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J. Phys. A: Math. Gen., Vol. 11, No. 7, 1978. Printed in Great Britain. © 1978

Relativistic electron scattering from a two-centre potential

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Received 9 May 1977, in final form 15 November 1977

Abstract. A method of studying the scattering of a high-energy electron from a two-centre Coulomb potential is presented. The Dirac equation for the problem is solved by a generalised form of the Sommerfeld–Maue approximation, using a spheroidal phase shift analysis at the final stage. For a screened potential, the total cross section has been calculated and averaged over a random orientation of the axes of the two-centre systems. For a long-range potential, the differential cross section can be obtained after the averaging is done numerically. The spheroidal phase shifts are obtained by comparing the asymptotic behaviour of the radial equation with that of the central Coulomb radial equation and using a generalised JWKB method. The method is studied by considering the simple case of two fixed point charges. Some results, for this case, are also presented.

1. Introduction

The scattering of a charged particle from a two-centre potential is of considerable physical interest. The process describes a number of well known problems of molecular, nuclear, and subnuclear physics. In a series of papers, Li (1971, 1972, 1973) has considered some of these problems. The scattering of low-energy electrons from a homonuclear molecule is an important problem of molecular physics. The Schrödinger equation describing this process is separable in spheroidal coordinates and the scattering cross section can be given in terms of spheroidal phase shifts. In recent years there has been a renewal of interest in problems with two-centre potentials. Müller *et al* (1973) have studied the bound states of an electron in the field of two Coulomb centres. They calculated the binding energies of a Dirac particle by a numerical method. The scattering problem with a relativistic electron has, however, not yet been studied. The difficulties involved can be seen by comparison with the spherical case. With a spherical potential, the Dirac equation gives a set of two linked radial equations and a phase shift analysis can still be made. The method has been used in the determination of the charge distribution in the nuclei, see Yennie *et al* (1954). However, with a two-centre potential, the Dirac equation is not at all separable. Even an approximate solution of the scattering problem will, therefore, be useful. The purpose of the present paper is to present an approximation method of studying this problem. Applications of this method to a number of physical problems will be presented elsewhere. We shall apply a generalised form (Mukherjee and Majumdar 1965) of the Sommerfeld–Maue approximation so that the solution of the

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Dirac equation can be constructed from that of a Schrödinger-like equation. The latter is separable in spheroidal coordinates for a class of potentials, and hence permits a spheroidal phase shift analysis. The relativistic scattering cross section is then obtained in terms of these spheroidal phase shifts. The phase shifts are determined by a semiclassical approximation. The method has been studied by considering the simple case of two fixed point charges.

For the two-centre problem it is convenient to work with the prolate spheroidal coordinates given by

$$\xi = \frac{r_a + r_b}{R}, \qquad \eta = \frac{r_a - r_b}{R}, \qquad \text{and} \qquad \phi, \tag{1.1}$$

where R is the distance between the two centres, r_a and r_b are the distances of the field point $\boldsymbol{r}$ from the two centres, and ϕ is the azimuthal angle which the plane of $\boldsymbol{R}$ and $\boldsymbol{r}$ makes with the plane of $\boldsymbol{R}$ and the z axis. We note that

$$\begin{aligned} x &= \tfrac{1}{2}R\sqrt{(\xi^2-1)(1-\eta^2)}\cos\phi, \\ y &= \tfrac{1}{2}R\sqrt{(\xi^2-1)(1-\eta^2)}\sin\phi, \\ z &= \tfrac{1}{2}R\xi\eta. \end{aligned} \tag{1.2}$$

The scheme of presentation is as follows. In § 2 we have solved the Dirac equation with a two-centre Coulomb potential by the Sommerfeld–Maue approximation. In § 3 we have considered a screened Coulomb potential and have obtained an expression for the total scattering cross section, averaged over a random distribution of the target axes. In § 4 we have given an outline of the generalised JWKB method, while the next two sections give an account of the application of this method to the present problem. Our conclusions are summarised in § 7.

2. Sommerfeld–Maue approximation for a two-centre potential

We consider the elastic scattering of a Dirac particle with an initial momentum $\boldsymbol{P}$ and energy ϵ from a two-centre potential Φ. To apply the Sommerfeld-Maue approximation, one must obtain ψ_0 from the equation

$$(\nabla^2 + P^2 + 2\epsilon V)\psi_0 = 0, \tag{2.1}$$

where $V = e\Phi$. The solution of the Dirac equation, in this approximation (Mukherjee and Majumdar 1965) is then given by

$$\psi = \psi_0 + \psi_1, \tag{2.2}$$

$$\psi_1 = A\psi_0 - \frac{\mathrm{i}}{2\epsilon}(\boldsymbol{\alpha}\cdot\nabla)\psi_0, \tag{2.3}$$

where the matrix A is to be chosen so as to normalise the incident wave, which is contained entirely in the function ψ_0. Thus ψ_1 is a correction to the scattered part only. The accuracy of this approximation has been studied by Bethe and Maximon (1954). In the case of a point charge scatterer, the exact scattering cross section of the Dirac equation differs from the approximate one only by terms of order $a^2/\epsilon \ln \epsilon$, with $a = \alpha Z$, where α is the fine structure constant and Z is the charge of the target in units of e. The approximation has been used extensively in the study of multiple scattering

of electrons and positrons (Mukherjee 1967, 1968, 1973) and also in calculating the Coulomb corrections to various electrodynamic processes (Bethe and Maximon 1954). The two-centre problem presents another case where the approximation can be applied with advantage.

