system–system scattering amplitude, a many-dimensional integral over the constituent particle coordinates and also a two-dimensional integral over the impact parameter need be calculated. In general, for the problem of an n-particle system scattering from a system of n' particles, one must evaluate an integral of $(3n - 3) + (3n' - 3) + 2$ dimensions. Only when rather simple functional forms are used for the system wavefunctions and particle–particle scattering amplitudes can one hope to evaluate these integrals explicitly. Previous calculations on particle-nucleus scattering [3] and elementary particle scattering in the quark model [4] have used Gaussians or sums of Gaussians for the functional forms of the constituent-particle scattering amplitudes and system wavefunctions or form factors. The introduction of more complex functions results in a many-dimensional integration that is at least formidable if not impossible to evaluate by analytic methods. It is the purpose of this paper to investigate how Monte Carlo techniques might be employed to obtain accurate numerical solutions to the many-dimensional integrals encountered in the Glauber theory.

Monte Carlo methods have increased in popularity as faster computing machines have been developed over the last few decades. Today, on present computers, one is able to evaluate a given statistical estimator many thousands of times in a matter of minutes. Such large sample sizes are needed in many Monte Carlo calculations to meet the accuracy requirements.

Schmid and others [5] have used Monte Carlo methods successfully to calculate binding energies of light nuclei, using a Rayleigh–Ritz variational procedure to minimize the expectation value of the Hamiltonian which included hard core potentials and functions with hard core factors. In this type of analysis one encounters many-dimensional integrals over the constituent nucleon coordinates which can be handled conveniently and accurately by Monte Carlo methods.

The accuracy of Monte Carlo methods is rather insensitive to the number of dimensions involved but very sensitive to large or rapid changes in the integrand as a function of any of the integration variables. In evaluating the Glauber integrals, the major problem lies in the integration over the impact parameter $\mathbf{b}$ because of the appearance of the oscillating factor $\exp(i\boldsymbol{\Delta} \cdot \mathbf{b})$, where $\boldsymbol{\Delta}$ is the momentum transferred between the colliding systems. As $\boldsymbol{\Delta}$ increases in magnitude, this factor destroys the "nice" behavior we would require of the integrand for Monte Carlo calculation. We will discuss this in more detail in the main text.

In this paper we will explore various methods of maximizing the efficiency of Monte Carlo evaluations of the many-dimensional integrals encountered in the Glauber theory.

In Section II we will exhibit the type of integral we plan to evaluate. A short explanation of how Monte Carlo techniques can be applied to evaluating integrals

will follow in Section III. We will then turn our attention to a particular problem, namely, the elastic scattering of two systems containing three particles each with hard core wavefunctions—i.e., proton–proton elastic scattering where the protons are composed of three quarks. In Section V we will discuss various approaches to evaluating the resulting integrals.

II. Glauber Approximation

The scattering amplitude as a function of the momentum transfer Δ for n-particle system–n'-particle system collisions in the Glauber approximation can be written as

$$F_{\mathrm{IF}}(\Delta) = k/2\pi i \int d^2b e^{i\Delta\cdot b} \int \cdots \int d\mathbf{q}_1 \cdots d\mathbf{q}_n \, d\mathbf{q}_1' \cdots d\mathbf{q}_{n'}'$$
$$\cdot u_{\mathrm{F}}(\mathbf{q}_1 \cdots \mathbf{q}_n) \, u_{\mathrm{F}}(\mathbf{q}_1' \cdots \mathbf{q}_{n'}') \left\{ \exp\left[i \sum_{ii'} \chi_{ii'}(\mathbf{b} - \mathbf{s}_i + \mathbf{s}_{i'}') \right] - 1 \right\}$$
$$\cdot u_{\mathrm{I}}(\mathbf{q}_1 \cdots \mathbf{q}_n) \, u_{\mathrm{I}}(\mathbf{q}_1' \cdots \mathbf{q}_{n'}'), \tag{1}$$

where k is the momentum of the incident system in the lab frame and $\mathbf{b}$ is the impact parameter which is the component of the displacement between centers of mass of the two systems in the plane having a normal in the direction $\mathbf{k}$. The coordinates $\mathbf{q}_1 \cdots \mathbf{q}_n$ and $\mathbf{q}_1' \cdots \mathbf{q}_{n'}'$ are the coordinates of the constituent particles of the incident and target systems, respectively. The coordinates $\mathbf{s}_1 \cdots \mathbf{s}_n$ and $\mathbf{s}_1' \cdots \mathbf{s}_{n'}'$ are projections of the $\mathbf{q}$-coordinates on the plane having normal $\mathbf{k}$. The wavefunctions of the systems initially and finally are given by the functions u_{I}, u_{I}' and u_{F}, u_{F}'. The χ-functions are called the phase shift functions and are related to the interaction potential between the constituent particles. The phase shift $\chi_{ii'}$ for the ith particle in the unprimed system scattering from the i'th particle in the primed system is

$$\chi_{ii'}(\mathbf{b} - \mathbf{s}_i + \mathbf{s}_{i'}) = \frac{-i}{\hbar v} \int_{-\infty}^{\infty} V_{ii'}(\mathbf{b} - \mathbf{s}_i + \mathbf{s}_i', z) \, dz, \tag{2}$$

where $V_{ii'}$ is the interaction potential. The summation $\sum_{ii'}$ in Eq. (1) is over all two-particle interactions; i.e., $11'$, $12'$,..., $1n'$, $21'$, $22'$,..., $2n'$,..., $n1'$,..., nn'. It is useful to define the profile function

$$\Gamma(\mathbf{b} - \mathbf{s}_i + \mathbf{s}_{i'}') = 1 - \exp[i\chi_{ii'}(\mathbf{b} - \mathbf{s}_i + \mathbf{s}_{i'}')] \tag{3}$$

so that the expression in curly brackets in Eq. (1) can be expanded as

$$\exp\left[i\sum_{ii'}\chi(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_{i'}')\right]-1=\sum_{ii'}\Gamma_{ii'}(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_{i'}')$$
$$+\sum_{\substack{ii'\\ii'>jj'}}\sum_{jj'}\Gamma_{ii'}(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_{i'}')\,\Gamma_{jj'}(\mathbf{b}-\mathbf{s}_j+\mathbf{s}_{j'}')$$
$$+\sum_{\substack{ii'\\ii'>jj'>kk'}}\sum_{jj'}\sum_{kk'}\Gamma_{ii'}(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_{i'}')\,\Gamma_{jj'}(\mathbf{b}-\mathbf{s}_j+\mathbf{s}_{j'}')$$
$$\times\,\Gamma_{kk'}(\mathbf{b}-\mathbf{s}_k+\mathbf{s}_{k'}')$$
$$+\cdots+\prod_{ii'=11'}^{nn'}\Gamma_{ii'}(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_i'),\tag{4}$$

where the summations are performed over all two-particle interactions that can occur between the two systems such that no combination appears twice. The profile functions $\Gamma_{ii'}$ are related to the free particle–particle scattering amplitudes as

$$f_{ii'}(\boldsymbol{\delta})=\frac{k}{2\pi i}\int e^{i\boldsymbol{\delta}\cdot\mathbf{b}}\Gamma_{ii'}(\mathbf{b})\,d^2b.\tag{5}$$

When Eq. (4) is substituted into Eq. (1), the expression for the total scattering amplitude becomes a sum of a large number of many-dimensional integrals, each containing a single Γ-term or product of more than one Γ, such as $\Gamma_{ii}\Gamma_{jj'}$ or $\Gamma_{ii'}\Gamma_{jj'}\Gamma_{kk'}$ or higher. The integrals which include only $\Gamma_{ii'}$ terms are called the single scatter contribution. Those having $\Gamma_{ii'}\cdot\Gamma_{jj'}$ terms are called double scattering contributions, etc. At $\Delta=0$, the single and double scatter terms dominate, accounting for greater than 95% of the contributions. As $|\Delta|$ increases, higher-order contributions become more important (see, for example, Ref. [4]).

