Born Series for Potential Scattering

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(Received 12 August 1971)

The Born series for the T matrix is considered with the class of potentials $V(r)=V_0\int_0^\infty dt A(t)\times e^{-tr^2}$. An explicit knowledge of $A(t)$ is not necessary since the resulting scattering amplitude can be expressed in terms of V. The exact expressions for the first and second Born approximations are utilized to approximate the general nth-order term in the series. The series is explicitly summed to yield an expression for the scattering amplitude which reduces at high energy to the previous impact-parameter amplitude of Blankenbecler and Goldberger. The continuation of the series beyond its radius of convergence is discussed and exemplified with an exponential potential $V=V_0 e^{-r/\sigma}$. A few specific numerical examples are considered to illustrate the behavior of the resulting scattering cross section. Improvement of low-energy total cross sections is noted, particularly for repulsive or weakly attractive potentials.

I. INTRODUCTION

The study of elastic scattering cross sections has yielded much information on chemical and nuclear interactions. It is a relatively easy task to compute the phase shifts and resulting cross sections (provided not too many partial waves are needed). Nevertheless it is still useful to have approximate closed form expressions for the scattering amplitude $f(\theta)$. Two such expressions are the impact-parameter approximations of Glauber[1] (G) and of Blankenbecler and Goldberger[2] (BG), given in Eqs. (1) and (2), respectively:

$$f_{\rm G}(\theta)=-iK\int_0^\infty db\, b\, J_0(|\vec{k}-\vec{k}'|b)[e^{2i\delta(b)}-1]\ , \qquad (1)$$

$$f_{\rm BG}(\theta)=2K\int_0^\infty db\ b\, J_0(|\vec{k}-\vec{k}'|b)\,\frac{\delta(b)}{1-i\delta(b)}\ , \qquad (2)$$

where

$$\delta(b)=-\frac{m}{\hbar^2K}\int_0^\infty dz\ V((b^2+z^2)^{1/2})$$

and b is the impact parameter. The total energy in the center-of-mass system is $E=\hbar^2K^2/2m$ and $|\vec{k}|=|\vec{k}'|=K$ above. The BG expression was originally suggested since it removed some singularities in the G result.[2] Both of these expressions satisfy unitarity at high energy. More recently Abul-Magd and Simbel[3] considered an extension of the BG result to obtain the off-shell scattering amplitude. In this paper an expression for the scattering amplitude will be derived which gives a modification of the BG result, and goes over to it at high energy. Special use will be made of Gaussian-like potentials.

II. BORN SERIES AND SCATTERING AMPLITUDE

The T matrix and the scattering amplitude are related by[4]

$$f(\Omega)=(-4\pi^2m/\hbar^2)\langle\vec{k}'|T|\vec{k}\rangle\ , \qquad (3)$$

where

$$\langle\vec{k}'|T|\vec{k}\rangle=\langle\vec{k}'|V|\vec{k}\rangle+\int dk''^3\,\frac{\langle\vec{k}'|V|\vec{k}''\rangle\langle\vec{k}''|T|\vec{k}\rangle}{E-\hbar^2k''^2/2m+i\epsilon}\ . \qquad (4)$$

V is the interaction potential and the states $|\vec{k}\rangle$ are eigenstates of the unperturbed kinetic energy operator. The well-known Born-series solution[4] to Eq. (4) is

$$\langle\vec{k}'|T|\vec{k}\rangle=\sum_{n=1}^\infty\langle\vec{k}'|T_n|\vec{k}\rangle\ , \qquad (5a)$$

where

$$\langle\vec{k}'|T_1|\vec{k}\rangle=\langle\vec{k}'|V|\vec{k}\rangle\ , \qquad (5b)$$

$$\langle\vec{k}'|T_n|\vec{k}\rangle=\frac{2m}{\hbar^2}\int dk''^3\ \frac{\langle\vec{k}'|V|\vec{k}''\rangle\langle\vec{k}''|T_{n-1}|\vec{k}\rangle}{K^2-k''^2+i\epsilon}\ ,\quad n\geq 2\ . \qquad (5c)$$

Consider the class of potentials expressible as

$$V(r)=V_0\int_0^\infty dt\,A(t)\,e^{-tr^2}\ , \qquad (6)$$

where $A(t)$ can be written as the inverse Laplace transform of V. It is not necessary to explicitly know the form of $A(t)$, since we will see that the scattering amplitude in Eq. (21) can be expressed in terms of V itself. To better illustrate the nature of the method we shall first consider $A(t)=\delta(t-t_0)$ and the more general case later. With $V(r)=V_0e^{-t_0r^2}$, Eq. (5) for $n=1, 2$ becomes

$$\langle \vec{k}' | T_1 | \vec{k} \rangle = \frac{V_0}{8\pi^{3/2} t_0^{3/2}} \exp(-|\vec{k}-\vec{k}'|^2/4t_0) \ , \tag{7}$$

$$\begin{aligned}\langle \vec{k}' | T_2 | \vec{k} \rangle &= \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right)^2 \frac{2m}{\hbar^2} \int dk''^3 \, \frac{\exp(-|\vec{k}''-\vec{k}'|^2/4t_0 - |\vec{k}-\vec{k}''|^2/4t_0)}{K^2 - k''^2 + i\epsilon} \\ &= \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right)^2 \left(\frac{4i\pi^2 m t_0}{\hbar^2}\right) \frac{1}{|\vec{k}+\vec{k}'|} \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{8t_0}\right) \\ &\quad \times \left[W\left(\frac{K}{(2t_0)^{1/2}} + \frac{|\vec{k}+\vec{k}'|}{2(2t_0)^{1/2}}\right) - W\left(\frac{K}{(2t_0)^{1/2}} - \frac{|\vec{k}+\vec{k}'|}{2(2t_0)^{1/2}}\right)\right] \ . \end{aligned} \tag{8}$$

The evaluation of the integral in Eq. (8) and the W functions are discussed in the Appendix. The on-shell second Born approximation to T for a Gaussian potential was reported by Wu[5] some time ago. Equation (8) is also valid off-shell. Note that both T_1 and T_2 have a Gaussian factor in $|\vec{k}-\vec{k}'|^2$, but the decay constant $\frac{1}{4}t_0$ for T_1 is twice that for T_2. Thus, as expected, larger momentum transfer is allowed with T_2.