For the solution of (2.1) we assume the form

$$\psi_0(\boldsymbol{r}, \boldsymbol{P}) = U(\boldsymbol{P})\, \mathrm{e}^{\mathrm{i}\boldsymbol{P}.\boldsymbol{r}} f(\boldsymbol{r}, \boldsymbol{P}), \tag{2.4}$$

where $U(\boldsymbol{P})$ is a plane wave Dirac spinor and $f(\boldsymbol{r}, \boldsymbol{P})$ is a slowly varying function of $\boldsymbol{r}$ as compared with $\mathrm{e}^{\mathrm{i}\boldsymbol{P}.\boldsymbol{r}}$. It then follows that

$$A = -\boldsymbol{\alpha}\,.\,\boldsymbol{P}/2\epsilon, \tag{2.5}$$

and the solution ψ is given by

$$\psi = \mathrm{e}^{\mathrm{i}\boldsymbol{P}.\boldsymbol{r}}\left(f(\boldsymbol{r}, \boldsymbol{P}) - \frac{\mathrm{i}}{2\epsilon}\boldsymbol{\alpha}\,.\,\nabla f(\boldsymbol{r}, \boldsymbol{P})\right) U(\boldsymbol{P}). \tag{2.6}$$

We now introduce a prolate spheroidal system fixed with the target. Equation (2.1) is written as

$$\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} + \left(\frac{1}{\xi^2-1} - \frac{1}{1-\eta^2}\right)\frac{\partial^2}{\partial\phi^2} + \frac{R^2}{4}(P^2+2\epsilon V)(\xi^2-\eta^2)\right]\psi_0 = 0. \tag{2.7}$$

in the asymptotic region

$$(\psi_0)_{\mathrm{scatt}} \xrightarrow[\xi\to\infty]{} \frac{P}{c\xi}\,\mathrm{e}^{\mathrm{i}c\xi} F(\eta, \phi; \boldsymbol{P}) U(\boldsymbol{P}), \tag{2.8}$$

where $c = \frac{1}{2}PR$. If the Coulomb potential is not screened, there is also a logarithmic phase factor. However, this factor will be of no consequence in the subsequent developments and will be omitted. It then follows from (2.4) and (2.8) that

$$f(\boldsymbol{r}, \boldsymbol{P}) \xrightarrow[\xi\to\infty]{} \frac{P}{c\xi} F(\eta, \phi; \boldsymbol{P}) \exp\left(\frac{\mathrm{i}R\xi}{2}[P - \sqrt{1-\eta^2}(p_1\cos\phi + p_2\sin\phi) - p_3\eta]\right), \tag{2.9}$$

where p_1, p_2, p_3 are the Cartesian components of $\boldsymbol{P}$ in the target-fixed frame. To determine the function in (2.6) we note that

$$\begin{aligned}\boldsymbol{\alpha}\,.\,\nabla \xrightarrow[\xi\to\infty]{} \frac{2}{R\xi}\Bigg[&\xi\sqrt{1-\eta^2}\left(\alpha_1\cos\phi + \alpha_2\sin\phi + \alpha_3\frac{\eta}{\sqrt{1-\eta^2}}\right)\frac{\partial}{\partial\xi} \\ &- \eta\sqrt{1-\eta^2}\left(\alpha_1\cos\phi + \alpha_2\sin\phi - \alpha_3\frac{\sqrt{1-\eta^2}}{\eta}\right)\frac{\partial}{\partial\eta} \\ &- \frac{1}{\sqrt{1-\eta^2}}(\alpha_1\sin\phi - \alpha_2\cos\phi)\frac{\partial}{\partial\phi}\Bigg].\end{aligned} \tag{2.10}$$

Using (2.10) we obtain

$$(\psi)_{\mathrm{scatt}} \xrightarrow[\xi\to\infty]{} \frac{P}{c\xi}\,\mathrm{e}^{\mathrm{i}c\xi}[1+M]U(\boldsymbol{P})F(\eta, \phi; \boldsymbol{P}), \tag{2.11}$$

where M is the Hermitian matrix

$$M=\frac{1}{2\epsilon}\begin{pmatrix} 0 & 0 & C & A-\mathrm{i}B \\ 0 & 0 & A+\mathrm{i}B & -C \\ C & A-\mathrm{i}B & 0 & 0 \\ A+\mathrm{i}B & -C & 0 & 0 \end{pmatrix} \tag{2.12}$$

with

$$\begin{aligned} A &= P\sqrt{1-\eta^2}\cos\phi - p_1, \\ B &= P\sqrt{1-\eta^2}\sin\phi - p_2, \\ C &= P\eta - p_3. \end{aligned} \tag{2.13}$$