III. Monte Carlo Evaluation of Definite Integrals

In this section we will discuss some of the basic ideas and techniques of Monte Carlo methods applied to evaluating definite integrals. Consider the m-dimensional integral

$$I=\int_{a_1}^{b_1}\int_{a_2}^{b_2}\cdots\int_{a_m}^{b_m}f(x_1,x_2,\ldots,x_m)\,dx_1\,dx_2\cdots dx_m\,.\tag{6}$$

The integration variables $x_1, x_2, \ldots, x_m$ can be considered continuous random

variables having a probability density function $P(x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m$ defined in $a_1 \leqslant x_1 \leqslant b_1$, $a_2 \leqslant x_2 \leqslant b_2, \ldots, a_m \leqslant x_m \leqslant b_m$ and normalized to unity. Rewriting Eq. (6) as

$$I = \int_{a_1}^{b_1} \int_{a_2}^{b_2} \cdots \int_{a_m}^{b_m} \left[\frac{f(x_1, x_2, \ldots, x_m)}{P(x_1, x_2, \ldots, x_m)}\right] P(x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m, \quad (7)$$

we see that the integral is just the expectation of the function

$$g(x_1, x_2, \ldots, x_m) = f(x_1, x_2, \ldots, x_m)/P(x_1, x_2, \ldots, x_m), \quad (8)$$

i.e.,

$$I = \mathscr{E}\{g(x_1, x_2, \ldots, x_m)\}. \quad (9)$$

An unbiased estimator of this expectation over N-observations of the random variables $x_1, x_2, \ldots, x_m$ is the simple average

$$I = \frac{1}{N} \sum_{i=1}^{N} g(x_1^i, x_2^i, \ldots, x_m^i), \quad (10)$$

where x_j^i is the ith observation of the random variable x_j. An unbiased estimator of the variance is

$$\mathrm{var}(I) = \frac{1}{N-1} \left\{ \sum_{i=1}^{N} [g(x_1^i, x_2^i, \ldots, x_1^i)]^2 - \frac{1}{N} \left[\sum_{i=1}^{N} g(x_1^i, x_2^i, \ldots, x_m^i) \right]^2 \right\} \quad (11)$$

and the standard error is

$$\Delta I = [\mathrm{var}(I)/N]^{1/2}. \quad (12)$$

For most problems, the probability density function is taken to be a product of single-variable functions, i.e.,

$$P(x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m = P_1(x_1)\, P_2(x_2) \cdots P_m(x_m)\, dx_1\, dx_2 \cdots dx_m. \quad (13)$$

This is done to facilitate the generation of the observations of the random variables since simplicity and speed of evaluation of Eqs. (10) and (11) are important factors in successful and accurate Monte Carlo. (For an example of conditional or biased Monte Carlo see Ref. [6].)

The accuracy of a Monte Carlo calculation depends on two basic elements, as can be seen from Eq. (12), i.e., the variance and the number of observations, N. To increase the accuracy of a given calculation, either the number of observations is increased or the variance is reduced. Some common variance-reducing techniques are stratified sampling, importance sampling, and control variates, among other. The simplest scheme is called crude Monte Carlo, where the probability density

function has the form of a product of rectangular or uniform distribution functions of the form

$$P(x_1, x_2, \ldots, x_m)\, dx_1\, dx_2 \cdots dx_m = U_1(x_1)\, U_2(x_2) \cdots U_m(x_m)\, dx_1\, dx_2 \cdots dx_m, \quad (14)$$

where

$$U_j(x_j)\, dx_j = \begin{cases} 1/(b_j - a_j), & a_j \leqslant x_j \leqslant b_j, \\ 0, & \text{otherwise.} \end{cases} \quad (15)$$

The estimator of the integral Eq. (6) becomes

$$I = \left[\frac{I}{N} \prod_{j=1}^{M} (b_j - a_j)\right] \cdot \sum_{i=1}^{N} f(x_1^i, x_2^i, \ldots, x_m^i). \quad (16)$$

Thus the integration is replaced by the simple average of the integrand over many observations of the random variables. When the integrand varies rapidly between the limits of integration, it is advantageous to break the integral into smaller parts and evaluate each part separately using crude Monte Carlo; this is called stratified sampling. Other times it may be possible to "subtract out" the rapidly varying part using an analytic function which can be readily integrated. This is a type of control variate procedure. Another popular technique is importance sampling and one which we employ in our calculations. Here the probability density functions for the random variables are chosen so that they behave on a gross scale much like the integrand itself. In a certain sense, importance sampling techniques "factor out" the variations of the integrand which would otherwise yield a large variance in crude Monte Carlo.

There is a compromise which one must make in all variance-reducing schemes; in attempting to reduce the variance of a calculation, one inherently increases the complexity and work to perform the generation of the random variables or evaluation of the integrand or both. Hence a profitable variance-reducing technique is one which will yield a more accurate result; i.e., smaller ΔI with the same amount of labor (or computer time).

IV. Glauber Approximation with Hard Cores

We consider the particular problem of the high-energy elastic scattering of two systems each containing three of the same type of particle. The scattering amplitude for the free scattering of these constituent particles will be Gaussian in form. This problem is of interest in high-energy elastic scattering of protons in the quark model, where each proton is composed of three quarks [4]. Also, if the constituent particles are nucleons, not distinguishing protons and neutrons, this would be

triton–triton elastic scattering. In any case, this problem exemplifies the general features of composite elastic scattering problems that are of interest in nuclear physics [3] and elementary particle scattering in the quark model [4].

For this problem, the expression for the phase shift function, Eq. (4), simplifies to

$$\begin{aligned}\left[\exp\left(i\sum_{ii'}\chi_{ii'}(\mathbf{b}-\mathbf{s}_i+\mathbf{s}_{i'}')\right)-1\right]&\\ =9\Gamma_{11'}(b-\mathbf{s}_1+\mathbf{s}_1')-[18\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1')\,\Gamma_{22'}(\mathbf{b}-\mathbf{s}_2+\mathbf{s}_2')&\\ +18\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1)\,\Gamma_{12'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_2')]&\\ +[6\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1')\,\Gamma_{22'}(\mathbf{b}-\mathbf{s}_2+\mathbf{s}_2')\,\Gamma_{33'}(\mathbf{b}-\mathbf{s}_3+\mathbf{s}_3')&\\ +36\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1')\,\Gamma_{12'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_2')\,\Gamma_{33'}(\mathbf{b}-\mathbf{s}_3+\mathbf{s}_3')&\\ +36\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1')\,\Gamma_{12'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_2')\,\Gamma_{22'}(\mathbf{b}-\mathbf{s}_2+\mathbf{s}_2')&\\ +6\Gamma_{11'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_1')\,\Gamma_{12'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_2')\,\Gamma_{13'}(\mathbf{b}-\mathbf{s}_1+\mathbf{s}_3')]&\\ +\text{HO terms.}&\end{aligned}\tag{17}$$

We will include only up to third-order terms in the Monte Carlo calculations. For most calculations this is sufficient. Placing Eq. (17) into Eq. (1), we see that the total scattering amplitude is seven multidimensional integrals.