Since the integral in Eq. (5c) is in general very difficult to evaluate for $n \geq 3$, it will be necessary to approximate $\langle \vec{k}' | T_2 | \vec{k} \rangle$ in order to obtain the higher-order terms. As the wave number K [or $A = K/(t_0)^{1/2}$] increases we would generally expect the scattering to become more peaked in the forward direction. We shall therefore approximate the "sum" variable $|\vec{k}+\vec{k}'| \sim 2K$, where we have used $|\vec{k}| \approx |\vec{k}'| \approx K$. Then $\langle \vec{k}' | T_2 | \vec{k} \rangle$ becomes

$$\langle \vec{k}' | T_2 | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right)^2 \left(\frac{4i\pi^2 m t_0}{\hbar^2}\right) \frac{1}{2K} \times \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{8t_0}\right) [W(K(2/t_0)^{1/2}) - 1] \tag{9}$$

where we have used the property[6] $W(0) = 1$. Equation (9) is a small-wavelength approximation of $\langle \vec{k}' | T_2 | \vec{k} \rangle$ which retains the strong dependence on the difference variable $|\vec{k}-\vec{k}'|$ and approximates the weaker dependence on $|\vec{k}+\vec{k}'|$. Note that the structure of Eqs. (9) and (7) are essentially the same, but with different coefficients (complex for T_2) and decay factors in the Gaussians.

Equation (9) can be used in Eq. (5c) to obtain $\langle \vec{k}' | T_3 | \vec{k} \rangle$, and the process continued to obtain $\langle \vec{k}' | T_n | \vec{k} \rangle$:

$$\begin{aligned}\langle \vec{k}' | T_n | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right) \left(\frac{im\sqrt{\pi}\, V_0}{2(t_0)^{1/2}\hbar^2 K}\right)^{n-1} \left[W\left(K\left(\frac{2}{t_0}\right)^{1/2}\right) - 1\right]\left[W\left(K\left(\frac{3}{2t_0}\right)^{1/2}\right) - 1\right] \\ \times \cdots \left[W\left(K\left(\frac{n}{(n-1)t_0}\right)^{1/2}\right) - 1\right] \frac{1}{n} \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{4nt_0}\right) \ , \quad n \geq 2 \end{aligned} \tag{10}$$

where the same small-wavelength approximation was made after each iteration. Equation (10) could be used to numerically sum the Born series; however, if we approximate all the $[W-1]$ factors by the second-order one $[W(K(2/t_0)^{1/2}) - 1]$, then the series can be summed explicitly.[7] Equations (10) and (5a) become

$$\langle \vec{k}' | T_n | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right) \left(\frac{m\sqrt{\pi}\, iV_0}{2(t_0)^{1/2}\hbar^2 K}\right)^{n-1} [W(K(2/t_0)^{1/2}) - 1]^{n-1} \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{4nt_0}\right) \ , \quad n \geq 1 \ . \tag{11}$$

$$\langle \vec{k}' | T | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2} t_0^{3/2}}\right) \frac{1}{X} \sum_{n=1}^{\infty} \frac{X^n}{n} \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{4nt_0}\right) \ , \tag{12}$$

where

$$X = \frac{m\sqrt{\pi}\, iV_0}{2(t_0)^{1/2}\hbar^2 K} [W(K(2/t_0)^{1/2}) - 1] \ .$$

It is interesting to note that $X = 2\langle \vec{k} | T_2 | \vec{k} \rangle / \langle \vec{k} | T_1 | \vec{k} \rangle$, with $|\vec{k}| = K$. As expected, each term in the Born series allows for increasing momentum transfer according to the relation for the nth term $\Delta K = |\vec{k}-\vec{k}'| \sim (4nt_0)^{1/2}$. Equation (12) can be rewritten as

$$\langle \vec{k}' | T | \vec{k} \rangle = 2\left(\frac{V_0}{8\pi^{3/2}(t_0)^{1/2}}\right) \frac{1}{X} \int_0^{\infty} db\, b\, J_0(|\vec{k}-\vec{k}'| b)$$

$$\times \sum_{n=1}^{\infty} (X e^{-t_0 b^2})^n \ , \quad (13)$$

where we have used the identity[8]

$$\exp(-r^2/4s)/s = 2\int_0^\infty db\, b\, J_0(br) e^{-sb^2} \ . \quad (14)$$

The series in Eq. (13) can be summed easily,

$$\sum_{n=1}^{\infty} (X e^{-t_0 b^2})^n = \frac{X e^{-t_0 b^2}}{1 - X e^{-t_0 b^2}} \quad (15)$$

and the resulting scattering amplitude is

$$f(\theta) = -\left(\frac{m\sqrt{\pi} V_0}{(t_0)^{1/2}\hbar^2}\right)\int_0^\infty db\, \frac{b J_0(|\vec{k}-\vec{k}'|b) e^{-t_0 b^2}}{1 - X e^{-t_0 b^2}} \quad (16)$$