In obtaining (2.11), we neglected the term ∇F, which is small compared with those retained which are of order PF. This is consistent with the assumption that $f(\boldsymbol{r}, \boldsymbol{P})$ is a slowly varying function of $\boldsymbol{r}$ as compared with $\mathrm{e}^{\mathrm{i}\boldsymbol{P}\cdot\boldsymbol{r}}$ for large $\boldsymbol{P}$. The approximation is, therefore, valid for $P \gg 1$. Also, the terms contributed by the logarithmic phase factor, if present, on differentiation, are neglected as they vanish as $1/\xi^2$. The magnitude of the scattered current density is given by

$$|\boldsymbol{J}_{\text{scatt}}| \xrightarrow[\xi\to\infty]{} \frac{P^2}{c^2\xi^2}|F(\eta, \phi; \boldsymbol{P})|^2\left(1+\frac{A^2+B^2+C^2}{4\epsilon^2}+\frac{Ap_1+Bp_2+Cp_3}{\epsilon^2}\right), \tag{2.14}$$

$$=\frac{P^2}{2c^2\xi^2}|F(\eta, \phi; |\boldsymbol{P}|, \omega, \alpha)|^2(1+\eta\cos\omega+\sqrt{1-\eta^2}\sin\omega\cos(\phi-\alpha)), \tag{2.15}$$

where ω, α are the polar and the azimuthal angles of the vector $\boldsymbol{P}$ in the target-fixed frame. For simplicity, we have put $\epsilon = P$ in (2.15). In the asymptotic region, $r^2|\boldsymbol{J}_{\text{scatt}}|$ will give the differential scattering cross section in the direction given by angles $(\cos^{-1}\eta, \phi)$ measured about the axis of symmetry of the target when the incident momentum $\boldsymbol{P}$ is in the direction (ω, α). The problem, therefore, reduces to the calculation of $F(\eta, \phi; |\boldsymbol{P}|, \omega, \alpha)$. This may be obtained by solving the equation (2.1), subject to the boundary condition (2.8), which is a simpler problem.

Equation (2.1) is separable in spheroidal coordinates if the potential is of the form:

$$2\epsilon V(\boldsymbol{r}) = \frac{U(\xi)+W(\eta)}{\xi^2-\eta^2}. \tag{2.16}$$

This form, though restrictive, includes a large class of physically interesting cases, including the case of two fixed point charges. If the point charges are of equal strength, we have, in addition,

$$W(\eta) = 0. \tag{2.17}$$

In this paper, we shall consider a potential which satisfies both (2.16) and (2.17). The solution of (2.1) is then well known, namely

$$\psi_0 \sim R_{ml}(c, \xi)S_{ml}(c, \eta)\,\mathrm{e}^{\mathrm{i}m\phi}, \tag{2.18}$$

where R and S satisfy the following equations:

$$\left(\frac{\mathrm{d}}{\mathrm{d}\xi}(\xi^2-1)\frac{\mathrm{d}}{\mathrm{d}\xi}+c^2\xi^2-\lambda_{ml}(c)-\frac{m^2}{\xi^2-1}+\frac{R^2}{4}U(\xi)\right)R_{ml}(c,\xi)=0, \tag{2.19}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}\eta}(1-\eta^2)\frac{\mathrm{d}}{\mathrm{d}\eta}-c^2\eta^2+\lambda_{ml}(c)-\frac{m^2}{1-\eta^2}\right)S_{ml}(c,\eta)=0, \tag{2.20}$$

where $\lambda_{ml}(c)$ is the separation constant and l is an ordering integer, $l=0,1,2,\ldots$. The angle function S_{ml} is independent of the potential because of the particular choice of the potential. The properties of the spheroidal functions and the separation constant can be found in Stratton *et al* (1956), Flammer (1957), Mott and Massey (1965), and Morse and Feshbach (1953). The standard spheroidal phase shift analysis can now be used (see, for example, Mott and Massey 1965) to obtain

$$F(\eta,\phi;|\boldsymbol{P}|,\omega,\alpha)$$
$$=\frac{1}{\mathrm{i}P}\sum_{l=0}^{\infty}\sum_{m=0}^{l}\left(\frac{2-\delta_{m0}}{N_{ml}(c)}\right)\cos m(\phi-\alpha)S_{ml}(c,\eta)S_{ml}(c,\cos\omega)(\mathrm{e}^{2\mathrm{i}\sigma_{ml}}-1), \tag{2.21}$$

where $N_{ml}(c)$ is the normalisation constant given by

$$\int_{-1}^{+1}\mathrm{d}\eta\, S_{ml'}(c,\eta)S_{ml}(c,\eta)=\delta_{ll'}N_{ml}(c), \tag{2.22}$$

δ is the Kronecker delta function, and σ_{ml} are the spheroidal phase shifts. Using (2.15) one can now express the relativistic differential scattering cross section in terms of these phase shifts. We are, however, interested in expressing the differential cross section in terms of the angles(Θ,Φ) measured in the laboratory frame, with $\boldsymbol{P}$ along its z direction. The connection between these two sets of angles, in the asymptotic region, is easily obtained from the addition theorem of cosine of angles. Thus to average over a random distribution of the target orientations, it is necessary to write $F(\eta,\phi;|\boldsymbol{P}|,\omega,\alpha)$ as $F(\Theta,\Phi;|\boldsymbol{P}|,\omega,\beta)$, where (ω,β) give the orientation of the target in the laboratory frame and then average the differential cross section over the range of (ω,β). This can be done numerically.

If the potential is screened, as in the case of diatomic molecules, one can also calculate the total cross section. The process of averaging is much simpler here, as will be shown in the next section.