When the system wavefunctions are chosen to the Gaussians or sums of Gaussians these integrals can be evaluated analytically (see Ref. [4]). When hard core factors are included the evaluation becomes extremely difficult if not impossible. Monte Carlo methods, and in particular, importance sampling techniques, can be applied to this problem in a natural way.

Let the system wavefunctions be of the form

$$|\,u(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)|^2 = C\exp\left\{\frac{1}{s^2}\sum_{i>j}r_{ij}^2\right\}\cdot\xi_{\mathrm{HC}}\cdot\delta(\mathbf{r}_1+\mathbf{r}_2+\mathbf{r}_3),\tag{18}$$

where, following Schmid [5],

$$\begin{aligned}\xi_{\mathrm{HC}} &= \prod_{i>j}g(r_{ij}) = g(|\,\mathbf{r}_1-\mathbf{r}_2\,|)\cdot g(|\,\mathbf{r}_2-\mathbf{r}_3\,|)\cdot g(|\,\mathbf{r}_3-\mathbf{r}_1\,|),\\ g(a) &= \begin{cases}0, & a>\beta,\\ \sin[(a-\beta)/(\alpha-\beta)], & \beta\leqslant a\leqslant\alpha,\\ 1, & a>\alpha,\end{cases}\\ r_{ij} &= |\,\mathbf{r}_i-\mathbf{r}_j\,|,\end{aligned}\tag{19}$$

and the scattering amplitude for the constituent particles when scattering as free particles is of the form

$$f_{ii'}(\Delta) = f(0)\exp\{-B^2\Delta^2/2\},\tag{20}$$

where $f(0)$ and B^2 are in general complex constants.

For elastic scattering $u_F = u_I$, $u_F' = u_I'$ in Eq. (1) and we take Eq. (18) as the wavefunction for both systems. The resulting expression for the total scattering amplitude to third-order scattering terms becomes

$$F_{\text{elastic}}(\Delta) = \frac{k}{2\pi i} \int d^2b\, e^{i\Delta\cdot\mathbf{b}} \left[\sum_{N=1}^{7} \Gamma_N(\mathbf{b}) \right], \tag{21}$$

where

$$\Gamma_N = \int d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3\, d\mathbf{r}_1'\, d\mathbf{r}_2'\, d\mathbf{r}_3' \mid u(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)|^2 \mid u(\mathbf{r}_1', \mathbf{r}_2', \mathbf{r}_3')|^2 \cdot \Gamma_N(\mathbf{b}, \mathbf{s}_1, \mathbf{s}_2, \mathbf{s}_3, \mathbf{s}_1', \mathbf{s}_2', \mathbf{s}_3') \tag{22}$$

and

$$\begin{aligned} \Gamma_1 &= 9\Gamma_{11'}, & \Gamma_2 &= -18\Gamma_{11'}\Gamma_{22'}, \\ \Gamma_3 &= -18\Gamma_{11'}\Gamma_{12'}, & \Gamma_4 &= 6\Gamma_{11'}\Gamma_{22'}\Gamma_{33'}, \\ \Gamma_5 &= 36\Gamma_{11'}\Gamma_{12'}\Gamma_{33'}, & \Gamma_6 &= 36\Gamma_{11'}\Gamma_{12'}\Gamma_{22'}. \\ \Gamma_7 &= 6\Gamma_{11'}\Gamma_{12'}\Gamma_{13'}, \end{aligned} \tag{23}$$

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Let us consider the seven integrals of Eq. (22), ignoring for the moment the integration over the impact parameter. It is convenient to make the following change of variables [5].

$$\begin{aligned} \mathbf{u} &= \mathbf{r}_1 + \mathbf{r}_2, & \mathbf{u}' &= \mathbf{r}_1' + \mathbf{r}_2', \\ \mathbf{v} &= \mathbf{r}_1 - \mathbf{r}_2, & \mathbf{v}' &= \mathbf{r}_1' - \mathbf{r}_2'. \end{aligned} \tag{24}$$

This change enables us to write Eq. (22), using Eq. (18), for the wavefunction, as

$$\Gamma_N(\mathbf{b}) = c^2 \int d\mathbf{u}\, d\mathbf{v}\, d\mathbf{u}'\, d\mathbf{v}' \exp[-(u^2/\sigma_u^2 + v^2/\sigma_v^2) - (u'^2/\sigma_u^2 + v'^2/\sigma_v^2)] \cdot \xi_{\text{HC}}(\mathbf{u}, \mathbf{v})\, \xi_{\text{HC}}(\mathbf{u}', \mathbf{v}') \cdot \Gamma_N(\mathbf{b}, \mathbf{u}, \mathbf{v}, \mathbf{u}', \mathbf{v}'). \tag{25}$$

This form of the integral has the feature that the integration variables in the exponential terms do not appear in cross terms like $\mathbf{u} \cdot \mathbf{v}$. The observations of the new coordinates will be generated according to the normal probability density functions

$$\begin{aligned} N(\sigma_u'^2, \mathbf{u}) &= (\pi\sigma_u'^2)^{-3/2} \exp\{-(1/\sigma_u'^2)(u_x^2 + u_y^2 + u_z^2)\}, \\ N(\sigma_v'^2, \mathbf{v}) &= (\pi\sigma_v'^2)^{-3/2} \exp\{-(1/\sigma_v'^2)(v_x^2 + v_y^2 + v_z^2)\}, \end{aligned} \tag{26}$$

with similar expressions for the primed coordinates.

For the "no hard core" case where the hard core is unity, i.e., $\alpha = \beta = 0$, the Γ_n's can be calculated analytically. Thus, we can use this limit to check the reliability of the Monte Carlo calculations. The parameters σ_u' and σ_v' are chosen carefully. As a rule of thumb they should be chosen slightly larger than the wavefunction parameters σ_u and σ_v. If they are chosen too small, poor convergence will result.

To illustrate this point, consider the integral

$$A = (2/\pi)^{1/2} \int_{-\infty}^{\infty} dx\, e^{-(1-x)^2} e^{-x^2/\alpha^2}. \tag{27}$$

Using the Monte Carlo method described in Section III we write this integral as

$$A = \int_{-\infty}^{\infty} [f(x)/g(x)]\, g(x)\, dx, \tag{28}$$

where $f(x) = (2/\pi)^{1/2} \exp[-(1-x)^2] \exp[-x^2/\alpha^2]$ and we choose $g(x) = [1/(\pi\alpha'^2)^{1/2}] \exp[-x^2/\alpha'^2]$. An estimate of A is the average over M observations of x,

$$A = (1/M)\, \sqrt{2}\, (\alpha'/\alpha) \sum_{j=1}^{M} \exp[-(1-x_j)^2] \cdot \exp[-x_j^2/\alpha^2], \tag{29}$$

where x_j is the jth observation. Choosing $\alpha = 1$, the exact value of this integral is $A = 0.6065$. Table I shows the results of the Monte Carlo calculation when α' is 0.1, 0.5, 1.0, and 1.5 for increasing sample sizes. It is seen that the results for $\alpha' = 0.1$ are quite a bit smaller than the exact result and the convergence to the correct result is slow at best. At $\alpha' = 0.5$, the results are beginning to look reasonable although the approach to the exact result is still slow. For $\alpha' = 1.0$ there is greater agreement and convergence is quite satisfactory, being accurate to about 1% with a sample size of 10,000.