It is easy to show that this reduces to the BG result with a Gaussian potential for $K/(t_0)^{1/2} \gg 1$, since $|W(K(2/t_0)^{1/2})| \ll 1$ in this limit.[6]

Now consider the more general potential in Eq. (6). Procedures exactly analogous to those used for the Gaussian potential also apply here. For example, Eqs. (7) and (8) for the exact first- and second-order terms become

$$\langle \vec{k}' | T_1 | \vec{k} \rangle = \frac{V_0}{8\pi^{3/2}} \int_0^\infty dt_1 \frac{A(t_1)}{t_1^{3/2}} \exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{4t_1} \right) , \quad (17)$$

$$\langle \vec{k}' | T_2 | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2}}\right)^2 \frac{2m}{\hbar^2} \int_0^\infty dt_1 \frac{A(t_1)}{t_1^{3/2}} \int_0^\infty dt_2 \frac{A(t_2)}{t_2^{3/2}} \int dk''^3 \frac{\exp(-|\vec{k}''-\vec{k}'|^2/4t_2 - |\vec{k}-\vec{k}''|^2/4t_1)}{K^2 - k''^2 + i\epsilon}$$

$$= \left(\frac{V_0}{8\pi^{3/2}}\right)\left(\frac{iV_0\sqrt{\pi}\, m}{2\hbar^2}\right) \int_0^\infty dt_1 \frac{A(t_1)}{(t_1)^{1/2}} \int_0^\infty dt_2 \frac{A(t_2)}{(t_2)^{1/2}} \frac{\exp[-|\vec{k}-\vec{k}'|^2/4(t_1+t_2)]}{|t_1\vec{k}' + t_2\vec{k}|}$$

$$\times \left[W\left(\frac{K}{2}\left(\frac{t_1+t_2}{t_1 t_2}\right)^{1/2} + \frac{|t_1\vec{k}' + t_2\vec{k}|}{2[t_1 t_2(t_1+t_2)]^{1/2}} \right) - W\left(\frac{K}{2}\left(\frac{t_1+t_2}{t_1 t_2}\right)^{1/2} - \frac{|t_1\vec{k}' + t_2\vec{k}|}{2[t_1 t_2(t_1+t_2)]^{1/2}} \right) \right] . \quad (18)$$

The Fourier transform of the potential $V(r)$ was assumed to exist. Even if the Fourier transform of $V(r)$ does not exist, regularization[9] procedures can sometimes be applied to circumvent this (an example of such a potential will be considered in Sec. III). With the assumption of small wave numbers and mostly forward scattering, the "sum" variable can be approximated, $|\vec{k}'t_1 + \vec{k}t_2| \sim K(t_1+t_2)$. The nth-order term becomes

$$\langle \vec{k}' | T_n | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2}}\right) \left(\frac{im\sqrt{\pi}\, V_0}{2\hbar^2 K}\right)^{n-1} \int_0^\infty \cdots \int_0^\infty dt_1 \cdots dt_n \frac{A(t_1)\cdots A(t_n)}{(t_1 \cdots t_n)^{1/2}}$$

$$\times \left[W\left(K\left(\frac{t_1+t_2}{t_1 t_2}\right)^{1/2}\right) - 1 \right] \left[W\left(K\left(\frac{t_1+t_2+t_3}{(t_1+t_2)t_3}\right)^{1/2}\right) - 1 \right] \cdots \left[W\left(K\left(\frac{(t_1+\cdots+t_n)}{(t_1+\cdots+t_{n-1})t_n}\right)^{1/2}\right) - 1 \right]$$

$$\times \frac{\exp[-|\vec{k}-\vec{k}'|^2/4(t_1+\cdots+t_n)]}{t_1+\cdots+t_n} . \quad (19a)$$

This could be used directly for numerical summation of the Born series, but there is an enormous simplification if the product of functions in brackets is approximated. We shall let

$$\left[W\left(K\left(\frac{(t_1+\cdots+t_n)}{(t_1+\cdots t_{n-1})t_n}\right)^{1/2}\right) - 1 \right] \rightarrow [W(K(2/t_n)^{1/2}) - 1] \ ;$$

this approximation can be viewed as a partial decoupling of the potentials in the nth-order term {the remaining factor

$$\frac{\exp[-|\vec{k}-\vec{k}'|^2/4(t_1+\cdots+t_n)]}{(t_1+\cdots+t_n)}$$

is not approximated}. This finally leads to

$$\langle \vec{k}' | T_n | \vec{k} \rangle = \left(\frac{V_0}{8\pi^{3/2}}\right)\left(\frac{mi\sqrt{\pi}\, V_0}{2\hbar^2 K}\right)^{n-1} \int_0^\infty dt_1 \frac{A(t_1)}{(t_1)^{1/2}}$$

$$\times \int_0^\infty dt_2 \frac{A(t_2)}{(t_2)^{1/2}} [W(K(2/t_2)^{1/2}) - 1] \int_0^\infty dt_3 \frac{A(t_3)}{(t_3)^{1/2}} [W(K(2/t_3)^{1/2}) - 1]$$

$$\cdots \int_0^\infty dt_n \frac{A(t_n)}{(t_n)^{1/2}} [W(K(2/t_n)^{1/2}) - 1] \frac{\exp[-|\vec{k}-\vec{k}'|^2/4(t_1 + \cdots t_n)]}{(t_1 + \cdots + t_n)} . \quad (19b)$$