3. Averaged total cross section

The total cross section can also be obtained by integrating over the range of η, ϕ in the asymptotic region, i.e.

$$\sum_t(\omega,\alpha)=\frac{1}{2P^2}\int\mathrm{d}\eta\,\mathrm{d}\phi\Big[(1+\eta\cos\omega+\sqrt{1-\eta^2}\sin\omega\cos(\phi-\alpha))$$
$$\times\sum_{m,l}\sum_{m',l'}\left(\frac{2-\delta_{m0}}{N_{ml}(c)}\right)\left(\frac{2-\delta_{m'0}}{N_{m'l'}(c)}\right)\cos m(\phi-\alpha)\cos m'(\phi-\alpha)(\mathrm{e}^{2\mathrm{i}\sigma_{ml}}-1)$$
$$\times(\mathrm{e}^{-2\mathrm{i}\sigma_{m'l'}}-1)S_{ml}(c,\eta)S_{ml}(c,\cos\omega)S_{m'l'}(c,\eta)S_{m'l'}(c,\cos\omega)\Big]. \tag{3.1}$$

To integrate over η, we make use of the expansion

$$S_{ml}(c,\eta)=\sum_{n=0,1}^{\infty}{}' d_n(c|m,l)P^m_{m+n}(\eta), \tag{3.2}$$

where Σ' indicates that the summation is over even values of n, if $(l-m)$ is even, and over odd values of n, if $(l-m)$ is odd. The appearance of different $P^m_{m+n}(\eta)$ in the angle function is indicative of the fact that in the present problem only the component of the angular momentum in the direction of the symmetry axis of the target is conserved. The expansion (3.2) is useful, because the series converges rapidly (even for $c=8$, one needs only about ten terms, the next coefficient $d_{21}(8|0,1)$ being as small as $8{\cdot}96\times10^{-8}$). Using the recurrence relations of $P^m_{m+n}(\eta)$, we get by a lengthy but straightforward calculation:

$$\begin{aligned}
\sum_l(\omega,\alpha)=\frac{\pi}{P^2}\sum_{l,m}\Bigg\{&\frac{4(2-\delta_{m0})}{N_{ml}(c)}|S_{ml}(c,\cos\omega)|^2\sin^2\sigma_{ml}\\
&+\sum_{l'}\sum_n{}'\frac{(2m+n)!(2-\delta_{m0})}{n!(2m+2n+1)N_{ml}(c)}(\mathrm{e}^{2\mathrm{i}\sigma_{ml}}-1)S_{ml}(c,\cos\omega)d_n(c|m,l)\\
&\times\Bigg[\frac{2\cos\omega(\mathrm{e}^{-2\mathrm{i}\sigma_{ml'}}-1)S_{ml'}(c,\cos\omega)}{N_{ml'}(c)}\Bigg(\frac{n\,d_{n-1}(c|m,l')}{2m+2n-1}\\
&+\frac{2m+n+1}{2m+2n+3}d_{n+1}(c|m,l')\Bigg)+\frac{\sin\omega(\mathrm{e}^{-2\mathrm{i}\sigma_{m+1,l'}}-1)}{N_{m+1,l'}(c)}S_{m+1,l'}(c,\cos\omega)\\
&\times\Bigg(\frac{n(n-1)}{2m+2n-1}d_{n-2}(c|m+1,l')-\frac{(2m+n+1)(2m+n+2)}{2m+2n+3}d_n(c|m+1,l')\Bigg)\\
&+\frac{(2-\delta_{m-1,0})(\mathrm{e}^{-2\mathrm{i}\sigma_{m-1,l'}}-1)}{2N_{m-1,l'}(c)}\sin\omega\,S_{m-1,l'}(c,\cos\omega)\\
&\times\Bigg(\frac{1}{2m+2n+3}d_{n+2}(c|m-1,l')-\frac{1}{2m+2n-1}d_n(c|m-1,l')\Bigg)\Bigg]\\
&+\sum_{l'}\sum_n{}'\frac{(\mathrm{e}^{2\mathrm{i}\sigma_{0l}}-1)(\mathrm{e}^{-2\mathrm{i}\sigma_{1l'}}-1)}{N_{0l}(c)N_{1l'}(c)}\sin\omega\,S_{0l}(c,\cos\omega)\\
&\times S_{1l'}(c,\cos\omega)\,d_n(c|0,l)\Bigg(\frac{n(n-1)}{(2n+1)(2n-1)}d_{n-2}(c|1,l')\\
&-\frac{(n+1)(n+2)}{(2n+1)(2n+3)}d_n(c|1,l')\Bigg)+\sum_{l'}\sum_n{}'\frac{(\mathrm{e}^{2\mathrm{i}\sigma_{1l}}-1)(\mathrm{e}^{-2\mathrm{i}\sigma_{0l'}}-1)}{N_{1l}(c)N_{0l'}(c)}\\
&\times\sin\omega\,S_{1l}(c,\cos\omega)S_{0l'}(c,\cos\omega)\,d_n(c|1,l)\Bigg(\frac{(n+1)(n+2)}{(2n+3)(2n+5)}\\
&\times d_{n+2}(c|0,l')-\frac{(n+1)(n+2)}{(2n+1)(2n+3)}d_n(c|0,l')\Bigg)\Bigg\}.
\end{aligned} \tag{3.3}$$

