Accurate momentum-space method for scattering by nuclear and Coulomb potentials*

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(Received 26 March 1974)

A coordinate-space boundary-matching method is used to solve the problem of including the long-range Coulomb interaction in momentum-space calculations of elastic scattering.

There has been considerable interest in momentum-space methods for solving the Lippmann-Schwinger equation for scattering problems. Although traditionally one solves the Schrödinger equation in coordinate space, and obtains phase shifts and differential cross sections from the solution of the Schrödinger equation, it is often advantageous to solve the scattering problem in momentum space. Particularly when one has to deal with nonlocal potentials, it may be easier to work in momentum space. One example is pion-nucleus scattering, where the optical potential derived from a multiple scattering theory is nonlocal.[1] Another example is the treatment of heavy-ion collisions,[2] in which the Pauli principle requires a strongly nonlocal optical potential.

The difficulty of incorporating the Coulomb interaction in momentum-space methods has discouraged their use, in spite of the attempts of several previous authors to solve this problem. One approach is to include the Coulomb potential in the Green's function that appears in the Lippmann-Schwinger equation, so that only the short-ranged part of the interaction need be represented in momentum space. The required momentum-space Coulomb Green's function is easily calculated[3]; however, its singularity is not a simple pole, which could be treated by a subtraction method,[4] but a complex power with negative real part, whose infinitely rapid oscillations demand the development of entirely new methods. A second approach uses a free Green's function, but adds the momentum-space representation of the Coulomb interaction to the nuclear interaction. Unfortunately, standard momentum-space methods then become invalid, because the Coulomb matrix elements $\langle \vec{k} | V_C | \vec{k}' \rangle$ are singular at $\vec{k} = \vec{k}'$. A mathematically correct (but numerically inefficient) method of overcoming this difficulty is to introduce an exponential screening factor in the Coulomb potential, and extrapolate calculated cross sections to the limit of infinite range of screening.[5] A third approach is to expand the scattering wave function in terms of regular Coulomb functions. The complete matrix of the short-ranged interaction between regular Coulomb functions is then required. Although this method is valid in principle, in practice it would require a very time-consuming calculation of large numbers of Coulomb functions.

Several quick approximate methods have been suggested. In one of these methods,[6] the nuclear phase shift is approximated by adding the nuclear phase shift produced by the deviation of the Coulomb potential from the point-charge form to the phase shift obtained without Coulomb forces. This is accurate if the phase shifts are small. In another method[7] the phase shift is calculated for the potential truncated at a distance R. Subtracting an asymptotic term of order $(kR)^{-1}$ then gives an approximation to the nuclear phase shift in the presence of the Coulomb interaction. By using the momentum-space method without regard to the singularity at $\vec{k} = \vec{k}'$, Chalmers and Saperstein[8] find empirically that the phase shift obtained for a point-Coulomb potential differs from the Coulomb phase shift σ_l by an amount α which is independent of l. They give a rough argument to explain this result, which enables them to calculate cross sections in the presence of the Coulomb interaction.

In this note, we show how the Coulomb interaction can be handled in momentum space by exactly the same boundary matching methods that are used in coordinate-space calculations.

For elastic scattering, the mathematical problem to be solved is to compute the so-called "nuclear phase shift" δ_{nl}, which is defined by

$$\psi_l(k, r) \propto F_l(kr, \eta) + \tan\delta_{nl}\, G_l(kr, \eta). \tag{1}$$

Here F_l and G_l are regular and irregular Coulomb functions with Sommerfeld parameter $\eta = Z_1 Z_2 e^2 \mu / \hbar k$ and ψ_l is a solution of the complete Schrödinger equation. Once δ_{nl} is known, the cross section can be computed from the "total amplitude" by the exact formula[5]

$$f(\theta) = f_C(\theta) + f_n(\theta), \tag{2a}$$

where the point-Coulomb and nuclear amplitudes

are, respectively,

$$f_C(\theta) = -\frac{\eta}{2k}\sin^2\left(\frac{\theta}{2}\right)\exp\left[2i\left(\sigma_0 - \eta\ln\sin\frac{\theta}{2}\right)\right], \tag{2b}$$

$$f_n(\theta) = \frac{1}{2ik}\sum_l (2l+1)\exp(2i\sigma_l)[\exp(2i\delta_{nl})-1]P_l(\cos\theta). \tag{2c}$$