Using Eqs. (5a), (14), and (19b) the Born series becomes

$$\langle \vec{k}' | T | \vec{k} \rangle = 2\left(\frac{V_0}{8\pi^{3/2}}\right) \int_0^\infty db\, b\, J_0(|\vec{k}-\vec{k}'|b) \int_0^\infty dt \frac{A(t)}{\sqrt{t}} e^{-tb^2} \frac{1}{X} \sum_{n=1}^{\infty} X^n , \quad (20)$$

where

$$X = \frac{mi\sqrt{\pi}V_0}{2\hbar^2 K} \int_0^\infty dt' \frac{A(t')}{(t')^{1/2}} e^{-t'b^2} \times [W(K(2/t')^{1/2}) - 1].$$

The geometric series in Eq. (20) can easily be summed to $X/(1-X)$, which is also the analytic continuation[10] of this series beyond its radius of convergence $|X| = 1$. The resulting scattering amplitude is

$$f(\theta) = 2K \int_0^\infty db \frac{b\, J_0(|\vec{k}-\vec{k}'|b)\delta(b)}{1 + \Delta_r(b) - i[\delta(b) + \Delta_i(b)]} , \quad (21)$$

where

$$\delta(b) = -\left(\frac{m\sqrt{\pi}V_0}{2\hbar^2 K}\right) \int_0^\infty dt \frac{A(t)}{\sqrt{t}} e^{-tb^2} , \quad (22a)$$

$$\Delta_r(b) = \left(\frac{mi\sqrt{\pi}V_0}{2\hbar^2 K}\right) \int_0^\infty dt \frac{A(t)}{\sqrt{t}} e^{-tb^2 - 2K^2/t} \times \mathrm{erf}(-i(2/t)^{1/2}K) , \quad (22b)$$

$$\Delta_i(b) = \left(\frac{m\sqrt{\pi}V_0}{2\hbar^2 K}\right) \int_0^\infty dt \frac{A(t)}{\sqrt{t}} e^{-tb^2 - 2K^2/t} , \quad (22c)$$

$$\Delta(b) = \Delta_r(b) - i\Delta_i(b) = \left(\frac{-im\sqrt{\pi}V_0}{2\hbar^2 K}\right) \int_0^\infty dt\, e^{-tb^2} \frac{A(t)}{\sqrt{t}} W(K(2/t)^{1/2}).$$

$f(\theta)$ in Eq. (21) should then be an approximate continuation of the *true* Born series.[11] The expressions in Eq. (22) explicitly depend on $A(t)$, but it is possible to express them in terms of V by using Eq. (6) and the identity[6]

$$W(K(2/t)^{1/2}) = 2(t/\pi)^{1/2} \int_0^\infty dz \exp(-tz^2 + iz2^{3/2}K)$$

to obtain

$$\delta(b) = (-m/\hbar^2 K) \int_0^\infty dz\; V((b^2+z^2)^{1/2}) , \quad (23a)$$

$$\Delta_r(b) = (m/\hbar^2 K) \int_0^\infty dz\; \sin(2^{3/2}Kz)\, V((b^2+z^2)^{1/2}) , \quad (23b)$$

$$\Delta_i(b) = (m/\hbar^2 K) \int_0^\infty dz\; \cos(2^{3/2}Kz)\, V((b^2+z^2)^{1/2}) . \quad (23c)$$

By comparison of Eqs. (2) and (21) it is clear that the new scattering amplitude differs from the BG result by the presence of Δ_r and Δ_i. The integrands in Eqs. (23b) and (23c) contain terms which oscillate in sign more rapidly as K increases. Therefore Δ_r and Δ_i will become negligible[12] for sufficiently large K and $f(\theta) \to f_{BG}(\theta)$ in this limit. Furthermore, all the amplitudes $f(\theta)$, $f_{BG}(\theta)$, and $f_G(\theta)$ eventually take the limiting form of the first Born approximation (assuming it exists for the particular potential) as K becomes very large.[13] Although we did not explicitly introduce the impact parameter b, the limiting behavior $f(\theta) \to f_{BG}(\theta)$ shows the connection between the series method here and the impact-parameter expression of BG. Since $f_{BG}(\theta)$ can be derived from $V(r)$ without relying on Eq. (6) (Refs. 2 and 3) and $f(\theta) \to f_{BG}(\theta)$ in the large K limit, it is interesting to speculate that the amplitude in Eq. (21) with the factors in Eq. (23) is more general than the use of the potential form in Eq. (6) might imply.[14]

The total cross section from Eq. (21) is given by

$$Q = \int d\Omega\, |f(\theta)|^2 = 8\pi K^2 \int_0^\infty db \frac{b\,\delta(b)}{1 + \Delta_r(b) - i[\delta(b) + \Delta_i(b)]} \times \int_0^\infty db' \frac{b'\delta(b')}{1 + \Delta_r(b') + i[\delta(b') + \Delta_i(b')]} \times \int_0^\pi d\theta \sin\theta\, J_0(b'|\vec{k}-\vec{k}'|)\, J_0(b|\vec{k}-\vec{k}'|) .$$

With our previous assumption that most of the scattering is in the forward direction, the angular integral[2] gives $(1/bK^2)\delta(b-b')$ to yield

$$Q = 8\pi \int_0^\infty db \frac{b\,\delta^2(b)}{[1 + \Delta_r(b)]^2 + [\delta(b) + \Delta_i(b)]^2} . \quad (24)$$