To average over a random distribution of the target axes, one requires almost identical

manipulations. The final result is given by

$$\left\langle \sum_t \right\rangle = \frac{\pi}{P^2} \sum_{l,m} \Bigg\{ 2(2-\delta_{m0}) \sin^2 \sigma_{ml}$$
$$+ \sum_n{}' \sum_N{}' \sum_{l'} \Bigg[\frac{(2m+n)!(2m+N)!(2-\delta_{m0})(e^{2i\sigma_{ml}}-1)}{(2m+2n+1)(2m+2N+1)n!N!N_{ml}(c)} d_n(c|m,l) d_N(c|m,l)$$
$$\times \Bigg(\frac{2(e^{-2i\sigma_{ml'}}-1)}{N_{ml'}(c)} D_1(n)D_1(N) + \frac{(e^{-2i\sigma_{m+1,l'}}-1)}{N_{m+1,l'}(c)} D_2(n)D_2(N)$$
$$+ \frac{(e^{-2i\sigma_{m-1,l'}}-1)(2-\delta_{m-1,0})}{2N_{m-1,l'}(c)} D_3(n)D_3(N) \Bigg) + \frac{(e^{2i\sigma_{0l}}-1)(e^{-2i\sigma_{1l'}}-1)}{N_{0l}(c)N_{1l'}(c)}$$
$$\times d_n(c|0,l) d_N(c|0,l) D_4(n)D_4(N) + \frac{(e^{2i\sigma_{1l}}-1)(e^{-2i\sigma_{0l'}}-1)}{N_{1l}(c)N_{0l'}(c)}$$
$$\times d_n(c|1,l) d_N(c|1,l) D_5(n)D_5(N) \Bigg] \Bigg\}, \tag{3.4}$$

where

$$D_1(x) = \frac{x}{2m+2x-1} d_{x-1}(c|m,l') + \frac{2m+x+1}{2m+2x+3} d_{x+1}(c|m,l'),$$
$$D_2(x) = \frac{x(x-1)}{2m+2x-1} d_{x-2}(c|m+1,l') - \frac{(2m+x+1)(2m+x+2)}{2m+2x+3} d_x(c|m+1,l'),$$
$$D_3(x) = \frac{1}{2m+2x+3} d_{x+2}(c|m-1,l') - \frac{1}{2m+2x-1} d_x(c|m-1,l'), \tag{3.5}$$
$$D_4(x) = \frac{x(x-1)}{(2x-1)(2x+1)} d_{x-2}(c|1,l') - \frac{(x+1)(x+2)}{(2x+1)(2x+3)} d_x(c|1,l'),$$
$$D_5(x) = (x+1)(x+2) \left(\frac{d_{x+2}(c|0,l')}{(2x+3)(2x+5)} - \frac{d_x(c|0,l')}{(2x+1)(2x+3)} \right).$$

The cross section is thus expressed in terms of the spheroidal phase shifts and the expansion coefficients d_n. Although the expression (3.4) involves multiple summations, its evaluation is not difficult if $c<1$. The coefficients $d_n(c|m,l)$ fall off rapidly as n increases and only a few of them will be required for the calculations. The method of calculating the phase shifts will be our concern in the following sections.

4. A semiclassical method for the phase shifts

Although the averaged differential cross section in the case of an unscreened potential can be obtained only numerically, as has been pointed out in § 2, a direct numerical calculation for the phase shifts may not be very convenient. The solution of the radial equation, even in the absence of a potential, is not a simple function. Moreover, for a given value of l, one has $l+1$ independent radial equations. It will, therefore, be advantageous to look for a suitable approximation method to calculate the phase shifts, particularly when we are obliged to make an approximation to begin with. The simple JWKB approximation has already been used to calculate the binding energies by

Arnold and Bates (1969). A generalised version of the JWKB method, first studied by Miller and Good (1953), and studied by a number of authors (Rosen and Yennie 1964, Lu and Measure 1972, Wald and Lu 1974, Wald *et al* 1975, and Berry and Mount 1972) has been found ideally suited for this purpose. The accuracy of this method has also been studied by Wald *et al* (1975). To summarise the method, let us assume that it is possible to write the radial equation as

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{t_1(y)}{\hbar^2}\right)G(y)=0. \tag{4.1}$$

Consider another equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}s^2}+\frac{t_2(s)}{\hbar^2}\right)U(s)=0, \tag{4.2}$$

which can be solved exactly. We shall call equation (4.2) a 'model equation' for the problem, provided $t_1(y)$ and $t_2(s)$ are similar in the following sense:

(i) They should have the same number of turning points, i.e. for every real physical y_t which makes $t_1(y_t)=0$, there should be a real, physical s_t giving $t_2(s_t)=0$.
(ii) The two functions $t_1(y)$ and $t_2(s)$ must have the same number of extrema.
(iii) They should have similar behaviour near the respective singular points.

If these conditions are satisfied, one looks for a solution

$$G(y)=T(y)U[s(y)], \tag{4.3}$$

where s is considered as a function of y. Substituting the expression (4.3) in equation (4.1) and using (4.2), one gets the consistency conditions:

$$\frac{T'}{T}=-\frac{1}{2}\frac{s''}{s'}, \tag{4.4}$$

and

$$s'^2t_2-t_1=\hbar^2\frac{T''}{T}. \tag{4.5}$$

Condition (4.4) is satisfied by the choice $T=1/\sqrt{s'}$. To satisfy the second condition, we expand both $s(y)$ and $t_2(s)$ in powers of $\hbar^2$ and consider terms up to a given order of $\hbar^2$. Thus, to the zeroth order in $\hbar^2$, the condition is

$$\sqrt{t_2(s)}\,\mathrm{d}s=\sqrt{t_1(y)}\,\mathrm{d}y, \tag{4.6}$$

which, on integration, gives

$$\int_{s_t}^{s}\sqrt{t_2(s)}\,\mathrm{d}s=\int_{y_t}^{y}\sqrt{t_1(y)}\,\mathrm{d}y. \tag{4.7}$$

