Finite second-order Born term for Coulomb wavepacket scattering

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It has been known for some time that, for nonrelativistic Coulomb scattering, the terms in the Born series of second and higher order diverge when using the standard method of calculation. In this paper we take the matrix elements between square-integrable wavepacket state vectors. We reproduce the Rutherford cross section from the first-order contribution. We find that the second-order contribution is finite and negligible compared to the first-order contribution, away from the forward direction. At first order, the contribution to the amplitude in the forward direction is found to be finite and physically reasonable. We comment on how a similar procedure applied to the divergences of quantum field theories might render them finite.
I. INTRODUCTION

The Born approximation (or time-dependent perturbation theory) is the most widely used method for calculating scattering cross sections in nonrelativistic quantum mechanics \[1,3\] and, with modifications, in relativistic quantum field theories \[4\]. In nonrelativistic quantum mechanics it gives an approximation of the full evolution operator as a series in powers of the potential. It is only useful, meaning that few terms are needed for a result of sufficient precision, when the interaction is weak, but this includes a wide variety of cases.

It has been known for a long time, as illustrated by the calculation of Dalitz \[5\], that for nonrelativistic Coulomb scattering the terms in the Born series of second and higher order diverge when using the standard method of calculation. As is well known, the same pattern of finiteness and divergences happens in relativistic quantum field theories. We will comment later on the possibility that the results obtained here can be extended to that domain. Before an investigation into the divergences of quantum electrodynamics, which will be the subject of a future work, we consider nonrelativistic Coulomb scattering. For that system, exact results \[1,6\] are available for comparison. The existence of exact solutions gives us information about the possibility of a power series solution. The exact Coulomb scattering amplitude \[1\] depends on $\Gamma(1 + i\eta)$, where $\eta$ is defined below in Eq. (22). Because $\Gamma(1 + i\eta)$ has a pole nearest to the real axis at $\eta = i$, we know that there is a series for this amplitude in powers of $\eta$ that converges only on $|\eta| < 1$. It is this series that we seek.

It is the aim of this paper to show that the second-order term (for nonrelativistic Coulomb scattering) becomes finite when square-integrable wavepackets are used instead of plane waves for the initial and final states, when the interaction time remains finite rather than infinite and when care is paid to the order in which integrals are performed.

The results of Dalitz \[5\] are in terms of an arbitrary, nonzero, regularization parameter with no physical meaning. The results diverge as this parameter is taken to zero. Our results will be finite partly because they depend on a nonzero parameter with physical meaning, the width in momentum space, $\sigma_p$, of the wavepackets. For simplicity, we choose wavepackets with a spherically symmetric distribution of momentum about the mean value. This width parameter is not the eigenvalue of an Hermitian observable, but it is measurable in the following sense. A state would have to be prepared the same way many times and momentum measurements performed. The distribution of these measurements allows calculation of the standard deviation in any direction.

Our construction of an ideal theoretical scattering experiment differs significantly from the standard method \[7\], in that a limit as interaction time goes to infinity is replaced by a sequence where the momentum width is made ever smaller, but never vanishes. This latter method was discussed in a previous work by this author \[6\]. We define a small dimensionless parameter

$$\epsilon = \frac{\sigma_p}{p},$$

where $p$ is the magnitude of the initial and final momenta. (We acknowledge that unperturbed energy is conserved in a scattering description, so we do not feel the need to prove this fact by choosing different energies for our initial and final states.) It is important to ensure that wavepacket spreading is negligible over the finite time of the interaction. A convenient choice to ensure this is to make the initial and final separations of the position wavepackets equal to

$$2R = \frac{2}{\sqrt{\epsilon}} \sigma_x,$$

where $\sigma_x \sigma_p = 1/2$ for minimal Gaussian wavepackets (setting $\hbar = 1$). (We choose Gaussian wavepackets to make the subsequent integrals tractable. It is beyond the scope of this paper to investigate the effects of wavepacket shapes on our results.)

Then as $\epsilon$ is made smaller, the resolutions of the momenta improve, the wavepacket spatial widths increase, but their initial and final separations increase at a greater rate, and the interaction time increases while wavepacket spreading remains negligible to order $\sqrt{\epsilon}$. So the small parameter for the approximations we will use must be taken as $\sqrt{\epsilon}$.