The total cross section from the optical theorem[4] is

$$Q = (4\pi/K)\,\mathrm{Im} f(0)$$

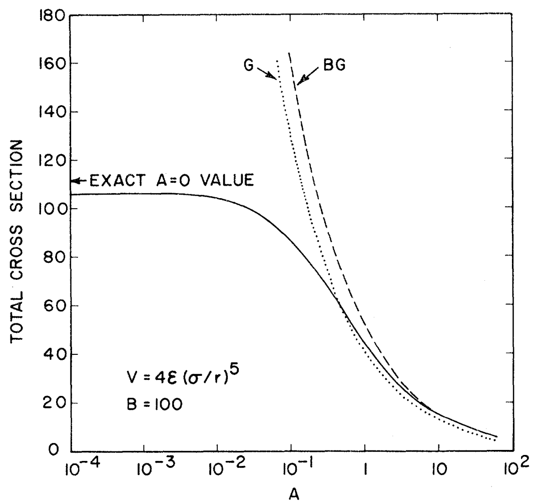

FIG. 1. Total cross section in units of $\pi\sigma^2$ shown for the potential $V=4\epsilon(\sigma/r)^5$ at $B=100$. The solid curve was computed from Eq. (25). It is approximately 5% in error at $A=0$ and approaches the BG results for $A \gtrsim 10$. The G curve is essentially exact for $A \gg 10$. Both the BG and G curves diverge for $A \to 0$.

$$= 8\pi \int_0^\infty db\, \frac{b\,\delta(b)[\delta(b)+\Delta_i(b)]}{[1+\Delta_r(b)]^2+[\delta(b)+\Delta_i(b)]^2} \quad . \quad (25)$$

The optical theorem and the integrated cross section will agree at high energy, since $\delta(b) \gg \Delta_i(b)$ in that limit.[12] The corresponding cross sections from $f_{BG}(\theta)$ and $f_G(\theta)$ are

$$Q_{BG} = 8\pi \int_0^\infty \frac{db\, b\,\delta^2(b)}{[1+\delta^2(b)]} \quad , \quad (26a)$$

$$Q_G = 8\pi \int_0^\infty db\, b \sin^2\delta(b) \quad . \quad (26b)$$

Q_{BG} and Q_G are *incorrectly* independent of an over-all sign change of the potential $(V \to -V)$, while Q in Eq. (25) does depend on such a sign change (due to the presence of Δ_r). Also note that Q_{BG} and Q_G diverge as $K \to 0$. Although Eq. (21) was derived with a small-wavelength approximation, we shall see in Sec. III that the result is also good at $K=0$ for some cases.

III. NUMERICAL EXAMPLES

In this section a few numerical examples will be considered to illustrate the behavior of the amplitude in Eq. (21) and the effect of the new terms Δ_r and Δ_i. The primary effect of Δ_r and Δ_i is expected to show up at low energy since $f(\theta) \to f_{BG}(\theta)$ at high energy. Rather than just use the special case of the simple Gaussian potential in Eq. (16) $[A(t)=\delta(t-t_0)$ in Eq. (21)], a few other potentials will be used to better illustrate the utility of Eq. (21). We shall first consider total cross sections from Eq. (25).

As a specific example consider the potential $V=4\epsilon(\sigma/r)^n$, $\epsilon>0$ and $n>3$, where ϵ and σ are in units of energy and length, respectively. For this case[14] we have

$$A(t) = t^{(n-2)/2}/\Gamma(\tfrac{1}{2}n) \quad .$$

The scattering amplitude for this potential is well behaved, but the Fourier transform of V and the Born series do not exist for such a singular potential.[9] In Sec. II the Fourier transform of V was assumed to exist. For this new case our summation of the Born series should be viewed in terms of a regularization of the potential.[9] This can conveniently be done by considering the potential $V=4\epsilon\sigma^n/(r+\alpha)^n$, $\alpha>0$ and letting $\alpha \to 0$ after summing the series. Also since the Born approximation does not exist for this singular potential, $f \to f_{BG}$ at high energy. It can be shown directly from Eq. (23) that

$$\delta(b) = -\frac{B\sqrt{\pi}}{A}\left(\frac{\sigma}{b}\right)^{n-1} \frac{\Gamma(\frac{1}{2}(n-1))}{\Gamma(\frac{1}{2}n)} \quad , \quad (27a)$$

$$\Delta_i(b) = \frac{2\sqrt{\pi}B}{A\Gamma(\frac{1}{2}n)}\left(\frac{\sqrt{2}A\sigma}{b}\right)^{(n-1)/2} \times K_{(n-1)/2}(2^{3/2}Ab/\sigma) \quad , \quad (27b)$$

$$\Delta_r(b) = \frac{2B}{A}\left(\frac{\sigma}{b}\right)^{n-1} \int_0^\infty dt\, \frac{\sin(2^{3/2}Abt/\sigma)}{(1+t^2)^{n/2}} \quad , \quad (27c)$$

where $A=K\sigma$, $B=2m\epsilon\sigma^2/\hbar^2$, and $K_\nu(\ )$ is a modified Bessel function.[15] For odd integer values of n the quantity Δ_r can be expressed in terms of Bessel and Struve functions,[15] but a more convenient computational form from Eq. (22b) is

$$\Delta_r(b) = \frac{\sqrt{\pi}B}{A\Gamma(\frac{1}{2}n)}\left(\frac{\sigma}{b}\right)^{n-1} \int_0^\infty dx\, e^{-x} x^{(n-3)/2} \times \mathrm{Im}\,W(A(2/x)^{1/2}b/\sigma) \quad . \quad (27d)$$