Bertocchi *et al* (1965), Lu and Measure (1972) and Wald and Lu (1974) have studied the higher-order terms in $\hbar^2$. Thus, to terms of order $\hbar^2$, the consistency condition is

$$\int_{s_t}p_2\,\mathrm{d}s+\tfrac{1}{8}\hbar^2\int_{s_t}\left(\frac{3p_2'^2}{p_2^3}-\frac{2p_2''}{p_2^2}\right)\mathrm{d}s=\int_{y_t}p_1\,\mathrm{d}y+\tfrac{1}{8}\hbar^2\int_{y_t}\left(\frac{3p_1'^2}{p_1^3}-\frac{2p_1''}{p_1^2}\right)\mathrm{d}y, \tag{4.8}$$

where $p_1^2=t_1(y)$ and $p_2^2=t_2(s)$. The integrands in the second term on each side are

divergent at the lower limit of integration. However, as has been pointed out by Bertocchi *et al* (1965), the divergences cancel out in the expression for the phase shift σ_{ml}. The point has been studied in detail by Wald and Lu (1974). If equations (4.1) and (4.3) both describe scattering phenomena, the phase shift corresponding to equation (4.1) can be determined, through the consistency condition, from the known phase shift corresponding to equation (4.2). The method has been applied to some simple cases by Wald and Lu (1974), and Wald *et al* (1975), and the results show fairly good agreement with exact results obtained otherwise. The next two sections will be devoted to the application of this method to the present problem.

5. The choice of a model equation

To study the semiclassical method of calculating the phase shifts, it will be useful to consider a specific example. Let us consider a target consisting of two point charges of strength Qe each, separated by a distance R. Applications to more realistic targets will be considered elsewhere. To write down the radial equation in the form (4.1), we eliminate the first-order derivative term by substituting

$$R_{ml}(c, \xi) = (\xi^2 - 1)^{-1/2} G_{ml}(c, \xi), \tag{5.1}$$

in the radial equation (2.19). This gives

$$\frac{\mathrm{d}^2 G_{ml}(y)}{\mathrm{d}y^2} + \frac{t_1(y)}{\hbar^2} G_{ml}(y) = 0, \tag{5.2}$$

where

$$\frac{t_1(y)}{\hbar^2} = \frac{1}{y^2 - c^2}\left(y^2 - \lambda_{ml}(c) + 2by - \frac{(m^2-1)c^2}{y^2 - c^2}\right), \tag{5.3}$$

with $y = c\xi$ and $b = 2\epsilon\alpha Q/P$. Equation (5.2) is written in a form so that the limit $c \to 0$ (i.e. $R \to 0$) exists and can be taken easily. This corresponds to the scattering from a central charge of strength $2Qe$ and the relevant equation is

$$\frac{\mathrm{d}^2 U_l(s)}{\mathrm{d}s^2} + \frac{t_2(s)}{\hbar^2} U_l(s) = 0, \tag{5.4}$$

where

$$\frac{t_2(s)}{\hbar^2} = 1 + \frac{2b}{s} - \frac{l(l+1)}{s^2}. \tag{5.5}$$

The solution of equation (5.4) is well known. We would, therefore, like to examine the possibility of taking (5.4) as the model equation for our problem. We note the following:

(i) In the asymptotic region, the solution $G_{ml}(y)$ can differ from $U_l(s)$ only by some additional phase. Thus

$$G_{ml}(y) \xrightarrow[y \to \infty]{} \sin(y + b \ln 2y - \tfrac{1}{2}l\pi + \sigma_{ml}), \tag{5.6}$$

and

$$U_l(s) \xrightarrow[s \to \infty]{} \sin(s + b \ln 2s - \tfrac{1}{2}l\pi + \sigma_l). \tag{5.7}$$

(ii) For $l \neq 0$, the function $t_2(s)$ has one real positive root, the classical turning point. The situation with $t_1(y)$ is more complicated. We find three different cases, depending on the value of m:

(*a*) For $m = 1$, the problem is similar to the central Coulomb case.

(*b*) For $m > 1$, the function $t_1(y)$ has four roots, we choose, as an example, $b = 0{\cdot}5$ and $c = 0{\cdot}3$, to locate these roots. Since for $c < 1$, $\lambda_{ml}(c) \sim l(l+1)$, it can be shown that only two of the roots are real and positive. There is, however, only one turning point, the other being less than c (note that $y \geqslant c$). Moreover, $t_1(y)$ has only one maximum beyond its turning point, just as in the corresponding central potential case.

The two functions $t_1(y)$ and $t_2(s)$ have similar behaviour near their singular points. Thus, while the Coulomb function is dominated at the origin by the centrifugal term, the two-centre function is dominated near $y \sim c$ by the 'geometric potential' $V_g = (m^2-1)c^2/(y^2-c^2)^2$. Both are repulsive inverse square potentials.

(*c*) The favourable situation no longer exists if $m = 0$. The term V_g now leads to an attractive inverse square potential near $y \sim c$ and it is well known that for $l = 0$, the solution for such a potential is not bounded at the singular point. The presence of the attractive singular term leads to some complication even for $l \neq 0$. One gets, in general, two turning points, and the Coulomb equation cannot be considered a suitable model equation in this case.