It is puzzling why more researchers do not use wavepackets in their calculations. Perhaps it is felt that they are an unnecessary complication. They are certainly a complication, as we will see. However it is the point of this paper to demonstrate that they are necessary if one wants to obtain finite results. A plane wave (a momentum eigenvector) has a position probability density spread evenly over the entire universe. This is hardly what we would call a realistic representation of a physical situation. In the standard derivation of the cross section \[3\], one must deal with the square of a Dirac delta function. No such problem arises in this presentation. Probability amplitudes can be defined in the relativistic domain \[8–11\], with well-defined Lorentz transformation properties.

In Section \[\text{III}\] we will present our results for all terms up to second order. Conclusions follow in Section \[\text{III}\].

Throughout this paper, we use Heaviside-Lorentz units, in which $\hbar = c = \epsilon_0 = \mu_0 = 1$. 

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\[\begin{align*}
\end{align*}\]
II. MATRIX ELEMENTS

The Hamiltonian we consider is, in position space,
\[ H = H_0 + V = \frac{1}{2m_0} \frac{\partial^2}{\partial r^2} + \frac{\alpha}{r}, \]  
(3)
with \( m_0 \) the mass, \( r = |r| \) and \( \alpha \) the fine structure constant (or \( Z_1 Z_2 \alpha \) for atomic number \( Z_1 \) of the target and \( Z_2 \) of the projectile).

For nonrelativistic quantum mechanics with a potential operator, \( V \), the Born series for the full evolution operator is [1], to second order,
\[ e^{-iHt} = e^{-iH_0t} - i \int_0^t e^{-iH_0(t-\tau)} V e^{-iH_0\tau} d\tau - \int_0^t e^{-iH_0(t-\tau_2)} V \int_0^\tau_2 e^{-iH_0(\tau_2-\tau_1)} V e^{-iH_0\tau_1} d\tau_1 d\tau_2 + \ldots \]  
(4)

Our initial and final momentum wavefunctions, normalized to unity, are given by
\[ \Psi_i(k) = e^{-(k-p_i)^2/4\sigma_p^2} e^{-ik \cdot R_i}, \]  
\[ \Psi_f(k) = e^{-(k-p_f)^2/4\sigma_p^2} e^{-ik \cdot R_f}, \]  
(5)
with
\[ R_i = -R \hat{z}, \quad p_i = +p \hat{z}, \]  
\[ R_f = +R(\sin \theta, 0, \cos \theta), \quad p_f = +p(\sin \theta, 0, \cos \theta) \]  
(6)
and \( \theta \) the scattering angle. The interaction time is the time for free evolution
\[ T = \frac{2R}{p/m_0}. \]  
(7)
(We do not attempt to calculate time delays or advancements here, as was done in [6].) Note that we are representing the special geometry of a head-on collision, as was done in [6].

We need to calculate the matrix elements
\[ \mathcal{M}(\theta) = \langle \psi_f | e^{-iHT} | \psi_i \rangle \]  
(8)
as contributions from each order. In anticipation of our result, we call these amplitudes finite amplitudes, using the notation introduced in [6]. They are such that their modulus squared is a probability. In contrast, scattering amplitudes, \( f(\theta) \), as defined in the literature [1] are such that the differential cross section is
\[ \frac{d\sigma}{d\Omega} = |f(\theta)|^2. \]  
(9)

We note that if Eq. (4) is, in fact, an approximation of a unitary operator, then we are guaranteed to find finite contributions by the Schwartz inequality [1]
\[ |\langle \psi_f | e^{-iHT} | \psi_i \rangle| \leq 1 \]  
(10)