TABLE I

Monte Carlo Estimates of Eq. (29) for Various Sample Sizes, M, and Various Values of the Parameter α', the Generation Parameter[a]

M \ α'	0.1	0.5	1.0	1.5
500	0.415	0.633	0.598	0.644
1000	0.379	0.612	0.593	0.618
5000	0.424	0.622	0.603	0.613
10,000	0.513	0.626	0.599	0.615

[a] The value of the integral for $\alpha = 1$ is 0.6065.

For the "no hard core" case the results of the Monte Carlo calculations are shown in Fig. 1. Each of the seven $\overline{\Gamma}(b)$ were calculated at 16 values of b using 1000 observations at each point. The exact result is also shown. The standard errors are smaller than the symbols, and so are not drawn in the figure. Agreement is quite good.

Two other quantities are also calculated simultaneously with the Γ's. The normalization constant, R_{norm}, defined by

$$R_{\text{norm}} = (\pi\sigma_u'^2)^{-3}\,(\pi\sigma_v'^2)^{-3} \int d^3u\, d^3v\, d^3u'\, d^3v' \mid u(\mathbf{u}, \mathbf{v})|^2 \mid u(\mathbf{u}', \mathbf{v}')|^2, \tag{30}$$

which for the "no hard core" calculation can be found exactly to be

$$R_{\text{norm}} = (\pi\sigma_u{}^2)^3\,(\pi\sigma_v{}^2)^3/(\pi\sigma_u'^2)^3\,(\pi\sigma_v'^2)^3 = (1.1)^{-6} = 0.56447, \tag{31}$$

when $\sigma_u'^2 = 1.1\sigma_u{}^2$ and $\sigma_v'^2 = 1.1\sigma_v{}^2$. Also the rms distance $\langle r^2\rangle^{1/2}$ is calculated

$$\langle r^2\rangle = \int d^3u\, d^3v\, r^2 \mid u(\mathbf{u}, \mathbf{v})|^2 \Big/ \int d^3u\, d^3v \mid u(\mathbf{u}, \mathbf{v})|^2 = \tfrac{3}{2}\sigma_u{}^2. \tag{32}$$

The value of $\overline{\Gamma_N}(b)$ is calculated using 1000 estimates at each value of b. Thus a total of 16,000 estimates is required to obtain the results shown in Fig. 1. Table II lists the values of $\langle r^2\rangle$ and R_{norm} for various runs. The values of the parameters used in these calculations are $\text{Re}\,B^2 = 3.75$, $\text{Im}\,B^2 = 5.0$, $\text{Re}\,f(0) = -0.18$, $\text{Im}\,f(0) = 1.1$, and $\sigma_u{}^2 + \text{Re}\,B^2 = 8.63$, where the units are $(\text{GeV/c})^{-2}$.

TABLE II

Values of Monte Carlo estimates of $\langle r^2\rangle$ and R_{norm} for three independent runs for the no hard core case

$\langle r^2\rangle$ Exact value = 7.32	R_{norm} Exact value = 0.5645	Sample size
7.35	0.5646	16,000
7.33	0.5649	16,000
7.39	0.5625	16,000

When the hard core is "turned on," we proceed in exactly the same manner, choosing the random observations to have the same probability density functions, Eq. (26). We expect that more estimates will be needed to achieve the same order of accuracy as in the "no hard core" case since many of the estimates will give zero contributions due to the hard core factors.

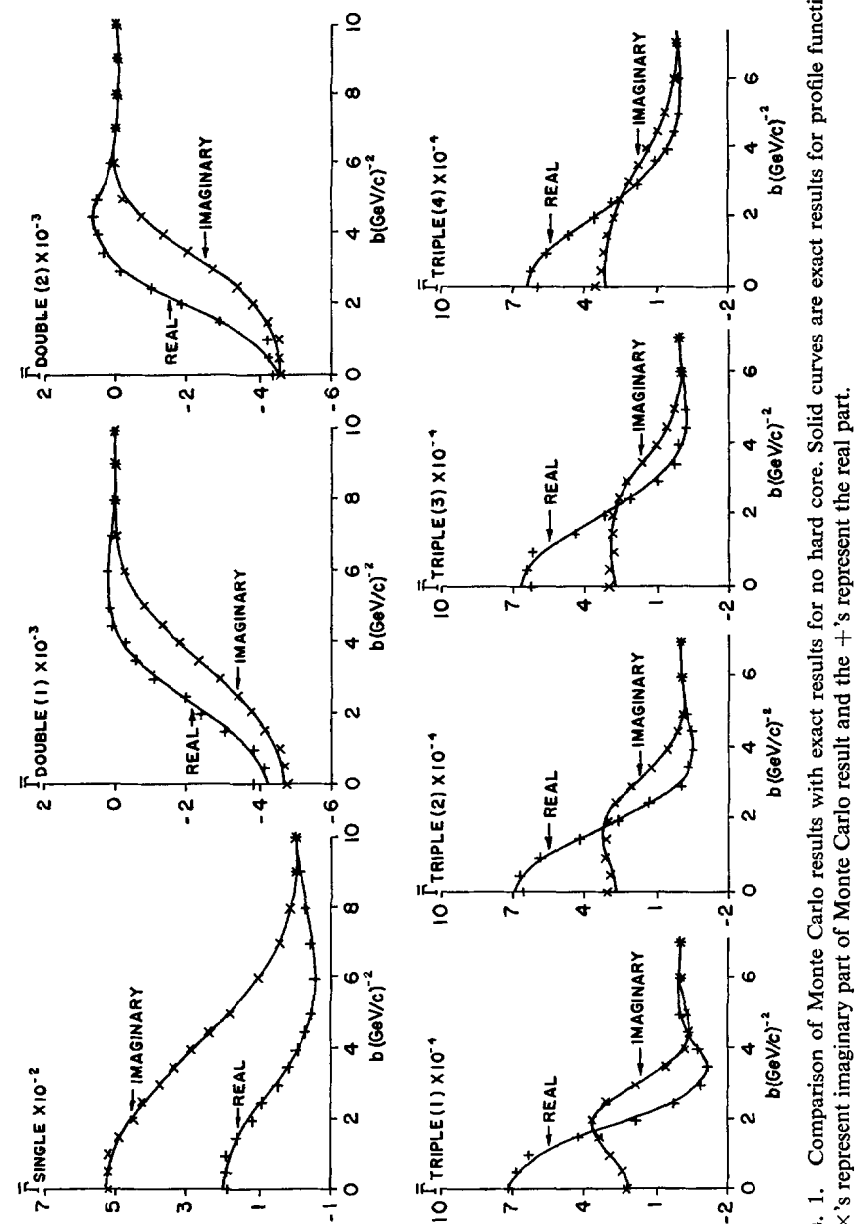

FIG. 1. Comparison of Monte Carlo results with exact results for no hard core. Solid curves are exact results for profile functions. The ×'s represent imaginary part of Monte Carlo result and the +'s represent the real part.