The total potential is the sum of nuclear and Coulomb parts

$$V = V_n + V_C. \tag{3}$$

The Coulomb potential is produced by the nuclear charge density. This can be separated into disjoint long- and short-ranged parts, as follows:

$$V = V_l + V_s, \tag{4a}$$

$$V_l = (V_n + V_C)\theta(r-R), \tag{4b}$$

$$V_s = (V_n + V_C)\theta(R-r), \tag{4c}$$

where θ is the Heaviside step function defined by

$$\theta(x) = \begin{cases} 1, & x>0; \\ 0, & x<0. \end{cases} \tag{5}$$

In addition, we assume that it is possible to choose R so that for $r>R$

$$V_n\psi = 0, \qquad V_C = Z_1Z_2e^2/r \quad (r>R). \tag{6}$$

It is best to choose R as small as possible, consistent with Eq. (6). With these approximations, the form (1) is exact for all $r>R$. Moreover, for $r<R$ the wave function is equal to a regular solution ψ_{sl} of the Schrödinger equation with potential V_s. If we know ψ_{sl}, we can determine δ_{nl} by matching the logarithmic derivatives of ψ_{sl} and ψ_l at $r=R$. This method in no way depends on how ψ_{sl} is calculated. Therefore, ψ_{sl} may as well be calculated by solving the Lippmann-Schwinger integral equation in momentum space, instead of a coordinate-space differential equation.

The matching procedure is as follows: Let δ_{sl} be the phase shift calculated for the potential V_s, so that

$$\psi_{sl}(r) \propto F_l(kr, \eta=0) + \tan\delta_{sl}G_l(kr, \eta=0). \tag{7}$$

The condition for this to match smoothly at $r=R$ with

$$\psi_l(r) \propto F_l(kr, \eta) + \tan\delta_{nl}\, G_l(kr, \eta)$$

is

$$\tan\delta_{nl} = \frac{\tan\delta_{sl}[F, G_0] + [F, F_0]}{[F_0, G] + \tan\delta_{sl}[G_0, G]}. \tag{8}$$

Here the subscript 0 indicates $\eta=0$, the square bracket is of Wronskian form, e.g.

$$[F, G_0] = \left[G_0\frac{dF}{dr} - F\frac{dG_0}{dr}\right]_{r=R}, \tag{9}$$

and the angular momentum label l has been omitted. We note that Coulomb functions are required only at the single radius R. Now that fast, accurate algorithms for the Coulomb functions are available, the matching involves negligible computation. No comparison calculations or extrapolations are necessary.

Often the momentum-space wave function is needed, in addition to the phase shift. Provided that only matrix elements of short-range operators are to be calculated, this presents no difficulty, because it then suffices to calculate the wave function only for $r<R$. The coordinate-space version of the wave function ψ_{sl} that is computed by solving the Lippmann-Schwinger equation is correct for $r<R$, except for an over-all constant factor. This factor is easily determined by comparing the properly normalized ψ_{sl} and ψ_l,

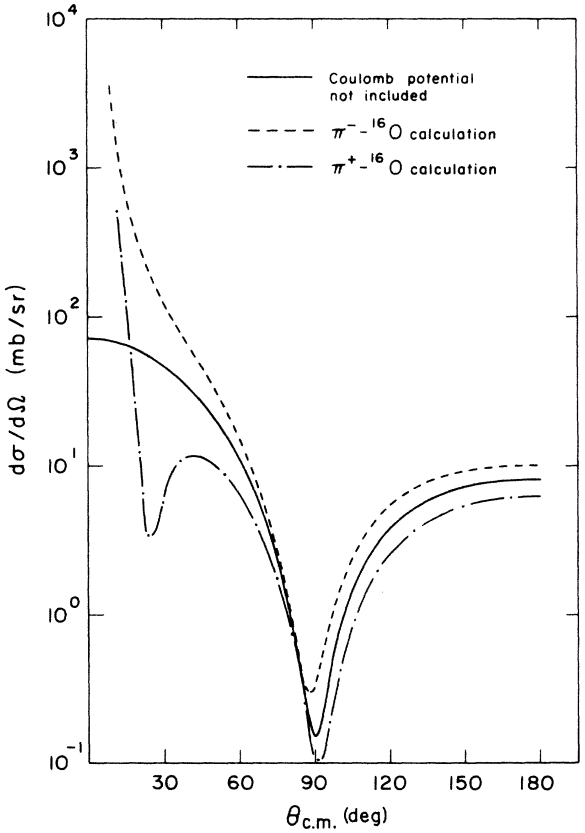

FIG. 1. A plot of differential cross section $d\sigma/d\Omega$ vs c.m. scattering angle θ. The pion kinetic energy (lab) is 30 MeV. Parameters involved in the calculation are explained in text. On this scale, coordinate-space and momentum-space calculations are indistinguishable.

both evaluated at $r = R$ in terms of F, G, F_0, G_0, and the known phase shifts δ_{sl} and δ_{nl}.