A. Zeroth order, \( \mathcal{M}_0(\theta) \)

First
\[ \mathcal{M}_0(\theta) = \int d^3k_1 \Psi_f^*(k_1) e^{-iE_1T} \Psi_i(k_1) \]  
\[ = \int d^3k_1 \frac{e^{-(k_1-p_f)^2/4\sigma_p^2}}{(2\pi\sigma_p^2)^{3/2}} \frac{e^{-(k_1-p_i)^2/4\sigma_p^2}}{(2\pi\sigma_p^2)^{3/2}} e^{i(k_1 \cdot (R_f-R_i))} e^{-iE_1T}, \]  
(11)
with \( E_n = k_n^2/2m_0 \). We will repeatedly use the identity
\[
(k - p_f)^2 + (k - p_i)^2 = 2(k - p_+)^2 + \frac{1}{2}(p_f - p_i)^2,
\]
with
\[
p_+ = \frac{1}{2}(p_f + p_i).
\]
Changing integration variables to \( \kappa = k_1 - p_+ \) involves a straightforward application of the integral \([12]\) (their Eq. (3.323.2))
\[
\int d^3\kappa e^{-\kappa^2/2\sigma_r^2} e^{i\kappa \cdot \xi} = (2\pi\sigma_r^2)^{3/2} e^{-\xi^2/8\sigma_r^2},
\]
which we will use frequently. The only point to note is that the phase factor \( e^{-i\kappa^2 T/2m_0} \) can be set to \( 1 + O(\sqrt{\epsilon}) \) with our scaling scheme to avoid wavepacket spreading.

We find
\[
M_0(\theta) = e^{+iET} e^{-\sin^2\frac{\theta}{2}/2\sigma^2} (1 + O(\sqrt{\epsilon})).
\]
Of course this is a function sharply peaked around zero scattering angle. Note that the modulus-squared of the amplitude \( M \) we calculate is a probability, and this probability is 1 for \( \theta = 0 \).

**B. First order, \( M_1(\theta) \)**

We want to evaluate the matrix elements in momentum space, as the free evolution operators take their simplest representation, as phase factors, in this basis. Multiplication of the position wavefunction by the factor \( \alpha/r \) from the Coulomb potential is equivalent to convolution of the momentum wavefunction. We find
\[
\Psi'(k) = \langle k | \frac{\alpha}{r} | \psi \rangle = \int \frac{d^3r}{(2\pi)^3} e^{-ik \cdot r} \frac{\alpha}{r} \int \frac{d^3k'}{(2\pi)^3} e^{ik' \cdot r} \Psi(k').
\]
Exchanging the order of the integrals gives
\[
\Psi'(k) = \int d^3k' \mathcal{V}(k - k') \Psi(k'),
\]
with
\[
\mathcal{V}(q) = \int \frac{d^3r}{(2\pi)^3} e^{-iq \cdot r} \frac{\alpha}{r} = \frac{\alpha}{2\pi^2q} \int_0^\infty dr \, \sin(qr).
\]
Integration in spherical polar coordinates cancels the zero of the denominator, a technique that we will use many times. Note that the integral for \( \mathcal{V} \), as written, diverges for all \( q \). The exchange of the order of integration was not justified. We interpret \( \mathcal{V} \) as a distribution \([13]\). If it is made finite by a regularization procedure, it can be used in integrals. Then, finally, the regularization is removed to give, possibly, a finite result. This procedure is what we are doing when we use Dirac delta functions. In this case, it is equivalent to what we would find if we kept the original integration order.

We insert a Yukawa regularization factor, \( e^{-\lambda r} \), in the last form of Eq. \([18]\) to find the regularized \( \tilde{\mathcal{V}} \)
\[
\tilde{\mathcal{V}}(q) = \frac{\alpha}{2\pi^2} \frac{1}{q^2 + \lambda^2}.
\]
We will refer to this as the potential kernel.

Then the first order matrix element is
\[
M_1(\theta) = -i \int_0^T d\tau \int d^3k \Psi_f(k) e^{-iE(k)(T-\tau)} \frac{\alpha}{2\pi^2} \int d^3k' \frac{1}{(k - k')^2 + \lambda^2} e^{-iE(k')\tau} \Psi_i(k').
\]
We can evaluate this quite simply for scattering sufficiently far from the forward direction. In that region, the Gaussians keep \( \mathbf{k} \) close to \( \mathbf{p}_f \) and \( \mathbf{k}' \) close to \( \mathbf{p}_i \). The potential kernel is slowly varying, so can be replaced by its value at the wavefunction peaks, with no singularity, and taken outside the integral. The remaining integrals are easily evaluated using the methods of the previous section.