It is easy to estimate the fraction of the observations which give zero contribution. We define the number of effective observations or estimates, N_{eff}, as the number of observations which give nonzero values for the wavefunction. To evaluate N_{eff} for a given value of b, we consider the probability density function of the inter-

$$P(\mathbf{v}) = (\pi\sigma_v'^2)^{-3/2} \exp[-\sigma_v'^{-2}(v_x^2 + v_y^2 + v_z^2)]. \tag{33}$$

The probability density function for the magnitude of v is found by integrating $P(\mathbf{v})$ over the angle variables:

$$P(|\, v \,|) = (\pi\sigma_v'^2)^{-3/2} \cdot 4\pi v^2 e^{-v^2/\sigma_v'^2}. \tag{34}$$

The probability that $|\, v \,|$ is less than or equal to β is the probability that the hard core factor $g(v)$ will be zero, i.e.,

$$P(|\, v \,| \leqslant \beta) = \int_0^\beta P(|\, v \,|)\, dv = 4\pi(\pi\sigma_v'^2)^{-3/2} \int_0^\beta v^2 e^{-v^2/\sigma_v'^2}\, dv. \tag{35}$$

Integrating by parts, this integral becomes

$$P(|\, v \,| \leqslant \beta) = 2\left[\int_0^\beta f(t)\, dt - \beta' f(\beta')\right], \tag{36}$$

where

$$\beta' = \sqrt{2}\, \beta/\sigma_v$$

and

$$f(t) = [1/(2\pi)^{1/2}] \cdot \exp(-t^2/2). \tag{37}$$

Equation (32) is the probability that an estimate will give zero contribution when the density function contains a hard core of size β. The integrand in the actual calculation contains six hard core factors corresponding to the three inter-particle displacements in each of the two protons. Thus the probability for a nonzero contribution is

$$[1 - P(|\, v \,| \leqslant \beta)]^6. \tag{38}$$

The number of effective estimates is given in terms of this probability and the actual number of estimates

$$N_{eff} = [1 - P(|\, v \,| \leqslant \beta)]^6 \cdot N_{\text{actual}}. \tag{39}$$

For hard cores of size $\beta = 1$, 2, and 3 $(\text{GeV}/c)^{-1}$ and for $N_{\text{actual}} = 1000$, the number of effective estimates is

$$N_{eff}(\beta = 1) = 941, \qquad N_{eff}(\beta = 2) = 598, \qquad N_{eff}(\beta = 3) = 215.$$

Using the criterion that the number of effective estimates for hard core calculations be equal to the total number of estimates for the "no hard core" case to obtain the same accuracy, we can approximate the number of estimates we need to achieve the same accuracy as in a calculation where no hard core factors are included, i.e., the calculation of the previous section. We adjust N_{actual} so that N_{eff} equals the number of estimates for the "no hard core" case. For example, to obtain results of the same accuracy as the previous section where 1000 estimates were used we would need

$$N_{\text{actual}} = 1000/0.941 = 1062 \quad \text{for} \quad \beta = 1.0\,(\text{GeV/c})^{-1},$$
$$N_{\text{actual}} = 1000/0.598 = 1672 \quad \text{for} \quad \beta = 2.0\,(\text{GeV/c})^{-1},$$
$$N_{\text{actual}} = 1000/0.215 = 4651 \quad \text{for} \quad \beta = 3.0\,(\text{GeV/c})^{-1}.$$

The function $\Gamma(b)$ for three different-sized hard cores, $\alpha = 1.5$ and $\beta = 1.0$, $\alpha = 2.5$ and $\beta = 2.0$, $\alpha = 3.5$ and $\beta = 3.0$, was investigated and in Table III we list the values of $\langle r^2 \rangle$ and R_{norm} obtained in these calculations. It is seen that $\langle r^2 \rangle$ is increased quite significantly over the "no hard core" case and increases as β increases. In Fig. 2, the function $\Gamma(b)$ is shown for the hard core parameters $\alpha = 3.5$ and $\beta = 3.0$, obtained by taking 6000 estimates at each value of b. Also shown are the "no hard core" analytic results (solid lines) so that the deviations can be more readily ascertained. The presence of hard core effects is observed in the reduced peaks of $\Gamma(b)$ near $b = 0$. Three independent runs were made for each of the three hard core sizes investigated. For $\alpha = 1.5$ and $\beta = 1.0$, 1100 estimates were used at each value of b. For $\alpha = 2.5$ and $\beta = 2.0$, 3000 estimates were used.

TABLE III

Values of $\langle r^2 \rangle$ and R_{norm} for Various Sizes for the Hard Core

Run identification	α	β	R_{norm}	$\langle r^2 \rangle$
1HC1	1.5	1.0	0.497	7.64
2HC1	1.5	1.0	0.495	7.60
3HC1	1.5	1.0	0.479	7.61
1HC2	2.5	2.0	0.277	8.54
2HC2	2.5	2.0	0.280	8.51
3HC2	2.5	2.0	0.279	8.48
1HC3	3.5	3.0	0.0829	10.30
2HC3	3.5	3.0	0.0833	10.31
3HC3	3.5	3.0	0.0829	10.26