As an example of the boundary-matching method, we present calculations for positive and negative pions on ^{16}O, using an optical potential

$$(2\mu/\hbar^2)\, V_n = -A[(b_0 + b_1)P_0^2\rho(r) + \tfrac{1}{2}b_1\nabla^2\rho(r)] \qquad (10)$$

where b_0 and b_1 are $(-0.7723 + 0.9499i)$ fm^3 and $(8.164 + 0.4438i)$ fm^3, respectively,

$$\mu = \frac{E_\pi(P_0)}{1 + E_\pi(P_0)/Mc^2}$$

is the reduced mass of the pion and the target of mass M, P_0 is the asymptotic wave number in the pion-nucleus c.m. frame, and $\rho(r)$ is the nucleon density. For $\rho(r)$ we used the modified harmonic oscillator form

$$\rho(r) = \rho_0(1 + \alpha r^2/r_0^2)\exp(-r^2/r_0^2)\ , \qquad (11)$$

with $\alpha = \frac{4}{3}$, $r_0 = 1.7$ fm and $\rho_0 = 1/[\pi^{3/2}r_0^3(1 + \frac{3}{2}\alpha)]$. The Coulomb potential V_C was taken as due to a uniformly charged sphere of radius 2.7 fm. An approximate Klein-Gordon equation

$$(\nabla^2 + P_0^2)\psi_s = (2\mu/\hbar^2)(V_n + V_C)\psi_s \qquad (12)$$

was solved in momentum space by the matrix-inversion method described in Ref. 4. In our calculation we chose $R = 7.5$ fm and used 24 grid points. The stability of the calculation under the change of number of grid points was checked by doing the calculation with 16 and 32 grid points. Results of this calculation were compared with those of a conventional coordinate-space calculation. The boundary-matching procedure did not perceptibly increase the computation time.

Figure 1 shows the cross section computed for a neutral projectile, compared with the Coulomb-corrected cross sections for π^+ and π^- projectiles, all calculations being done at $E_\pi(\text{lab}) = 30$ MeV. On the scale of these graphs, the momentum-space and coordinate-space calculations are indistinguishable. Similar accuracy was found at other energies. The influence of the Coulomb attraction and repulsion and the Coulomb-nuclear interference effects are clearly visible.

TABLE I. Nuclear phase shifts δ_{nl} for point-Coulomb potentials for $P_0 = 0.776$ fm^{-1}. The exact values are identically zero. The tabulated values were calculated by applying boundary matching to the results of a momentum-space calculation with n grid points. The accuracy is seen to decrease somewhat for large Z_1Z_2.

l	$Z_1Z_2 = 1$ $n = 24$	$R = 10$ fm $n = 32$	$Z_1Z_2 = 10$ $n = 24$	$R = 10$ fm $n = 32$
0	3.6×10^{-6}	-3.7×10^{-6}	4.2×10^{-4}	-2.1×10^{-4}
1	1.1×10^{-6}	-7.9×10^{-7}	2.5×10^{-4}	-7.2×10^{-5}
2	2.7×10^{-6}	1.1×10^{-7}	3.9×10^{-4}	3.9×10^{-5}
3	-8.9×10^{-7}	-4.3×10^{-8}	5.5×10^{-5}	2.6×10^{-5}
4	4.1×10^{-7}	-4.9×10^{-8}	1.7×10^{-4}	3.3×10^{-5}

In order to indicate the numerical accuracy of the method, we present the results of the calculation in which the total potential was just the point-Coulomb potential ($V_C = Z_1Z_2e^2/r$). The exact nuclear phase shifts for this problem are identically zero. The results of momentum-space calculations are presented in Table I. The errors may be larger here than in the realistic case because of the singularity at $r = 0$.

We believe that this simple accurate method removes what previously seemed a serious obstacle to the use of momentum-space methods in problems where the Coulomb force is important. The method can easily be extended to other cases (such as inelastic scattering) as long as the nuclear potential can be treated as of strictly finite range.[9]

ACKNOWLEDGMENTS

We wish to thank G. A. Miller and R. A. Eisenstein for instruction in the use of their coordinate-space elastic scattering code, and F. Tabakin for the encouragement he gave us in several discussions.

*Work supported in part by the National Science Foundation.

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[9]Some modification of the method may be useful in treating potentials V_n that fall off more slowly than an exponential. In particular, the r^{-2} potential that arises in a correct treatment of the Klein-Gordon equation with the Coulomb potential can be removed from V_n if F and G are replaced by more appropriate hypergeometric functions.