We find

\[
\mathcal{M}_1(\theta) = -i e^{+iE T} \alpha \frac{\sigma_p^2}{p} \frac{1}{E \sin^2 \frac{\theta}{2}} = -i e^{+iE T} 2 \eta e^2 \frac{1}{\sin^2 \frac{\theta}{2}}, \quad \text{for } \theta \neq 0,
\]

(21)

where

\[
\eta = \frac{\alpha}{p/m_0} \tag{22}
\]

is a commonly used dimensionless measure of the strength of the Coulomb interaction \([1]\).

Then we use a formula from \([6]\), derived for Gaussian wavepackets, that relates probabilities, \( P \), and differential cross sections:

\[
\frac{d\sigma}{d\Omega} = \frac{p^2}{16 \sigma_p^4} P.
\]

(23)

Since \( \mathcal{M}_0(\theta) \) essentially vanishes in this region, we have

\[
\frac{d\sigma}{d\Omega} = \frac{p^2}{16 \sigma_p^4} |\mathcal{M}_1|^2 = \frac{\alpha^2}{16 E^2 \sin^4 \frac{\theta}{2}}.
\]

(24)

This is the well-known Rutherford cross section \([14]\), known to be in good agreement with experiment in the nonrelativistic regime and where spin contributions are negligible \([15]\). It is possible that the dependence on the wavepacket shape cancels out to give this expression. Investigation of that possibility must await a future work.

C. First order in the forward direction, \( \mathcal{M}_1(0) \)

For forward scattering, in Eq. \([20]\), we set \( \mathbf{p}_f = \mathbf{p}_i = p \hat{z} \) and \( \mathbf{R}_f = -\mathbf{R}_i = R \hat{z} \). While the integrals are regularized with a nonzero value of \( \lambda \), we can change integration variables to \( \mathbf{k} = \mathbf{k} - \mathbf{k}' \) and \( \mathbf{k}_+ = \mathbf{k} + \mathbf{k}' \), with \( d^3k \, d^3k' = \frac{1}{8} d^3k_+ d^3k_- \). In the integral over \( k_- \), \( \lambda \) can now be set to zero as the integration measure in spherical polar coordinates cancels the divergence. We find, using MATHEMATICA \([16]\),

\[
\int d^3k_- e^{-k_-^2/8\sigma_p^2} \frac{1}{k_+^2 + \lambda^2} e^{i2\sigma_p k_- (\tau - \frac{T}{2})} \rightarrow \pi^2 \frac{\text{erf} \left( \sqrt{2} v_+ (\tau - \frac{T}{2})/\sigma_+ \right)}{v_+ (\tau - \frac{T}{2})},
\]

(25)

with \( v_+ = k_+/m_0 \). The argument of this function varies by only \( O(\sqrt{\epsilon}) \) as \( k_+ \) changes by \( \sigma_p \), while it changes by order unity as \( \tau \) changes by order \( \sqrt{\epsilon} \). The function is peaked at the origin with a width of order unity. So, since the function is slowly varying with respect to momentum, it can be set to its value at \( k_+ = 2p \) and taken outside the \( k_+ \) integral.

This gives

\[
\mathcal{M}_1(0) = -i \frac{\alpha}{2\pi^2} \frac{1}{(2\pi \sigma_p^2)^2} \frac{1}{8} \int_0^\infty d\tau \sqrt{2} \text{erf} \left( \frac{\sqrt{2} v (\tau - \frac{T}{2})}{\sigma} \right) \int d^3k_+ e^{+ik_+ \cdot \mathbf{R}_f \cdot e^{-i(2p)^2/8\sigma_p^2} e^{-iE_+ T/4}}.
\]

(26)

Evaluating the \( k_+ \) integral gives

\[
\mathcal{M}_1(0) = -e^{+iE T} i \frac{i \eta}{4} \int_\text{Z} dz \frac{\text{erf} \left( z \right)}{z},
\]

(27)

with \( Z = \sqrt{8}/\epsilon \). Numerical integration with MATHEMATICA \([16]\) gives an approximate expression

\[
\mathcal{M}_1(0) \cong -e^{+iE T} i \frac{i \eta}{4} (2.00 \ln(\sqrt{\frac{8}{\epsilon}}) + 1.96).
\]

