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The integration of the Lippmann-Schwinger equation

with the Monte-Carlo method

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A Monte-Carlo method to integrate the Lippmann-Schwinger equation for elastic scattering is presented. Advantages and limitations of this algorithm are compared with traditional methods of computation.

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The Lippmann-Schwinger equation¹⁾ has been used extensively in the past to solve the problem of potential scattering. In its operator form it is written²⁾ as

$$T = V + V G_0 T \quad (1)$$

where T is the t -operator, V is the potential and G_0 the free particle propagator. In the non-relativistic momentum representation²⁾, the matrix form of Eq. (1) for spinless particles is

$$t(\vec{K}', \vec{K}) = v(\vec{K}', \vec{K}) + 2m \int_{\Gamma} \frac{d\vec{p}}{k^2 - p^2 + i\epsilon} v(\vec{K}', \vec{p}) t(\vec{p}, \vec{K}) \quad (2)$$

where $\vec{K}$ and $\vec{K}'$ are the initial and final momenta and $v(\vec{p}, \vec{p}')$ is the Fourier transform of the potential $V(\vec{r})$. The integral extends over the whole space Γ of $\vec{p}$.

We propose in this paper a new procedure to integrate Eq. (2) based on the Monte-Carlo (MC) method³⁾. This algorithm has been used in the past⁴⁾ to solve the Schrödinger equation in configuration space and to determine the energy eigenvalues and wave functions of ground state bound systems. It is now used extensively as a non-perturbative method to determine the properties of hadrons⁵⁾ in gauge field theories on a 4-dimensional lattice, as suggested originally by K. Wilson⁶⁾.

In order to integrate Eq. (2) we begin by transforming it into a transport type equation by introducing a new parameter $s = \pm 1$ and separating the real and imaginary parts of the propagator and the potential. We then have

$$t_s(\vec{K}', \vec{K}) = v_s(\vec{K}', \vec{K}) + \sum_{s'} \int_{\Gamma} d\vec{p} v_s(\vec{K}', \vec{p}; s') t_{s'}(\vec{p}, \vec{K}) \quad (3)$$

and the kernel in Eq. (3) is

$$K(s, \vec{p}; s', \vec{p}') = \frac{2m}{(k^2 - p^2 + i\epsilon)^2} \left\{ [(k^2 - p^2 + i\epsilon)^2]_{s, s'} + \epsilon \delta_{s, -s'} [v_1(\vec{p}, \vec{p}') + \epsilon \delta_{s, s'} - s(k^2 - p^2 + i\epsilon) \delta_{s, -s'}] v_{-1}(\vec{p}, \vec{p}') \right\}, \quad (4)$$

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where the indices $s = +1$ and -1 correspond to the real and the imaginary parts of t and v respectively. The quantity ε is small and positive. The Eq. (3) can now be integrated using standard Monte-Carlo techniques³⁾ by choosing two probability densities $g_s(\vec{p})$ and $Q(s, \vec{p}; s', \vec{p}')$ with the following properties,

$$\begin{aligned} 0 < g_s(\vec{p}) \quad \text{and} \quad \sum_s \int_{\Gamma} d\vec{p} \, g_s(\vec{p}) &= 1 \\ 0 < Q(s, \vec{p}; s', \vec{p}') \quad \text{and} \quad \sum_s \int_{\Gamma} d\vec{p} \, Q(s, \vec{p}; s', \vec{p}') &= 1. \end{aligned} \quad (5)$$

We also introduce a function $h_s(\vec{p}, \vec{k})$ which must satisfy $\int_{\Gamma} d\vec{p} \, h_s(\vec{p}, \vec{k}) < \infty$. It can be shown³⁾ that by performing a random walk in momentum and s space $(s_0, \vec{p}_0) \rightarrow (s_1, \vec{p}_1) \rightarrow (s_2, \vec{p}_2) \dots (s_l, \vec{p}_l)$, where the initial state $(s_0, \vec{p}_0)$ has a probability $g_s(\vec{p})$ and each successive step a probability $Q(s_l, \vec{p}_l; s_{l+1}, \vec{p}_{l+1})$, one can calculate an estimator η defined as

$$\eta_l(h) = \frac{h_{s_0}(\vec{p}_0)}{g_{s_0}(\vec{p}_0)} \sum_{j=0}^{l-1} w_j s_j \left(\vec{p}_j, \vec{k} \right) \quad (6)$$

with

$$w_j = \frac{K(s_0, \vec{p}_0; s_1, \vec{p}_1) K(s_1, \vec{p}_1; s_2, \vec{p}_2) \dots K(s_{j-1}, \vec{p}_{j-1}; s_j, \vec{p}_j)}{Q(s_0, \vec{p}_0; s_1, \vec{p}_1) Q(s_1, \vec{p}_1; s_2, \vec{p}_2) \dots Q(s_{j-1}, \vec{p}_{j-1}; s_j, \vec{p}_j)}, \quad (7)$$

$$w_0 \equiv 1$$

which has the property

$$f_s(\vec{k}', \vec{k}) = \int_{\Gamma} d\vec{p} \, t_s(\vec{p}, \vec{k}) h_s(\vec{p}, \vec{k}') = \lim_{l \rightarrow \infty} E[\eta_l(h)]. \quad (8)$$

The $E[\eta_l]$ in Eq. (8) indicates the expectation value of the estimator η_l over a number of independent walks. The steps l of these walks are not on a fixed grid and can take any value on the $(s, \vec{p})$ space. The multiplicative estimator η in Eq. (6) is not the only possible one for this type of calculation, but has the advantage of an intuitive physical interpretation as shown later. The convergence of Eq. (6) requires that

$$\sum_{s, s'} \int_{\Gamma} d\vec{p} \, d\vec{p}' K(s, \vec{p}; s', \vec{p}') < \infty,$$

and that $|K|$ should have a spectral radius less than unity.