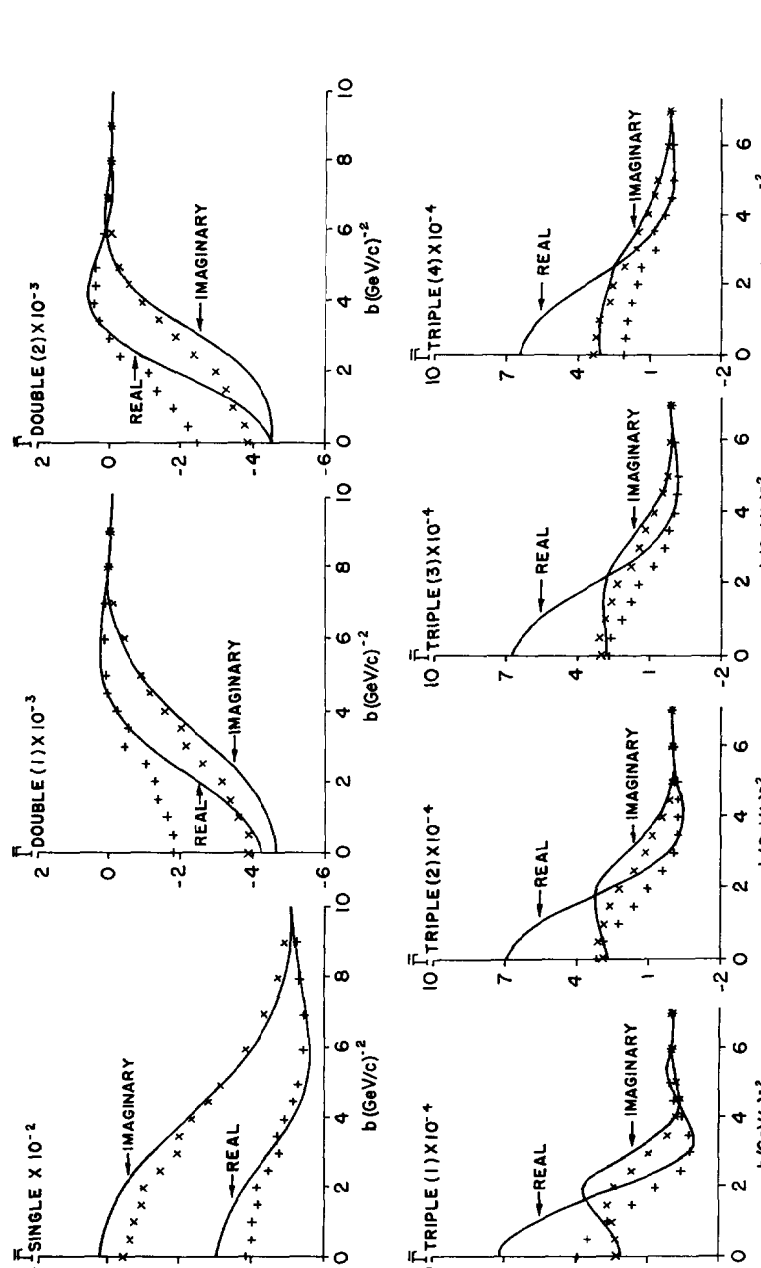

FIG. 2. The Monte Carlo evaluation of the profile functions $\tilde{I}^{\nu}(b)$. Results to third order are shown. The hard core parameters are $\alpha = 3.5$, and $\beta = 3.0$. The solid line is the exact result for the no hard core case. The flattening effect near $b = 0$ is characteristic of the hard core calculations.

Of course the object of this calculation is to obtain the scattering amplitude and differential cross section. To achieve this end we must take the Fourier transform of the functions $\bar{\Gamma}_N(b)$ to obtain the scattering amplitude. Using a grid method for integrating the transform integral of the point by point functions $\bar{\Gamma}_N(b)$ obtained by the Monte Carlo calculations of the previous sections works well for small values of the momentum transfer squared, Δ^2, but due to the oscillating factor $\exp(i\boldsymbol{\Delta} \cdot \mathbf{b})$ this method gives poor results for large values of Δ^2, specifically, for this problem, $\Delta^2 > 0.5\,(\mathrm{GeV/c})^2$. An alternate procedure, which is the one we describe here, is to χ^2-fit the numerical functions $\bar{\Gamma}_i(b)$, $i = 1, 7$ determined by Monte Carlo methods to analytic functions whose transform properties are known. The goodness of the fits will be the most significant factor in determining whether the amplitude obtained in this way is a reliable result or not. A set of different runs is necessary in order to obtain an idea of the accuracy of the results, i.e., for each set of parameters the complete calculation of the amplitude and cross section is to be repeated several times with independent sets of estimates so as to test for reproducibility and accuracy. It is reasonable to fit our Monte Carlo $\bar{\Gamma}_i(b)$-functions to a series of Gaussians of the form

$$\overline{\Gamma_i^{\mathrm{FIT}}}(b) = \sum_{j=1}^{N} T_i^{(j)} \exp(-jE_i b^2) = T_i^{(1)} \exp(-E_i b^2) + T_i^{(2)} \exp(-2E_i b^2) + \cdots, \tag{40}$$

where the subscript i specifies the scattering process, i.e., $i = 1, 7$ and $T_i^{(j)}$ and E_i are complex. Each scatter contribution is fit separately, which gives a total of seven fits for each run.

Having obtained E_i and $T_i^{(j)}$, we can find the scattering amplitude for each type of scatter by taking the Fourier transform of the fitting function, which is

$$f_i(\Delta) = \sum_{j=1}^{N} (T_i^{(j)}/E_i) \cdot \exp(-\Delta^2/4jE_i) \tag{41}$$

and the total scattering amplitude, up to third order in scatter processes, i.e., $i = 1, 7$, is

$$F_{pp}(\Delta) = \sum_{i=1}^{7} \sum_{j=1}^{N} (T_i^{(j)}/E_i) \exp[-\Delta^2/4jE_i]. \tag{42}$$

The χ^2-fitting procedure minimizes the function

$$\chi_i^{\,2} = \sum_{k=1}^{M} \{(\overline{\Gamma_i^{\mathrm{MC}}}(b_k) - \overline{\Gamma_i^{\mathrm{FIT}}}(b_k))/\overline{\Delta\Gamma_i^{\mathrm{MC}}}(b_k)\}^2, \tag{43}$$

where M is the number of values of b at which $\overline{\Gamma_i^{\mathrm{MC}}}(b_k)$ has been evaluated using Monte Carlo methods and $\overline{\Delta\Gamma_i^{\mathrm{MC}}}(b_k)$ is the standard error. The superscript MC

represents the Monte Carlo values while FIT denotes the value of the fitting function given by Eq. (40).

We will require that the fits have at least a confidence level of 0.01. In terms of the maximum allowable value for χ^2 as a function of the number of degrees of freedom, ν, this means that for

$$\nu = 24, \qquad \chi^2_{\text{MAX}} = 43.0;$$

$$\nu = 25, \qquad \chi^2_{\text{MAX}} = 44.3;$$

$$\nu = 26, \qquad \chi^2_{\text{MAX}} = 45.6.$$

The number of degrees of freedom is defined as the number of data points minus the number of parameters in the fitting function. The number of parameters in the fitting function of Eq. (40) is $2N + 2$, where N is the number of terms in the expansion. The total number of data points, M, is twice the number of points at which $\overline{\Gamma_i^{\text{MC}}}(b)$ is calculated using Monte Carlo methods since $\overline{\Gamma_i^{\text{MC}}}(b)$ has both real and imaginary parts. Thus the number of degrees of freedom for these fits is

$$\nu = M - 2N - 2. \tag{44}$$

As we have mentioned before, three independent runs were made for each of the three hard core sizes investigated, i.e., $\alpha = 3.5$, $\beta = 3.0$; $\alpha = 2.5$, $\beta = 2.0$; and $\alpha = 1.5$, $\beta = 1.0$. The results of the fits of the Monte Carlo function $\bar{\Gamma}_i$'s for the "no hard core" case and the three different-sized "hard core" cases to the function $\overline{\Gamma_i^{\text{FIT}}}(b)$ of Eq. (40) are shown in Table IV. The values of χ_i^2, for $i = 1, 7$, for the different runs indicate that the fits are acceptable.

The differential cross section in terms of the scattering amplitude is found using

$$d\sigma/dt = \pi \mid F_{pp}(\Delta)\mid^2 = \pi \left| \sum_{i=1}^{7} f_i(\Delta) \right|^2. \tag{45}$$

The $f_i(\Delta)$'s are the Fourier transforms of the fit functions $\overline{\Gamma_i^{\text{FIT}}}$ of Eq. (41). Figs. 3–6 show the differential cross sections for the "no hard core" case and the three "hard core" cases. The "no hard core" results in Fig. 3 are compared to the exact result and agreement is seen to be quite good. The dashed lines in the figures indicate the extreme values of $d\sigma/dt$ determined by the Monte Carlo–Fit method we have been describing. The solid lines in Figs. 4–6 for the "hard core" cases are the exact calculations where the density function parameter σ_u^2 has been adjusted to match the values of $\langle r^2 \rangle$ in Table III for the various hard core sizes.