(28)

We see that this expression contains the same phase factor, \( \exp(+iET) \), as \( \mathcal{M}_0(0) \). It is proportional to \( \eta \) with a factor that depends only logarithmically on \( \epsilon \). For example, with \( \epsilon = 0.001 \), it takes the form

\[
\mathcal{M}_1(0) \cong -e^{+iE T} i 2.74 \eta.
\]

(29)
The second order matrix element is

\[ M_2(\theta) = -\int_0^T d\tau_2 \int_0^{\tau_2} d\tau_1 \int d^3 k_2 \Psi_f^*(k_3) e^{-iE_3(T-\tau_2)} \int d^3 k_2 \frac{\alpha}{2\pi^2} \frac{1}{(k_3 - k_2)^2 + \lambda^2} e^{-iE_2(\tau_2 - \tau_1)} \times \int d^3 k_1 \frac{\alpha}{2\pi^2} \frac{1}{(k_2 - k_1)^2 + \lambda^2} e^{-iE_1 \tau_1} \Psi_i(k_1). \] (30)

If we tried to evaluate the intermediate \( k_2 \) integral first, with two potential kernel factors

\[ D = \frac{1}{(k_2 - k_3)^2 (k_2 - k_1)^2} \]

in the integrand, we would not be able to cancel divergences at both \( k_3 \) and \( k_1 \). So we perform the \( k_1 \) integral first, then the \( k_3 \) integral and finally the \( k_2 \) integral.

First we evaluate

\[ I_1 = \int d^3 k_1 \frac{1}{(k_1 - k_2)^2 + \lambda^2} e^{-iE_1 \tau_1} \Psi_i(k_1). \] (32)

While the potential kernel is regularized, we can change integration variables to \( \kappa = k_1 - k_2 \). Then we can set \( \lambda = 0 \) since, in spherical polar coordinates, the factor \( \kappa^2 \) from the integration measure cancels the factor \( \kappa^2 \) in the denominator. We then find

\[ I_1 = \int d^2 \kappa e^{-ik_2 \cdot R} e^{-i(k_2 - p_i)^2/4\sigma_i^2} \int_0^\infty d\kappa' \int d^2 \kappa' e^{-\kappa'^2/4\sigma_i^2} \int d\kappa \int d\kappa' \sqrt{\lambda^2 + \kappa^2} e^{-iE(k) \tau_1} e^{i\kappa \xi_i}, \] (33)

where

\[ \xi_i = -\frac{k_2 - p_i}{2\sigma_i^2} - i(R_i + v(k_2)\tau_1). \] (34)

We will use the notation

\[ E(k) = \frac{k^2}{2m_0} \quad \text{and} \quad v(k) = \frac{k}{m_0}. \] (35)

The factor \( \exp(-\frac{(k_2 - p_i)^2}{4\sigma_i^2}) \) will not, in fact, survive once we find the dependence on \( k_2 \) of the remaining integrals. But another factor will emerge that regularizes the \( k_2 \) integral, as we will see below. Remarkably, the regularizing influence of the initial wavefunction is extended to the intermediate \( k_2 \) integral.

We know that

\[ \int d^2 \kappa e^{A \kappa} = 4\pi \frac{\sinh(\sqrt{A^2} \kappa)}{\sqrt{A^2} \kappa} \quad \text{and} \quad \int d^2 \kappa e^{iB \kappa} = 4\pi \frac{\sin(\sqrt{B^2} \kappa)}{\sqrt{B^2} \kappa}. \] (36)

These functions are both even and entire, with power series that contain only integral powers of \( A^2 \) and \( B^2 \), respectively. If we put \( A = iB \) in the first formula, we get the second formula. So, by analytic continuation,

\[ \int d^2 \kappa e^{(A + iB) \kappa} = 4\pi \frac{\sinh(\sqrt{(A + iB)^2} \kappa)}{\sqrt{(A + iB)^2} \kappa}. \] (37)