This difficulty can be removed if one introduces Langer's substitution. The motivation for introducing this substitution is well studied (Bertocchi *et al* 1965, Berry and Ozorio de Almeida 1973, Crothers 1976). A simple way to understand the motivation is to note that the JWKB method is based essentially on the classical picture of the motion of a particle in one dimension, where the variable has a spectrum of values from $-\infty$ to $+\infty$. But the variable in the radial equation under consideration has a restricted range (for example, s in (5.4) has a range from 0 to ∞). A correct correspondence can be established if a new variable (e.g. $\ln s$ instead of s) is chosen and the phase relationship is obtained in terms of this new variable. For the two-centre problem, one has to introduce the variable $z = \ln(y-c)$. It is now easy to see that this substitution can cure the bad behaviour of the two-centre problem for $m = 0$. With Langer's substitution, we have, for the two-centre function

$$t_1^{\mathrm{L}}(y) = \frac{1}{y^2-c^2}\left(y^2+2by-\lambda_{ml}(c)-\frac{(m^2-1)c^2}{y^2-c^2}\right)-\frac{1}{4(y-c)^2}, \tag{5.8}$$

so that as $y \to c$,

$$t_1^{\mathrm{L}}(y) \to \left(-\frac{(m^2-1)}{4}-\frac{1}{4}\right)\frac{1}{(y-c)^2}+\mathrm{O}\left(\frac{1}{y-c}\right)+\ldots. \tag{5.9}$$

Thus the offensive inverse square term is cancelled by Langer's counter-term when $m = 0$. Note that for $m \neq 0$, the inverse square singularity is not cancelled, but then the singular term changes sign to become a repulsive potential.

If one introduces Langer's substitution in $t_1(y)$, one must do the same in the corresponding Coulomb case, so that both the variables y and s have the same spectrum of values ($-\infty$ to $+\infty$). This has the additional advantage that the altered Coulomb function $t_2(s)$ for $l = 0$ now develops a real turning point, much to our

advantage. The altered Coulomb function is given by

$$t_2^{\mathrm{L}}(s) = 1 + \frac{2b}{s} - \frac{(l+\frac{1}{2})^2}{s^2}, \tag{5.10}$$

when expressed in terms of the original variable s. It may be pointed out that with Langer's substitution the relation (4.8) is slightly modified. The details will be given in another paper.

When Langer's substitution is made for $m = 0$ and any l, the function $t_1^{\mathrm{L}}(y)$ retains only one real root (instead of two, as discussed earlier), thus eliminating the cumbersome procedure of matching across the turning point. Also, both $t_1^{\mathrm{L}}(y)$ and $t_2^{\mathrm{L}}(s)$ for $m = 0$ show only one maximum beyond the respective turning points. To summarise the situation, we may take the central Coulomb equation as a model equation provided Langer's counter-term is added to both. When $m \neq 0$, the effect of Langer's substitution will be small. Since we are actually determining the difference in the phase shifts, even this small effect will almost be cancelled out. It is, in fact, more convenient to work with the original set of equations and not to invoke Langer's substitution unless necessary, as in the $m = 0$ case. We shall do the same in the next section.

Although we analysed the functions $t_1(y)$ and $t_2(s)$ for the simple case of two fixed point charges and only for a certain range of values of b and c, some of the observations are of more general validity. A realistic target will not give rise to a potential as singular as $1/y^2$ and hence the behaviour near the point $y \sim c$ will still be dominated by the V_g term. The choice of a model equation will, however, depend on the nature of the problem.

6. Phase shifts for scattering from two fixed point charges

As in the previous section, we consider a target consisting of two fixed point charges with $b = 0{\cdot}5$ and $c = 0{\cdot}3$. To zeroth order in $\hbar^2$, the phase shifts can be obtained from relation (4.7), keeping the asymptotic behaviours (5.6) and (5.7) in mind. However, we shall have to extract the typical logarithmic phase term out of both sides of equation (4.7). This can be done in the following way. We choose a large y, say $\tilde{y}$, for which the term $(m^2-1)\, c^2/(y^2-c^2)^2$ becomes negligible compared with the other terms. We can write

$$\int_{y_t}^{y} \sqrt{t_1(y)}\,\mathrm{d}y \simeq \int_{y_t}^{\tilde{y}} \sqrt{t_1(y)}\,\mathrm{d}y + \int_{\tilde{y}}^{y} \frac{1}{y}(y^2+2by-\lambda_{ml})^{1/2}\,\mathrm{d}y. \tag{6.1}$$

The second term, in the limit $y \to \infty$, yields the logarithmic phase term. Thus for $m \neq 0$, we have

$$\begin{aligned}
\sigma_{ml} - \sigma_l &= \lim_{\substack{y\to\infty \\ s\to\infty}} \left(s - y + b \ln \frac{s}{y}\right) \\
&= \sqrt{l(l+1)}\left[\sin^{-1}\left(\frac{b}{\sqrt{b^2+l(l+1)}}\right) + \frac{\pi}{2}\right] \\
&\quad - \sqrt{\lambda_{ml}}\left[\sin^{-1}\left(\frac{b}{\sqrt{b^2+\lambda_{ml}}}\right) - \sin^{-1}\left(\frac{b\tilde{y}-\lambda_{ml}}{\tilde{y}\sqrt{b^2+\lambda_{ml}}}\right)\right]
\end{aligned}$$

$$+b\ln\left(\frac{s_t+b}{\sqrt{\tilde{y}^2+2b\tilde{y}-\lambda_{ml}}+\tilde{y}+b}\right)-\sqrt{\tilde{y}^2+2b\tilde{y}-\lambda_{ml}}+\int_{y_t}^{\tilde{y}}\sqrt{t_1(y)}\,\mathrm{d}y. \qquad (6.2)$$

