Blankenbecler-Goldberger approximation in inelastic e-H and e-He scattering

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The Blankenbecler-Goldberger approximation to the scattering amplitude is applied to the inelastic e-H $(1s \rightarrow 2s)$ and e-He $[(1s)^2 \rightarrow (1s)(2s)]$ scattering. The results for the differential cross section indicate a very good agreement with the Glauber approximation, but the Blankenbecler-Goldberger method is more difficult to evaluate than the Glauber approximation.

I. INTRODUCTION

The application of the Glauber approximation¹ to atomic problems is well documented.² In addition we list the following papers individually: Tai *et al.*,³ Thomas and Gerjuoy,⁴ Franco,⁵ and Thomas and Chan.⁶ In an earlier work⁷ one of us had applied an alternate technique, the Blankenbecler-Goldberger (BG) approximation,⁸ to the elastic scattering of electrons on H and He. The BG amplitude and the sequence of approximations needed to obtain it are discussed in Ref. 9. The experience⁷ gathered from the *e*-H and *e*-He elastic scattering was that the BG amplitude fares very well when compared to the Glauber ampli-tude.

In the use of the Glauber approximation one does not need to evaluate the eikonal $\chi(b)$. The evaluation of the scattering amplitude employs the most expedient sequence of integrations which bypasses the evaluation of $\chi(b)$ [or the overlap function $\Gamma(b)$] $= 1 - e^{i\chi(b)}$]. In contrast to this the eikonal is an input in the BG approximation and must first be extracted. In Sec. II we follow the technique used earlier for the elastic problem to extract the eikonal for the e-H inelastic scattering in which the hydrogen atom is excited to the 2s state. As a check on our calculation we substituted this eikonal in the Glauber amplitude and carried out the last remaining b integration to reproduce the known⁴ inelastic amplitude. This eikonal is finally substituted in the BG form and the final bintegration done to generate the inelastic scattering amplitude from which the differential cross section is calculated. In Sec. III we do a similar calculation for inelastic e-He scattering in which one of the electrons is excited from the 1s ground state to 2s excited state without spin flip, i.e., the final state is $1s2s^{1}S$. The differential cross section is calculated at 100 eV. A brief discussion of results is given in Sec. IV.

The Glauber amplitude for two-body scattering is written as,¹

$$F(q) = \frac{ik}{2\pi} \int e^{i\vec{q}\cdot\vec{b}} (1 - e^{i\chi(b)}) d^2b , \qquad (1.1)$$

where k is the incident momentum, \vec{q} is the momentum transfer, b is the impact parameter, and $\chi(b)$ is the eikonal which for a potential $V(\vec{b},z)$ is defined as¹

$$\chi(b) = \frac{1}{\hbar v} \int_{-\infty}^{\infty} V(\mathbf{b}, z) dz . \qquad (1.2)$$

v is the incident velocity. The BG amplitude⁸ is, in contrast,

$$F(\vec{q}) = \frac{k}{2\pi} \int e^{i\vec{q}\cdot\vec{b}} \frac{\chi(b)}{1 - (i/2)\chi(b)} d^2b.$$
(1.3)

To order $\chi^2(b)$ the two amplitudes are identical.

II. EIKONAL FOR e-H INELASTIC SCATTERING

If the target (H or He) is treated as infinitely heavy the reduced mass in the problem is the electron mass. The Glauber amplitude for the scattering of an electron by a neutral atom such that the initial atom, in state i, is left finally in state f, is

$$F_{fi}(q) = \frac{ik_i}{2\pi} \int u_f^*(\vec{\mathbf{r}}) u_i(\vec{\mathbf{r}}) \Gamma(\vec{\mathbf{b}},\vec{\mathbf{r}}) e^{i\vec{\mathbf{d}}\cdot\vec{\mathbf{b}}} d^2\vec{\mathbf{b}} d^3r , \quad (2.1)$$

where $u_i(\vec{\mathbf{r}})$ and $u_f(\vec{\mathbf{r}})$ are the initial and final wave functions of the atom. r stands for $\{r_1, r_2, \ldots, r_Z\}$ the positions of Z electrons in the atom and d^3r stands for $\prod_{i=1}^{Z} d^2 \vec{\mathbf{r}}_i$. $\vec{\mathbf{b}}$ is the impact parameter, $\vec{\mathbf{q}} = \vec{\mathbf{k}}_i - \vec{\mathbf{k}}_f$ is the three-momentum transfer, and $\vec{\mathbf{k}}_i$ and $\vec{\mathbf{k}}_f$ are the initial and final momenta of the electron. The relation between the mass and momentum is $\hbar \vec{\mathbf{k}} = m\vec{\mathbf{v}}$. Let us define a function $\Gamma(\vec{\mathbf{b}}, \vec{\mathbf{r}})$ in terms of a phase $\chi(\vec{\mathbf{b}}, \vec{\mathbf{r}})$ as