In the remaining integral, we can replace

\[ e^{-iE(\kappa)\tau_1} \to 1 + O(\sqrt{\epsilon}) \] (38)

within the peak region of the Gaussian \( \exp(-\kappa^2/4\sigma_p^2) \). Then we have

\[ \int_0^\infty d\kappa e^{-\kappa^2/4\sigma_p^2} \frac{\sinh(\sqrt{\xi_i^2 \kappa})}{\sqrt{\xi_i^2 \kappa}} = \frac{1}{\sigma_p} \frac{\sqrt{\pi}}{2} g(\frac{\xi_i^2}{4\sigma_p^2}), \] (39)
with
\[ g(x) = \frac{2}{\sqrt{\pi}} \int_0^\infty dz \, e^{-z^2} \frac{\sinh(\sqrt{4x} z)}{\sqrt{4x} z} = \frac{\sqrt{\pi}}{2} \text{erf}(i\sqrt{x}), \]

normalized to \( g(0) = 1 \). The last integral was evaluated using MATHEMATICA \textsuperscript{[16]}. So our result for \( I_1 \) is

\[ I_1 = \frac{4\pi}{(2\pi\sigma_p^2)^{3/2}} e^{-iE_2T_1} e^{-ik_2 R_1} e^{-(k_2-p_i)^2/4\sigma_p^2} \frac{\sqrt{\pi}}{2} g\left(\frac{\xi_i^2}{4\sigma_x^2}\right). \]  

(41)

Similarly, we find

\[ I_3 = \int d^3k_3 \frac{1}{(k_3-k_2)^2} e^{-iE_3(T-\tau_2)} \psi_f^*(k_3) \]

\[ = \frac{4\pi}{(2\pi\sigma_p^2)^{3/2}} e^{-iE_3(T-\tau_2)} e^{+ik_2 R_f} e^{-(k_2-p_i)^2/4\sigma_p^2} \frac{\sqrt{\pi}}{2} g\left(\frac{\xi_f^2}{4\sigma_x^2}\right), \]

(42)

with

\[ \xi_f = -\frac{k_2-p_f}{2\sigma_p^2} - i(R_f+v(k_2)(T-\tau_2)). \]  

(43)

Then we find

\[ \mathcal{M}_2(\theta) = -\frac{\alpha^2}{\pi \sigma_x^2} \int_0^T d\tau_2 \int_0^{\tau_2} d\tau_1 \int d^3k_2 \frac{1}{(2\pi\sigma_p^2)^{3/2}} e^{-(k_2-p_f)^2/4\sigma_p^2} e^{-(k_2-p_i)^2/4\sigma_p^2} \times \]

\[ \times e^{-iE_2T} e^{ik_2(R_f-R_i)} g\left(\frac{\xi_f^2}{4\sigma_x^2}\right) g\left(\frac{\xi_i^2}{4\sigma_x^2}\right). \]  

(44)

Combining Gaussian exponents using Eq. \textsuperscript{[12]} gives

\[ \mathcal{M}_2(\theta) = -\frac{\alpha^2}{\pi \sigma_x^2} e^{-(p_f-p_i)^2/8\sigma_p^2} \int_0^T d\tau_2 \int_0^{\tau_2} d\tau_1 \int d^3k_2 \frac{1}{(2\pi\sigma_p^2)^{3/2}} e^{-(k_2-p_+)^2/2\sigma_p^2} e^{-iE_2T} e^{ik_2(R_f-R_i)} g\left(\frac{\xi_f^2}{4\sigma_x^2}\right) g\left(\frac{\xi_i^2}{4\sigma_x^2}\right), \]  

(45)

with \( p_+ \) as in Eq. \textsuperscript{[13]}. Then we change variables to \( \kappa = k_2 - p_+ \).

We use two properties of the \( g \) function that we have verified numerically. The arguments of the \( g \) function, \( \xi_i^2/4\sigma_x^2 \) and \( \xi_f^2/4\sigma_x^2 \), both contain a large, real, positive term (\( M = \sin^2 \frac{\theta}{2} / 4\kappa^2 \) for \( |\theta| \gg \epsilon \) in our case) and other terms that remain of order unity. We find

\[ g(M) \to \frac{e^M}{\pi M} \quad \text{for} \quad M \gg 1. \]  

(46)

Then for proportionally small fluctuations around that large, positive value,

\[ \frac{g(M+z)}{g(M)} \to e^z \quad \text{for} \quad M \gg 1 \quad \text{and} \quad |z| \ll M. \]  

(47)

These two results are consistent.