The W function was computed by the method of Salzer[16] and the integral was done by Gauss-Laguerre quadrature.[17] Figure 1 shows a plot of the total cross section $Q^* = Q/\pi\sigma^2$ (Figs. 2 and 3 are also in units of $\pi\sigma^2$) as a function of A for $n=5$ and $B=100$. The solid curve is from the optical theorem in Eq. (25) and the arrow indicates the exact result[9] at $A=0$. Equation (25) is 5% in error at $A=0$,[18] while the BG and G results diverge as expected. At zero energy Eq. (25) reduces to

$$Q = \frac{32\pi m^2}{\hbar^2} \int_0^\infty \frac{db\, b\rho_0(b)\rho_2(b)}{[1+(2^{3/2}m/\hbar^2)\rho_1(b)]^2} \,, \quad (28)$$

where

$$\rho_i(b) = \int_0^\infty dz\, z^i\, V((b^2+z^2)^{1/2}) \quad .$$

For inverse-power potentials this becomes

$$Q^* = \frac{2\pi\Gamma(\frac{1}{2}(n-1))\Gamma(\frac{1}{2}(n-3))[2^{3/2}B\Gamma(\frac{1}{2}(n-2))/\Gamma(\frac{1}{2}n)]^{2/(n-2)}\,\Gamma(2/(n-2))\Gamma((2n-3)/(n-2))}{\Gamma^2(\frac{1}{2}(n-2))(n-2)}\,, \quad n>3. \tag{29}$$

This expression agrees best with the exact result[9] for small values of n; the error is ~ 5% for $n < 20$, 10% at $n \sim 100$, and ~ 20% for $n \to \infty$. Finally, in the limit $A \gg 10$ the G curve is essentially exact[19] and can be considered as a reference for comparison (as noted before $Q \to Q_{BG} \sim Q_G$ for $A \gg 10$).

Consider the case of an exponential potential $V = V_0 e^{-r/\sigma}$. As A increases Q, Q_{BG}, and Q_G all go to the first Born approximation for the total cross section. At the other extreme of $A = 0$ it is interesting to look at the total cross section as a function of $B = 2mV_0\sigma^2/\hbar^2$ (Q_{BG} and Q_G again diverge here). Equation (28) becomes

$$Q^* = 8B^2\int_0^\infty dy\, \frac{y^4K_1(y)K_2(y)}{[1+\sqrt{2}Be^{-y}(1+y)]^2}\,. \tag{30}$$

Figure 2 shows Eq. (30) (solid curve) along with the first Born and exact results[20] for the repulsive potential case $V_0 > 0$. The good agreement of Eq. (30) with the exact result for B even greater than unity is related to the continuation of the Born series beyond its radius of convergence.[11] For the series in Eq. (20) to converge it was required that $|X| < 1$, and for this case $X = \sqrt{2}Be^{-y}(1+y)$. Therefore the radius of consequence is $|B| = 1/\sqrt{2}$.[21] Figure 2 shows that Eq. (30) produces a fairly accurate continuation beyond $B = 1/\sqrt{2}$. More generally, note that the denominator of the integrand in Eq. (28) is never zero for a repulsive potential, regardless of its strength.

The attractive exponential $V_0 < 0$ case behaves differently. Q should go through successive zero-energy resonances as the potential well supports more bound states (i.e., as $-B$ increases). The first bound-state resonance[21] is at $-B = 1.44$; Eq. (30) becomes singular for $B < -1/\sqrt{2}$. Therefore, for the attractive case Eq. (30) does not give an accurate continuation of the series. The location of the first zero-energy resonance is somewhat sensitive to the approximation of

$$\left[W\left(K\left(\frac{(t_1+\cdots+t_n)}{(t_1+\cdots+t_{n-1})t_n}\right)^{1/2}\right)-1\right]$$

in going from Eq. (19a) to Eq. (19b), and may likewise be sensitive for other potentials.

These results indicate that, for cases where V is repulsive or perhaps just has a weakly attractive well (i.e., it does not support any bound states), the total cross section in Eq. (25) should give fairly accurate results for $A \geq 0$. However, if V can support at least one bound state, then Eq. (25) will become a poor approximation for small values of A. The precise region where Eq. (30) breaks down in the latter case is not clear, but it is reasonable to expect it to occur for $A \lesssim (|B|)^{1/2}$. This corresponds to the region where the scattering wave undergoes a large distortion.

As an example to illustrate this behavior, consider a Lennard-Jones 12-6 potential of depth ϵ, $V = 4\epsilon[(\sigma/r)^{12} - (\sigma/r)^6]$. Figure 3 shows the total cross section from Eq. (25) (solid curve) and the

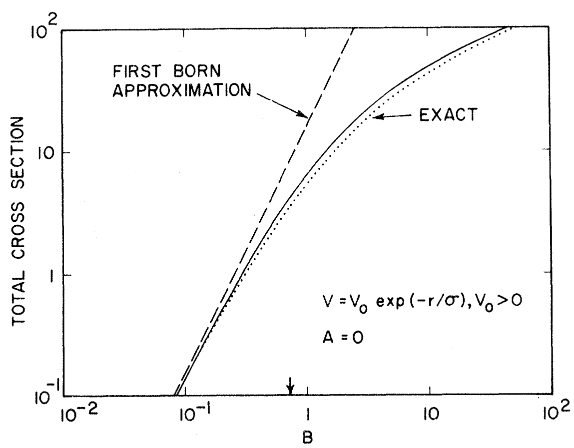

FIG. 2. Total cross section in units of $\pi\sigma^2$ at $A = 0$ shown for the exponential potential. The solid curve, computed from Eq. (30), agrees fairly well with the exact curve. The arrow on the B axis indicates the radius of convergence of the series in Eq. (20).