There is no noticeable difference between the "no hard-core" cross sections with $\langle r^2 \rangle$ the same as in the hard core case and the corresponding hard core results. Thus we conclude for the range of hard core values we have investigated that for a fixed rms quark distance $\langle r^2 \rangle^{1/2}$ there is no hard core effect on the proton–proton differential cross sections.

TABLE IV

Results of χ^2 Fits for Three Independent Runs[a]

Run identification	Degrees of freedom (ν)	χ^2_{MAX} for confidence levels 0.05	0.01	χ_1^2	χ_2^2	χ_3^2	χ_4^2	χ_5^2	χ_6^2	χ_7^2
1NHC	24	36.4	43.0	12	12	21	24	18	33	10
2NHC	24	36.4	43.0	20	17	16	23	30	26	17
3NHC	24	36.4	43.0	26	23	19	21	32	25	11
1HC1	26	38.9	45.6	22	17	26	12	26	28	19
2HC1	26	38.9	45.6	35	19	28	20	21	18	27
3HC1	26	38.9	45.6	41	24	25	16	19	37	24
1HC2	24	36.4	43.0	19	20	15	22	22	18	19
2HC2	24	36.4	43.0	25	33	18	10	26	30	21
3HC2	24	36.4	43.0	23	37	17	26	33	41	24
1HC3	24	36.4	43.0	25	20	12	17	22	18	28
2HC3	24	36.4	43.0	20	19	28	20	35	30	48*
3HC3	26	38.9	45.6	20	17	29	25	33	19	42

[a] Runs are for each of the following: (1) NHC, no hard core case; (2) HC1, hard core $\alpha = 1.5$, $\beta = 1.0$; (3) HC2, hard core $\alpha = 2.5$, $\beta = 2.0$; (4) HC3, hard core $\alpha = 3{,}5$, $\beta = 3.0$. The χ^2 values for the fits to the seven scattering terms, which include up to third-order scattering terms, are shown in the last seven columns. Also listed is the maximum value of χ^2 for the two confidence levels 0.05 and 0.01.

This method of fitting the $\overline{\Gamma_i^{MC}}(b)$-functions has the advantage of avoiding the evaluation of the Fourier transform integral by numerical methods.

The complete integration of the expression for the total scattering amplitude, $F(\Delta)$ of Eq. (1), including the Fourier transform integration over the impact parameter, can be done by Monte Carlo methods. This can be accomplished by generating random values of the impact parameter and the nucleon coordinates and evaluating the multidimensional integral of Eq. (1) by the importance sampling technique of Section III. We have attempted to calculate $F(\Delta)$ with no hard core present using this "brute force" method. Each Monte Carlo estimate consists of 14 numbers; u_x, u_y, u_z, v_x, v_y, v_z, u_x', u_y', u_z', v_x', v_y', v_z', b_x, and b_y. The resulst

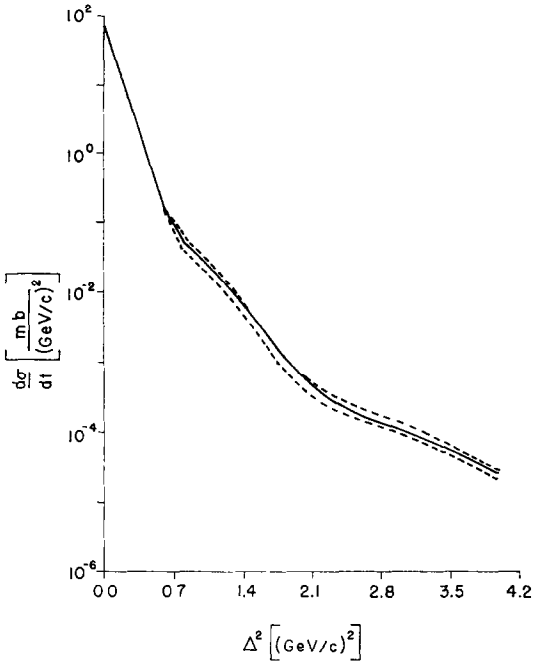

FIG. 3. The differential cross section as obtained by Monte Carlo fit method for no hard core falls within the dashed line region. The exact result is the solid line.

for values of Δ^2 from 0 to 1.0 GeV/c^2 at intervals of 0.1 (GeV/c)^2 are shown in Table V. Each 1000 estimates requires 19 sec of central processing (cp) time on the Lehigh CDC 6400 computer. The scattering amplitude $F(\Delta)$ can be found fairly accurately for small values of Δ^2. However, for values of Δ^2 greater than 0.4 (GeV/c)^2 with sample sizes of 2000 or greater, the standard errors are greater than the values of the scattering amplitude.

Since we know the exact result for the "no hard core" (NHC) case we can estimate the amount of cp time necessary to achieve a given accuracy. If we require that $d\sigma/dt$ be calculated to an accuracy of about 50% for the 11 points between $\Delta^2 = 0$ and 1.0 at intervals of 0.1, we can estimate the amount of cp time necessary in the following way. First of all, from Table V we notice that the variance in the calculated values of both Re $F(\Delta)$ and Im $F(\Delta)$ is statistically constant over the desired range of Δ^2. Also the standard errors for Re $F(\Delta)$ and Im $F(\Delta)$ are approximately equal for a given sample size. Thus

$$n'/n = (\Delta I/\Delta I')^2. \tag{46}$$

Taking $n' = 1000$, then from Table V, $\Delta I' \approx 0.35$. To find the number of estimates

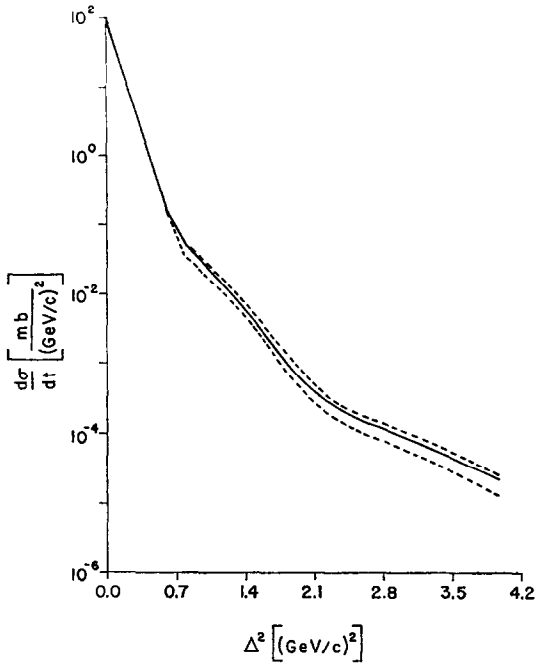

FIG. 4. The differential cross section as obtained by Monte Carlo fit procedure for hard core size $\alpha = 1.5$ and $\beta = 1.0$ falls within the dashed line region. The solid line is the exact result when the no hard core wavefunction is adjusted to give the same $\langle r^2 \rangle$ as in Table IV for this hard core size.

n needed to obtain the accuracy ΔI for the real or imaginary part of the scattering amplitude we use

$$n = (0.35/\Delta I) \cdot 1000.$$

To meet the requirement of $\sim 50\,\%$ accuracy in $d\sigma/dt$ at each value of Δ, we will need about $25\,\%$ accuracy in the larger of the real or imaginary part of the scattering amplitude since

$$d\sigma/dt = \pi[\mathrm{Re}^2 F(\Delta) + \mathrm{Im}^2 F(\Delta)]. \tag{47}$$

The estimated sample sizes and cp times needed to fulfill the stated requirements for each value of Δ^2 are shown in the last two columns of Table V.