Using these approximations gives

\[ g\left(\frac{\xi_f^2}{4\sigma_x^2}\right) g\left(\frac{\xi_i^2}{4\sigma_x^2}\right) \to \frac{4e^{4\epsilon^\sin^2 \frac{\theta}{2} / 2\kappa^2} e^{-\epsilon^2 / 2\kappa^2} e^{-\sin^2 \frac{\theta}{2} e^{-\cos^2 \frac{\theta}{2}(\tau_1+\tau_2-T)^2 / 2\kappa^2}} \times \]

\[ \times e^{-(\kappa+p_+(\tau_1-\tau_2))/T^2 / 2\kappa^2} e^{i\epsilon^\sin^2 \frac{\theta}{2} / e^{\kappa^2} e^{i\kappa^2 \chi}}, \]  

(48)

with

\[ \chi = v_1(\tau_1 - \frac{T}{2}) - v_2(\tau_2 - \frac{T}{2}). \]  

(49)
We note the cancellations
\[ e^{-(p_1-p_2)^2/8\sigma_p^2} e^{+ \sin^2 \frac{\theta}{2e^2}} = 1 \quad \text{and} \quad e^{-(k_2-p_2)^2/2\sigma_p^2} e^{+ \kappa^2/2\sigma_p^2} = 1. \]  
(50)

Changing variables again, to \( \kappa' = \kappa + p_+ (\tau_1 - \tau_2)/T \), gives a remaining constraining factor \( \exp(-\kappa'^2/2\epsilon p^2) \), as mentioned earlier. The width of this function is \( \sqrt{\epsilon p} \), wider than the previous \( \epsilon p = \sigma_p \).

The remaining \( \kappa' \) integral is performed using Eq. (14). Then, for the time integrals, we use a change of variables
\[ \int_0^T d\tau \int_0^{\tau_2} d\tau_1 \rightarrow \frac{1}{2} T^2 \int_{-\infty}^{\infty} dx_+ \int_{-\infty}^0 dx_-, \]  
(51)

with
\[ x_\pm = \frac{\tau_1 - T \eta}{T} \pm \frac{T - \tau_2}{T}. \]  
(52)

Finally, using Eq. (14) twice in the case \( \xi = 0 \) (the \( x_- \) integral is the integral of an even function on the half line, equal to one half the integral on the full line),
\[ \int_{-\infty}^{\infty} dx_+ \int_{-\infty}^0 dx_- e^{-\sin^2 \frac{\theta}{2e^2} / 2e^2} e^{-2\cos^2 \frac{\theta}{2e^2} / e^2} = \left( \frac{2\pi e^2}{\sin^2 \frac{\theta}{2}} \right) \frac{1}{2} \left( \frac{\pi e^2}{2 \cos^2 \frac{\theta}{2}} \right)^{1/2}. \]  
(53)

Our final result is
\[ \mathcal{M}_2(\theta) = -e^{+i\epsilon T} e^{i \sin^2 \frac{\theta}{2e^2}} \frac{16}{\pi^2} \eta^2 e^{i \frac{\theta}{2e}} e^{-\sin^2 \frac{\theta}{2e^2}} \frac{1}{\sin^2 \frac{\theta}{2} \cos \frac{\theta}{2}} \]  
(54)

for \( \theta \neq 0 \).

The presence of a half-integral power of \( \epsilon \) comes about because the width of the distribution \( \exp(-\kappa'^2/2\epsilon p^2) \) is \( \sqrt{\epsilon p} \).

We see that this term gives a correction to \( \mathcal{M}_1(\theta) \) that is negligible everywhere except close to the forward direction, where the approximations used to derive this term become no longer valid.

**E. Second order in the forward direction, \( \mathcal{M}_2(0) \)**

We fully expect that calculation of the second-order contribution in the forward direction will lead to a finite result. The calculation is challenging and will be left for future work. From what we saw for \( \mathcal{M}_1(0) \), we expect the result to be proportional to the same phase factor \( \exp(+i\epsilon T) \), so that it can interfere with \( \mathcal{M}_0(0) \), and to be proportional to \( \eta^2 \) with a factor that is neither very large nor very small and depends only weakly on \( \epsilon \). In the calculation of \( \mathcal{M}_1(0) \), we accomplished our intention to show that this forward amplitude is finite and has the correct dependence on the parameters.