Although the choice of h , g and Q is free, their form will affect the convergence of Eq. (6), the limit in Eq. (8) and the computing time. We choose the following

$$g_s(\vec{p}, \vec{k}') = \frac{-h_s(\vec{p}, \vec{k}')}{(2\pi)^2 m} = \delta_{s, s_0} \delta^3(\vec{p} - \vec{k}') \quad (9)$$

and

$$Q(s, \vec{p}; s', \vec{p}') = \frac{\varepsilon}{(2\pi)^2 p' [(k^2 - p'^2)^2 + \varepsilon^2]}. \quad (10)$$

With these definitions, the function $f(\vec{k}', \vec{k})$ in Eq. (8) is the scattering amplitude, and the sum in Eq. (6) is a modified form of the Born series. To generate new steps in $(s, \vec{p})$ space with the probability distribution Q of Eq. (10) we define

$$\begin{aligned} s' &= +1 \text{ or } -1 \text{ if } u_1 > \frac{1}{2} \text{ or } u_1 < \frac{1}{2} \text{ resp.} \\ \psi' &= 2\pi u_2 \\ \cos \theta' &= 2 \left(u_3 - \frac{1}{2} \right) \\ p'^2 &= k^2 + \varepsilon \operatorname{tg} \left[\pi \left(u_4 - \frac{1}{2} \right) \right], \end{aligned} \quad (11)$$

where ψ' and θ' are the angle coordinates of $\vec{p}'$ and the u_i are random numbers between 0 and 1 with uniform distribution. Individual walks begin at the final momentum $\vec{k}'$ and after a number of steps at intermediate momenta $\vec{p}$, they finish at the initial momentum $\vec{k}$. Thus we may interpret Q as the probability of transporting the particles between successive collisions where their momenta are changed with probability $v_s(\vec{p}, \vec{p}')$.

We wrote and tested a program that performs the algorithm described above. We compared the results of the computations with Coulomb, Yukawa and square well potentials. No difficulty occurs with

the singularity in the Coulomb potential which, with other methods of integration require special care⁷). For the Yukawa potential the first and second Born terms can be calculated analytically²), and their comparison with our calculation allowed a detailed check on the program and estimates of the accuracy of the result for different numbers of walks. In the case of the square well we calculated analytically the partial wave amplitudes and summed them to compare with our computation. In all of the above cases the computed results agreed with the analytical calculations within the variance of the computation. We used typically 4 to 10 steps in each walk and 10^3 to 10^5 walks, and obtained uncertainties of 1 to 5% in the scattering amplitude. A typical computing time for 4 steps and 10^3 walks was 5 to 10 seconds of CPU in an Amdahl V-8 computer.

We also compared results from our method with recent low energy π^+ + ^{12}C elastic scattering data⁸). The potential used in this calculation assumed no absorption and a zero spin-isospin target⁹), and contained only two free parameters. Its form was

$$V_1(\vec{p}, \vec{p}') = \left(\frac{Ze^2}{q^2} + C + D\vec{p} \cdot \vec{p}' \right) \exp \left[-\left[\frac{(Rq)^2}{4} \right] \right], \quad (12)$$

and

$$\vec{q} = \vec{p} - \vec{p}'.$$

The result of the calculation is shown in Fig. 1 where the two full lines indicate the 68% confidence level of the computation. The values of C and D where $C = 2.20 \times 10^{-5} \text{ MeV}^{-2}$ and $D = -5.4 \times 10^{-9} \text{ MeV}^{-4}$. The radius of ^{12}C used was $R = 3.20 \text{ fm}$. The calculation had four steps and 10^4 walks. It was repeated four times with different random numbers to determine the variance. The total CPU time was 250 seconds. These

results show that the MC method agrees with more conventional types of calculations of the pion-nuclear interaction.

Due to its statistical nature, the method described above will not provide exact answers and the variance of the result can either be estimated by repeating the computation several times with different random numbers, or can be calculated more accurately by computing

$$\sigma^2 = E[\eta^2] - [E[\eta]]^2. \quad (13)$$

This procedure requires longer computing time and is only justified when the uncertainty of the result must be known accurately.

Traditional methods rely on the partial wave expansion to separate variables. In our case this is not necessary and therefore this algorithm is especially useful for potentials without spherical symmetry. Long range or singular potentials can also be solved advantageously using the Monte-Carlo method.

The value of the parameter ϵ in Eq. (10) is arbitrary but its choice will affect the variance. A small ϵ will improve the accuracy of the $s' = s$ steps while a large ϵ decreases the variance of the $s' = -s$ steps. Its optimal value must be determined for each case, but the result is of course independent of ϵ .

In conclusion, we have described a novel method to integrate the momentum space Lippmann-Schwinger equation using the Monte-Carlo method, which offers distinct advantages for some types of potentials.

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FIGURE CAPTION

Fig. 1. Experimental values and the result of the MC integration for elastic scattered pions on ^{12}C at 13.9 MeV. The full lines indicate the 68% confidence level of the computation.