Of course the accuracy requirements here are by no means stringent. Also it should be kept in mind that the maximum value of Δ^2 for this proposed calculation is only $1.0\,(\mathrm{GeV/c})^2$. Furthermore, we should stress that these estimated cp times

TABLE V

Results of "Brute Force" Method[a]

	Re $f(\Delta)$				Im $f(\Delta)$				$d\sigma/dt$			50%	
Δ^2 (GeV/c)^2	Exact result	Monte Carlo result	Standard error	Variance	Exact result	Monte Carlo result	Standard error	Variance	Exact result (GeV/c)^2	MC result (GeV/c)^2	Sample size	Estimated sample size	Estimated cp-time (CDC 6400)
0	−1.85	−1.85	0.260		8.09	8.03	0.360		83.9	82.7	1000	1000	19
0.1	0.214	0.144	0.369	136	5.08	5.23	0.340	115	31.5	33.4	1000	1000	19
0.2	0.981	0.889	0.374	140	2.91	3.38	0.356	127	11.5	14.9	1000	1000	19
0.3	1.084	0.545	0.309	143	1.47	1.39	0.295	130	4.06	2.73	1500	1000	19
0.4	0.897	0.320	0.263	138	0.589	0.141	0.266	141	1.40	0.149	2000	2800	53
0.5	0.625	0.623	0.214	138	0.102	−0.105	0.216	141	0.489	0.486	3000	8100	154
0.6	0.370	0.093	0.192	148	−0.131	−0.006	0.188	141	0.188	0.011	4000	16,900	321
0.7	0.170	−0.252	0.172	147	−0.212	0.060	0.172	148	0.090	0.082	5000	49,000	931
0.8	0.0325	−0.066	0.155	144	−0.211	−0.025	0.154	142	0.055	0.006	6000	49,000	931
0.9	−0.0509	−0.100	0.143	143	−0.172	0.020	0.142	141	0.039	0.013	7000	66,000	1254
1.0	−0.0932	−0.038	0.133	142	−0.122	−0.141	0.132	139	0.029	0.026	8000	73,000	1387

[a] Values of the differential cross section for the no hard core case for Monte Carlo brute force method discussed in text as compared to the exact results. Also shown are the cp times required to perform the calculations.

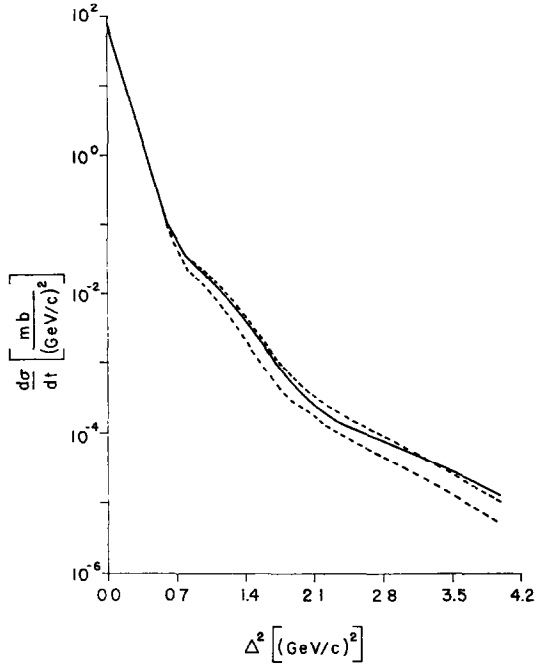

FIG. 5. The differential cross section as obtained by Monte Carlo fit procedure for a hard core size $\alpha = 2.5$ and $\beta = 2.0$ falls within the dashed line region. The solid line is the exact result when the no hard core wavefunction is adjusted to give the same $\langle r^2 \rangle$ as in Table IV for this hard core size.

are for NHC calculations. When we include the hard core part of the density function, the computation time will increase depending on the size of the hard core. In short, if we should perform a "brute force" calculation of this type requiring 50% accuracy in $d\sigma/dt$ at each value of Δ^2 between 0 and 1.0 $(GeV/c)^2$ at intervals of 0.1 (GeV/c), the total amount of cp time would be approximately 5000 sec. This is rather a large amount of time for such poor accuracy and small range of Δ^2.

In comparison, the cp time required to obtain the NHC results of Fig. 3 was 1020 sec. This number includes the 300 sec to generate each of the three sets of $\overline{\Gamma_i^{MC}}(b)$-functions and 40 sec to fit each set.

For the hard core cases, Figs. 4–6, the amount of time required increases rapidly as the value of β in Eq. (19) is increased. The cp times required for the HC calculations are shown in Table VI. The larger hard core sizes as discussed previously necessitated many more estimates due to the many "zero" contributions.

Perhaps the major drawback of the Monte Carlo–Fit method is the fitting phase. It may not always be possible to construct an analytic function as we did in Eq. 40

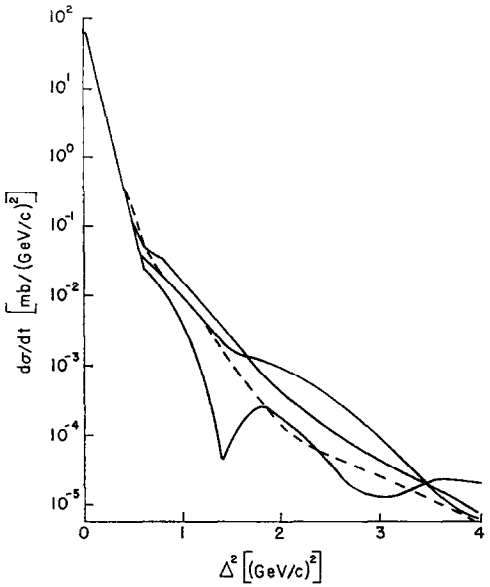

FIG. 6. The differential cross section as obtained by Monte Carlo fit procedure for a hard core size $\alpha = 3.5$ and $\beta = 3.0$ for the three computer runs. The dashed line is the exact result when the no hard core wavefunction is adjusted to give the same $\langle r^2 \rangle$ as in Table IV for this hard core size.

TABLE VI

Summary of cp Times: The cp Times Required (on the CDC 6400) to Perform Monte Carlo Fit Calculations for Three Runs for the Various Hard Core Sizes Investigated

β	α	Number of estimates at each b	Monte Carlo cp time/run sec	Number of runs	Fitting cp time (sec)	Total cp time (sec)
1.0	1.5	1100	~330	3	~40	~1110
2.0	2.5	3000	~750	3	~55	~2415
3.0	3.5	6000	~1500	3	~60	~4680

which would fit the $\overline{\Gamma_i^{MC}}(b)$-functions in a reliable way. In summary, we should note that the basic requirements of the fitting function are:

(1) It must be able to fit the point-by-point $\overline{\Gamma_i^{MC}}(b)$-functions well.

(2) It must have known Fourier transform properties.

CONCLUSIONS

In conclusion, we find that the Monte Carlo method can be used to solve the multidimensional integrals that occur in Glauber theory. We find no noticeable effect of a quark hard core for a given rms quark distance for the hard core values and wavefunctions we have investigated in proton–proton scattering.

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