 $\Gamma(\vec{\mathbf{b}},\vec{\mathbf{r}}) = 1 - e^{i\chi(\vec{\mathbf{b}},\vec{\mathbf{r}})}, \qquad (2.2)$

where $\vec{\mathbf{r}}$ again stands for the coordinate set $\{r_1, r_2, \ldots, r_z\}$ and $\chi(\vec{\mathbf{b}}, \vec{\mathbf{r}})$ is defined in terms of the potential through

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Using the Coulomb potential one obtains⁵

$$\chi(b, r) = 2\eta \ln(|b - \bar{s}|/b),$$
 (2.4)

where $\eta = -e^2/\hbar v_i$ for electron scattering by a neutral atom. The inelastic scattering amplitude can be written as

$$F_{fi}(\vec{\mathbf{q}}) = \frac{ik_i}{2\pi} \int e^{i\vec{\mathbf{q}}\cdot\vec{\mathbf{b}}} \Gamma_{\mathrm{H}}^{\mathrm{inel}}(\vec{\mathbf{b}}) d^2\vec{\mathbf{b}}, \qquad (2.5)$$

where

$$\Gamma_{\rm H}^{\rm inel}(\mathbf{\dot{b}}) = \int u_f^*(\mathbf{\dot{r}}) u_i(\mathbf{\dot{r}}) \Gamma(\mathbf{\dot{b}}, \mathbf{\dot{r}}) d^3 \gamma .$$
(2.6)

Note that due to the orthogonality of state *i* and *f*, if $i \neq f$, the unit factor in the definition of $\Gamma(\mathbf{b}, \mathbf{r})$ in Eq. (2.2) does not contribute to $\Gamma_{\rm H}^{\rm inel}(\mathbf{b})$.

Thomas and Gerjuoy⁴ have shown that the over-

$$\begin{split} \Gamma_{\rm H}^{\rm inel}\left(b\right) &= -i\frac{2^{11/2}}{3^4} \left[(1+i\eta)_1 F_2(1;1+i\eta,1+i\eta;y^2/4) - (2i\eta)_1 F_2(1;i\eta,1+i\eta;y^2/4) \right. \\ &\quad \left. + (i\eta-1)_1 F_2(1;i\eta-1,i\eta+1;y^2/4) \right] \\ &\quad \left. + 2^{9/2} \frac{\Gamma^2(1+i\eta)}{3^4(y/2)^{2\,i\eta}} \left[(2i\eta)(1+i\eta)_0 F_1(1;y^2/4) - (4i\eta)(y/2)_0^2 F_1(2;y^2/4) + (y/2)_0^4 F_1(3;y^2/4) \right] . \end{split}$$

(2.8)

This is the final form for the inelastic 1s - 2soverlap function for hydrogen atom. Having derived the overlap function we can do the *b* integration indicated in (2.5) to check our result with the known result⁴ for F(q) for 1s - 2s excitation in the Glauber approximation. The final result agrees with that of Thomas and Gerjuoy.⁴ This provides us with the check that our eikonal (overlap function) is correctly evaluated. The real and imaginary parts of the overlap function $\Gamma_{\rm H}^{\rm inel}(b)$ for 1s - 2sare plotted in Fig. 1 as a function of *b*.

With the eikonal $\chi(b)$ extracted from (2.8) through $\Gamma(b) = 1 - e^{i\chi(b)}$ we can evaluate the inelastic amplitude in the BG approximation,

$$F_{\rm H}^{\rm inel}(\mathbf{\bar{q}}) = k \int_0^\infty \frac{\chi(b)}{1 - (i/2)\chi(b)} J_0(qb) b \, db \,. \tag{2.9}$$

This integral had to be done numerically. The expansion of the hypergeometric functions in powers of y^2 in (2.8) was convenient for $b \sim 12a_0$. For integration beyond this value we used the asymptotic form⁶ for the modified Lommel functions,

$$\mathcal{L}_{\mu,\nu}(iy) = S_{\mu,\nu}(iy) - 2^{\mu-1}\Gamma\left(\frac{1+\mu-\nu}{2}\right)\Gamma\left(\frac{1+\mu+\nu}{2}\right)\frac{2}{\pi} e^{-i\pi\nu/2} \times \cos\left(\frac{\pi}{2}(\mu-\nu)\right)K_{\nu}(y), \qquad (2.10)$$