In [3], we used a wavepacket treatment that made the partial wave series converge for Coulomb scattering. We found that for \( \eta = \pm 1 \), the amplitude in the forward direction was very small. It will be of value to calculate \( \mathcal{M}_2(0) \) using the methods of this paper to allow estimation of the probability for forward scattering to order \( \eta^2 \). This will allow comparison between these two very different calculation methods for the same physical description, and to potentially observe a falloff of the probability of forward scattering with increasing \( \eta \).

Probabilities in the forward direction are not experimentally measurable. As discussed in [6], in an experiment such as a beam of alpha particles incident on a gold foil, projectiles with sufficiently large impact parameters relative to the nuclei are expected to pass by largely undisturbed and contribute to a strong peak of flux around the forward direction. This would obscure any attempt to measure probability in the forward direction. The calculation presented in this paper used the particular geometry of zero impact parameter.

**III. CONCLUSIONS**

If the matrix element for the second-order Born approximation to nonrelativistic Coulomb scattering is calculated between plane-wave state vectors (momentum eigenvectors), the result diverges. Calculating the matrix element between square-integrable wavepacket state vectors gives results that are everywhere finite, including in the forward
direction, and with the correct physical properties. We found that the finite second-order term makes a negligible contribution to the scattering away from the forward direction. This is reassuring, as the first-order result already gives an excellent agreement with experiment and the exact result for the cross section is just the Rutherford formula [1].

If these results can be extended to relativistic quantum field theory, quantum electrodynamics for example, it will greatly change the character of the renormalization program. The physical essence of renormalization is that the mass and charge input to the theory acquire corrections to become the observed, physical, mass and charge. The results presented here suggest that this might be done with finite corrections, rather than by manipulating regularized infinities.

Whether this is the case must await future investigation.

[1] Messiah A. Quantum Mechanics. vol. 1 and 2. North-Holland, Amsterdam and John Wiley and Sons, N.Y.; 1961.
[2] Cohen-Tannoudji C, Diu B, Laloë F. Quantum Mechanics. vol. I and II. Hermann and John Wiley and Sons, Inc.; 1977.
[3] Sakurai JJ. Modern Quantum Mechanics. Revised edition ed. Addison-Wesley, Reading, MA; 1994.
[4] Itzykson C, Zuber JB. Quantum Field Theory. 1st ed. McGraw-Hill Inc.; 1980.
[5] Dalitz RH. On higher Born approximations in potential scattering. Proc Roy Soc Lond A: Math, Phys and Eng Sci. 1951;206:509.
[6] Hoffmann SE. Prediction of deviations from the Rutherford formula for low-energy Coulomb scattering of wavepackets. Journal of Physics B: Atomic, Molecular and Optical Physics. 2017;50:215302.
[7] Newton RG. Scattering theory of waves and particles. 2nd ed. Springer-Verlag, N.Y.; 1982.
[8] Hoffmann SE. Relativistic probability amplitudes I. Massive particles of any spin. arXiv:180400548. 2018;
[9] Rosenstein B, Horwitz LP. Probability current versus charge current of a relativistic particle. J Phys A: Math Gen. 1985;18:2115.
[10] Fong R, Rowe EGP. The bra-ket formalism for free relativistic particles. Ann Phys. 1968;46:559.
[11] Foldy LL. Synthesis of covariant particle equations. Phys Rev. 1956;102:568.
[12] Gradsteyn IS, Ryzhik IM. Tables of Integrals, Series and Products. Corrected and enlarged ed. Academic Press, Inc., San Diego, CA; 1980.
[13] Richards JI, Youn HK. The theory of distributions: a nontechnical introduction. CUP Archive; 1995.
[14] Rutherford E. The scattering of α and β rays by matter and the structure of the atom. Phil Mag. 1911;Series 6, vol. 21:669.
[15] Geiger H, Marsden E. On a diffuse reflection of the alpha particles. Proc Roy Soc. 1909;82:495.
[16] Mathematica; 2019. Wolfram Research Inc.