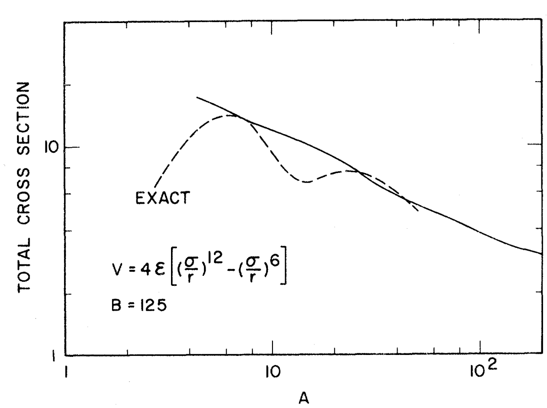

FIG. 3. The total cross section in units of $\pi\sigma^2$ shown at $B = 125$ for a Lennard-Jones 12-6 potential. The solid curve was computed from Eq. (25); it begins to break down for $A \lesssim 20 \sim \sqrt{B}$, where the large quantal oscillations appear in the exact result. For values of A greater than shown here, Eq. (25) goes over to the BG result with the potential $V = 4\epsilon(\sigma/r)^{12}$.

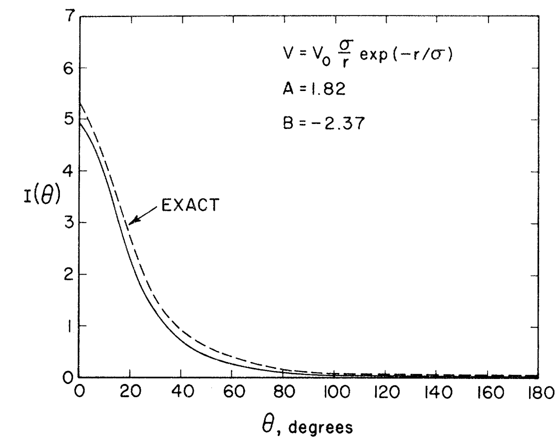

FIG. 4. Differential cross section shown in units of σ^2 for a Yukawa potential with $A = 1.82$ and $B = -2.37$. The solid curve was computed from the amplitude in Eq. (21). The accuracy is best for $0° \lesssim \theta \lesssim 90°$ and poorest at $\theta = 180°$, where the calculated and exact results differ by a factor of 3 (0.015 and 0.049, respectively).

exact results[22] for $B = 125$. Equation (25) begins to break down near $A \lesssim 20 \sim \sqrt{B}$, where large-amplitude quantal oscillations appear in the exact result.

As a final example, consider the calculation of the differential cross section $I(\theta) = |f(\theta)|^2$ with $f(\theta)$ from Eq. (21) using a Yukawa potential

$$V(r) = V_0(\sigma/r)e^{-r/\sigma}, \quad V_0 < 0$$

and[14]

$$A(t) = \frac{1}{(\pi t)^{1/2}} e^{-(1/4)\sigma^2 t} .$$

The calculation is rather straightforward, but a little more difficult than calculating total cross sections. The problem stems from the oscillatory nature of J_0 (Ref. 15) in the integrand of Eq. (21). The integration over b in Eq. (21) was done by Gauss-Legendre quadrature[17] on finite intervals; sufficient intervals were taken so as to obtain convergence. Equations (22) and (23) yield

$$\delta(b) = (-B/2A)K_0(b/\sigma) ,$$

$$\Delta_i(b) = \frac{B}{2A} K_0(b(1+8A^2)^{1/2}/\sigma) ,$$

$$\Delta_r(b) = \frac{B}{4A} \int_0^\infty dt \, \frac{\exp[-tb^2 - 1/(4\sigma^2 t)]}{t} \times \operatorname{Im} W(A(2/t)^{1/2}/\sigma) .$$

Figure 4 shows the calculated differential cross section (solid curve) along with the exact result[23] for $A = 1.82$ and $B = -2.37$. The angular distribution is most accurate in the forward direction, $0° \lesssim \theta \lesssim 90°$ (recall that mostly forward scattering was assumed in the derivation in Sec. II). Note that this potential can support one bound state and $A \sim (-B)^{1/2}$ in Fig. 4 so that the conditions in this case should be close to the estimated breakdown region for the amplitude in Eq. (21). As A decreases below ~ 1 the accuracy decreases (more rapidly in the backward direction), while as A increases the accuracy improves and the cross section finally approaches the first Born limit. Also note that f is complex in Eq. (21) while $f_{\text{1st Born}}$ is real, and $f \to f_{\text{1st Born}}$ as A increases.

The few examples in this section certainly do not present a complete analysis or test of the scattering amplitude in Eq. (21). In particular, a more thorough test of angular distribution calculations would be useful. Nevertheless, the examples do give an indication of the expected range of validity and accuracy of the amplitude. It is clear that Eq. (21) shows an improvement over the BG results in Eq. (2), particularly for low energy total cross sections. Finally, $V(r)$ was assumed to be real here, but a complex optical potential could just as easily be handled. Likewise if specific internal states $|i\rangle$ are present and if $\langle i|V(r)|j\rangle$ can be written as $\int_0^\infty dt A_{ij}(t) e^{-tr^2}$, then the treatment in Sec. II can be carried out with specific inelastic channels (the quantities δ, Δ_r, and Δ_i will become matrices).

ACKNOWLEDGMENT

I would like to thank Dr. R. Conn for useful and interesting discussions during the initial stages of this research.