lap function for the 1s - ns excitation of hydrogen atom is

$$\Gamma_{\rm H}^{\rm inel}(\vec{b}) = 2\pi A_n \sum_{j=0}^{n-1} \alpha_j(n) (-1)^{j+1} \frac{\partial^{j+1}}{\partial \lambda^{j+1}} \frac{1}{(2\pi)^2} \\ \times \int_0^\infty \frac{e^{-\lambda r}}{r} \left[1 - \left(\frac{|\vec{b} - \vec{s}|}{b}\right)^{2i\eta} \right] d^3 r,$$
(2.7)

where $\lambda = [(1 + 1/n)/a_0]$, a_0 is the first Bohr radius for H,

$$A_n = \left(\frac{2}{a_0}\right)^3 \frac{1}{4} \left(\frac{n!}{n^4(n-1)!}\right)^{1/2} = \left(\frac{2}{a_0}\right)^3 \frac{1}{4} n^{-3/2}$$

and

$$\alpha_j(n) = \frac{(1-n)_j}{(2)_j} j! \left(\frac{2}{na_0}\right)^j$$

 $(a)_j$ is the Pochhammer symbol¹⁰ with $(a)_0 = 1$ for all a. We obtain

where the asymptotic form of $S_{\mu,\nu}(iy)$ is known.¹¹ The exponential fall of $K_{\nu}(y)$ asymptotically allows us to ignore this term for $b \ge 12a_0$.



FIG. 1. Real and imaginary parts of $\Gamma_{\rm H}^{\rm inel}(b)$ for 1s $\rightarrow 2s$ transition in hydrogen.

The differential cross section for inelastic scattering 1s - 2s is then generated in the usual way. In Fig. 2 we have plotted $d\sigma_{fi}/d\Omega$ (in πa_0^2) versus q^2 (in a_0^{-2}) for incident electron energy of 100 eV and 1s - 2s excitation of hydrogen. We find that the BG approximation works just as well as the Glauber approximation. As the differential cross sections are so very close there will be no discernable difference in the total cross section either.

III. EIKONAL FOR e-He INELASTIC SCATTERING

In order to be able to use the BG form for He excitation we have to extract the corresponding eikonal $\chi(b)$. The analog of Eq. (2.1) for *e*-He inelastic scattering is

$$F_{\text{He}}^{\text{inel}}(\vec{q}) = \frac{ik_i}{2\pi} \int e^{i\vec{q}\cdot\vec{b}} d^2\vec{b} \int u_i(\vec{r}_1,\vec{r}_2) u_f^*(\vec{r}_1,\vec{r}_2) (1 - e^{i\chi(\vec{b},\vec{s}_1,\vec{s}_2)}) d^3r_1 d^3r_2 \equiv \frac{ik_i}{2\pi} \int e^{i\vec{q}\cdot\vec{b}} \Gamma_{\text{He}}^{\text{inel}}(\vec{b}) d^2\vec{b}, \qquad (3.1)$$

where $\mathbf{\tilde{r}} = (\mathbf{\tilde{s}}, z)$ and

$$\Gamma_{\rm He}^{\rm inel}(\vec{b}) = -\prod_{j=1}^{2} \int u_{f}^{*}(\vec{r}_{1},\vec{r}_{2})u_{i}(\vec{r}_{1},\vec{r}_{2}) \left(\frac{|\vec{b}-\vec{s}_{j}|}{b}\right)^{2in} d^{3}r_{1}d^{3}r_{2}.$$
(3.2)

For the purposes of comparison of the BG approximation with the Glauber approximation we use the wave functions given by Morse *et al.*¹² for an electron in the 1s state:

$$\phi(r) = \frac{1}{\sqrt{\pi}} \left(\frac{\alpha}{a_0}\right)^{3/2} e^{-\alpha r/a_0}; \qquad (3.3)$$

for an electron in 2s state:

$$\psi(r) = \left(\frac{\mu^5}{3\pi N a_0^3}\right)^{1/2} \left(\frac{r}{a_0} e^{-\mu r/a_0} - \frac{3A}{\mu} e^{-\mu B r/a_0}\right),\tag{3.4}$$

where

$$\alpha = 1.69,$$

$$\mu = 0.61,$$

$$\mu \beta = 1.57,$$

$$A = \frac{\mu(\alpha + \mu \beta)^3}{(\alpha + \mu)^4},$$

$$N = \left(1 - \frac{48A}{(1 + \beta)^4} + \frac{3A^2}{\beta^3}\right).$$
(3.5)