For $m=0$, the expression for $\sigma_{ml}-\sigma_l^{\mathrm{L}}$ is obtained from (6.2) by replacing s_t by s_t^{L}, y_t by y_t^{L}, $t_1(y)$ by $t_1^{\mathrm{L}}(y)$ and $l(l+1)$ by $(l+\frac{1}{2})^2$. The phase shifts σ_l^{L} can be obtained by applying the same method and are given by, up to terms of order $\hbar^2$,

$$\sigma_l^{\mathrm{L}}=b-(l+\tfrac{1}{2})\sin^{-1}\frac{b}{\sqrt{\beta}}-\frac{b}{2}\ln\beta-\frac{b}{24\beta}, \qquad (6.3)$$

where

$$\beta=b^2+(l+\tfrac{1}{2})^2. \qquad (6.4)$$

To obtain (6.3), we compared the Coulomb radial equation with the free radial equation, after making the Langer substitution. The Coulomb phase shifts are, of course, known exactly, namely

$$\sigma_l=\arg\Gamma(l+1-\mathrm{i}b). \qquad (6.5)$$

Thus, the accuracy of the present method can be checked by comparing (6.3) and (6.5). This has been done in table 1, where some phase shifts for $b=0{\cdot}5$ have been shown. It may be noted that the method reproduces accurately the Coulomb phase shifts, the agreement being excellent beyond $l=2$.

Table 1. Coulomb phase shifts: the exact phase shifts are given by σ_l and those calculated by the present method with Langer's substitution by σ_l^{L} ($b=0{\cdot}5$).

l	σ_l	σ_l^{L}
0	+0·24406	+0·23892
1	−0·21959	−0·22003
2	−0·46457	−0·46464
3	−0·62972	−0·62974
4	−0·75407	−0·75408
5	−0·85374	−0·85374
6	−0·93688	−0·93688
10	−1·17606	−1·17606
15	−1·37059	−1·37059

The knowledge of σ_l now permits us to determine σ_{ml} from the relation (6.2). We chose $b=0{\cdot}5$ and $c=0{\cdot}3$ and evaluated the integrals in (6.2) numerically. Some of these phase shifts, in the zeroth order, are shown in table 2. Some general features of the spheroidal phase shifts may be mentioned here:

(*a*) The phase shift difference $\sigma_{ml}-\sigma_l$ falls off as l increases. Thus in the example considered, $\sigma_{1,1}=-0{\cdot}1940$ and $\sigma_1=-0{\cdot}2196$, while $\sigma_{1,15}=-1{\cdot}3728$ and $\sigma_{15}=-1{\cdot}3706$. This fall is expected also on physical grounds since partial waves with large l cannot probe the region near the origin in detail and are, therefore, insensitive to the deviation of the spherical symmetry caused by a small separation of the two charges.

(*b*) The variation of the phase shifts with m is another novel feature of the two-centre problem. For a large l the phase shifts σ_{ml} are almost m independent and can be replaced by the central potential phase shifts σ_l.

Table 2. The spheroidal phase shifts ($b = 0{\cdot}5$, $c = 0{\cdot}3$).

l	m	$\sigma_{ml} - \sigma_l$	σ_{ml}
0	0	−0·213	+0·031
1	0	−0·043	−0·263
1	1	+0·026	−0·194
2	0	−0·015	−0·479
2	1	+0·003	−0·462
2	2	0·000	−0·465
3	0	−0·008	−0·638
3	1	0·000	−0·630
3	2	−0·001	−0·631
3	3	−0·002	−0·632

In the above, we have not taken into account the first-order correction to the spheroidal phase shifts. The calculation for the correction term involves some technical problems (see Wald *et al* 1975), which will be considered in a following paper. It may be pointed out that the simple JWKB method does not give the values of the spheroidal phase shifts as accurately as is obtained by the present method. The spheroidal phase shifts calculated up to the first-order term in $\hbar^2$ show a dependence on the choice of model equation. Naturally, one has to make the most appropriate choice for the model equation. The ordinary JWKB method involves the choice of a particular model equation for all problems and is, therefore, inadequate for the purpose.

7. Discussion

We can now summarise the method of solving the problem of high-energy electron scattering from a two-centre potential. If the potential is screened, the first step is to calculate the constants $\lambda_{ml}(c)$, $N_{ml}(c)$ and the coefficients $d_n(c|m, l)$ to the desired accuracy. The phase shifts σ_{ml} are determined by the semiclassical method, taking a suitable and solvable model equation. The averaged total cross section is then given by (3.4). To obtain the differential scattering cross section, the averaging must be done numerically. For unscreened potentials, the phase shifts σ_{ml}, however, approach σ_l, the corresponding central Coulomb phase shifts, as l increases and, beyond a certain value of l, one can safely replace σ_{ml} by σ_l. The semiclassical method used to calculate the phase shifts presents a convenient tool to calculate, with remarkable simplicity, the phase shifts for those cases where conventional direct methods are not useful. It is hoped that a variety of non-spherical potentials which appear in various branches of physics, can be studied with this technique. We shall consider some of these in a future publication.

Acknowledgments

One of us (SM) would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. He is grateful to Professor L Bertocchi for useful

discussions and to Dr I Ahmad for his help in the computational work. One of us (SSC) is thankful to University Grants Commission (UGC), New Delhi, for financial assistance.

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