APPENDIX

To derive Eqs. (8) and (18), integrals of the type

$$I(r,s) = \int dk''^3 \, \frac{\exp(-|\vec{k}'' - \vec{k}'|/4r - |\vec{k} - \vec{k}''|^2/4s)}{K^2 - k''^2 + i\epsilon} \tag{31}$$

must be performed (the $\lim_{\epsilon \to 0_+}$ is implied). After completing the square in the exponential the integral becomes

$$I(r,s) = \exp\left(-\frac{(k'^2 s + k^2 r)}{4rs}\right) \times \int dk''^3 \, \frac{\exp(-ak''^2 + \vec{b}\cdot\vec{k}'')}{K^2 - k''^2 + i\epsilon} ,$$

where $a = (r+s)/4rs$ and $\vec{b} = (s\vec{k}' + r\vec{k})/4rs$. The angular integrations can be performed to obtain

$$I(r,s) = \frac{2\pi}{b} \exp\left(-\frac{(k'^2 s + k^2 r)}{4rs}\right) \frac{\partial}{\partial b} \exp\left(\frac{b^2}{4a}\right) \times \int_{-\infty}^{+\infty} dk'' \, \frac{\exp[-a(k'' - b/2a)^2]}{K^2 - k''^2 + i\epsilon} .$$

Let $t = \sqrt{a}\,(k'' - b/2a)$ and separate the denominator by partial fractions to obtain

$$I(r,s)=\frac{\pi}{Kb}\exp\left(-\frac{(k'^2s+k^2r)}{4rs}\right)\frac{\partial}{\partial b}\exp\left(\frac{b^2}{4a}\right)\int_{-\infty}^{+\infty}dt\exp(-t^2)\left(\frac{1}{\sqrt{a}K+(b/2\sqrt{a})+i\epsilon-t}+\frac{1}{\sqrt{a}K-(b/2\sqrt{a})+i\epsilon-t}\right)$$
$$=\frac{-\pi^2 i}{Kb}\exp\left(-\frac{(k'^2s+k^2r)}{4rs}\right)\frac{\partial}{\partial b}\exp\left(\frac{b^2}{4a}\right)\left[W\left(\sqrt{a}K+\frac{b}{2\sqrt{a}}\right)-W\left(\sqrt{a}K-\frac{b}{2\sqrt{a}}\right)\right], \qquad (32)$$

where $W(x)=e^{-x^2}\operatorname{erfc}(-ix)$ and the $\lim_{\epsilon\to 0_+}$ has been taken after performing the integration.[24] A few properties of the W functions for real argument are

$$W(0)=1,\quad \operatorname{Re}W(x)=e^{-x^2}$$
$$\operatorname{Im}W(x)=i\exp(-x^2)\operatorname{erf}(-ix)\gtrless 0\ ,$$
$$\lim_{x\gg 1}\operatorname{Im}W(x)\sim(1/\sqrt{\pi}x)+O(1/x^3)\ .$$

Finally, after performing the differentiation $\partial/\partial b$ and using the definitions of a and $\vec{b}$, it is easy to obtain

$$I(r,s)=\frac{2i\pi^2 rs}{|s\vec{k}'+r\vec{k}|}\exp\left(-\frac{|\vec{k}-\vec{k}'|^2}{4(r+s)}\right)\times\left[W\left(\frac{K}{2}\left(\frac{r+s}{rs}\right)^{1/2}+\frac{|s\vec{k}'+r\vec{k}|}{2[rs(r+s)]^{1/2}}\right)-W\left(\frac{K}{2}\left(\frac{r+s}{rs}\right)^{1/2}-\frac{|s\vec{k}'+r\vec{k}|}{2[rs(r+s)]^{1/2}}\right)\right]. \qquad (33)$$

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[6]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1965), Chap. 7.

[7]The factor

$$\left[W\left(K\left(\frac{n}{(n-1)t_0}\right)^{1/2}\right)-1\right]$$

ranges from $[W(K(2/t_0)^{1/2})-1]$ to $[W(K(1/t_0)^{1/2})-1]$ as n goes from 2 to ∞, respectively. We have chosen the approximation $[W(K(2/t_0)^{1/2})-1]$ so that the result is correct out to second order.

[8]See Ref. 6, p. 486.

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[11]For a discussion of the convergence properties of the Born series see Ref. 4, p. 284 and H. Davies, Nucl. Phys. 14, 465 (1960).

[12]The function Δ_r decreases much more slowly than Δ_i as K increases; this can be seen from the properties of the W function (Ref. 6) in Eqs. (22b) and (22c).

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[14]The function $A(t)$ may only be given numerically in some cases. A large variety of common potentials with specific forms of $A(t)$ are known. See, for example, G. E. Roberts and H. Kaufman, *Tables of Laplace Transforms* (Saunders, New York, 1966).

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[17]Reference 6, Chap. 25.

[18]The solid curve in Fig. 1 remains flat down to $A=0$.

[19]R. B. Bernstein and K. H. Kramer, J. Chem. Phys. 38, 2507 (1963).

[20]See Ref. 4, p. 420.

[21]The *true* Born series, not the approximate one in Eq. (20), has a radius of convergence $|B|=1.44$, the first zero of $J_0(2\sqrt{B})$.

[22]R. B. Bernstein, J. Chem. Phys. 34, 361 (1961).

[23]These values of A and B correspond to the ^3S neutron-proton interaction at $E=75$ MeV. See E. Gerjuoy and D. S. Saxon, Phys. Rev. 94, 478 (1954).

[24]There are other methods of evaluating $I(r,s)$, but this seemed to be the simplest. The final integral in Eq. (32) and further properties of the W functions are given in Ref. 6.