A and N are so chosen that ϕ and ψ are orthogonal and both are unit normalized. One obtains in a straightforward way,

$$\Gamma_{\rm He}^{\rm inel}\left(\stackrel{+}{\mathbf{b}}\right) = \frac{16\pi\,\alpha^{3}b^{6}}{a_{0}^{3}} \left(\frac{\alpha^{3}\mu^{5}}{3\pi^{2}Na_{0}^{6}}\right)^{1/2} \left(-\frac{2}{y^{3}} - \frac{(2i\eta)^{2}(2+2i\eta)}{y(iy)^{2+2\,in}} \pounds_{2\,i\eta-1,\,0}(iy) + \frac{i(2i\eta)^{2}(2i\eta-2)}{(iy)^{2+2\,in}} \pounds_{2\,i\eta-2,\,1}(iy)\right) \\ \times \left[\frac{b}{a_{0}}\left(\frac{6}{y_{1}^{4}} + \frac{(2i\eta)^{2}(2+2i\eta)(3+2i\eta)}{y_{1}^{2}(iy_{1})^{2+2\,in}} \pounds_{2\,i\eta-1,\,0}(iy_{1}) - \frac{i(2i\eta)^{2}(2i\eta-2)(4i\eta+3)}{y_{1}(iy_{1})^{2+2\,in}} \pounds_{2\,i\eta-2,\,1}(iy)\right) \\ - \frac{(2i\eta)^{2}(2i\eta-2)(2i\eta-4)}{(iy_{1})^{2+2\,in}} \pounds_{2\,i\eta-3,\,2}(iy_{1})\right) \\ + \frac{3A}{\mu} \left(-\frac{2}{y_{2}^{3}} - \frac{(2i\eta)^{2}(2+2i\eta)}{y_{2}(iy_{2})^{2+2\,i\eta}} \pounds_{2\,i\eta-1,\,0}(iy_{2}) + \frac{i(2i\eta)^{2}(2i\eta-2)}{(iy_{2})^{2+2\,i\eta}} \pounds_{2\,i\eta-2,\,1}(iy_{2})\right) \right],$$

$$(3.6)$$

where

$$y_1 = \lambda_1 b, \quad \lambda_1 = (\alpha + \mu)/a_0,$$

$$y_2 = \lambda_2 b, \quad \lambda_2 = (\alpha + \mu \beta)/a_0, \quad (3.7)$$

and

$$y = \lambda b$$
, $\lambda = 2\alpha/a_0$.

The eikonal $\chi(b)$ defined through $\Gamma(b) = 1 - e^{i\chi(b)}$ is

then extracted from (3.6). The remaining procedure is a repeat of what we did for the hydrogen problem. In Fig. 3 we have plotted the real and the imaginary parts of the overlap function for e-He inelastic scattering $1s^2 - 1s2s$. In Fig. 4 we compare the two cross sections $(d\sigma_{fi}/d\Omega)(\ln \pi a_0^2)$ versus q^2 (in a_0^{-2}) for the inelastic $1s^2 - 1s2s$ *e*-He scattering of a 100-eV electron. We notice that



FIG. 2. $d\sigma/d\Omega$ for $1s \rightarrow 2s$ transition in hydrogen. Incident electron energy = 100 eV.

there is a discernable difference in the backward direction. However, as the differential cross section has also dropped by more than an order of magnitude, we do not anticipate any significant difference in the calculated total cross section in the two approximations. In the numerical integration of (2.9) to generate the BG amplitude the power-series expansion for hypergeometric functions up to $b \approx 6.5a_0$ and the asymptotic form for the modified Lommel functions for $b \gtrsim 6.5a_0$.

IV. CONCLUSION

We have extended a previous calculation⁷ which used the BG approximation for the elastic e-He and e-He scattering to the inelastic e-H and e-He scattering. We find that as in the elastic case the BG approximation works well for the inelastic scattering also when compared to the Glauber approximation. We suspect that this has to do more with the fact that the electromagnetic coupling is involved than any other subtle effect.

The advantage of using the Glauber form is that the amplitude can be evaluated with some effort in a closed form. The disadvantage of the BG form is that the eikonal has first to be evaluated and the last integral has to be done numerically. The excitation to each state has to be handled sep-



FIG. 3. Real and imaginary parts of $\Gamma_{\text{He}}^{\text{inel}}(b)$ for $1s^2 \rightarrow 1s2s$ transition in helium.

arately as against the Glauber form where an analytic result⁴ can be obtained for excitation to any state. The BG approximation, however, compares very well with the Glauber approximation for s - sexcitation.

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FIG. 4. $d\sigma/d\Omega$ for $1s^2 \rightarrow 1s^{2s}$ transition in helium. Incident electron energy = 100 eV.

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