Phase shifts for electron scattering from a two-centre potential

1979 J. Phys. A: Math. Gen. 12 329

(http://iopscience.iop.org/0305-4470/12/3/008)

J. Phys. A: Math. Gen., Vol. 12, No. 3, 1979. Printed in Great Britain

Phase shifts for electron scattering from a two-centre potential

S S Chandel† and S Mukherjee‡

† Department of Physics, Himachal Pradesh University, Simla 171005, India
‡ Department of Physics, North Bengal University, Darjeeling, West Bengal 734430, India

Received 13 January 1978, in final form 17 August 1978

Abstract. The spheroidal phase shifts for high-energy electron scattering from a target consisting of two point charges are calculated by a semiclassical method. The calculations include the contribution of terms linear in $\hbar^2$ for two different model equations, and the results obtained are compared. Some general features of the spheroidal phase shifts are pointed out. The variation of the phase shifts with the separation between the charges is also studied.

1. Introduction

The problem of an electron in a two-centre potential has become the subject of renewed interest (Müller *et al* 1973, Marinov *et al* 1975). In an earlier paper (Mukherjee and Chandel 1978, referred to hereafter as I), we made an attempt to study the scattering of high-energy electrons from a two-centre potential. The Dirac equation with a two-centre potential was reduced to a Schroedinger-like equation with the help of a generalised Sommerfeld–Maue approximation (Mukherjee and Majumdar 1965). The solution of the Dirac equation is then constructed from that of the Schroedinger-like equation. The latter is separable in spheroidal coordinates for a class of potentials. A spheroidal partial wave analysis can now be done. The phase shifts are determined by a generalised JWKB method (Miller and Good 1953, Rosen and Yennie 1964, Lu and Measure 1972, Berry and Mount 1972). We considered as an example a target consisting of a pair of fixed equal point charges. The method essentially consists of comparing the solution of the problem with the known solution of a suitable model equation. The method is ideally suited for our problem, provided an appropriate model equation can be found. We have considered a specific case and have studied the suitability of the radial equation of the central Coulomb field problem as the model equation of our problem. It has been observed that, except for the $m = 0$ cases, the central Coulomb radial equation serves well as the model equation if one restricts oneself to the zeroth-order approximation. The problem with $m = 0$ cases, as well as the divergence difficulties encountered in calculating the first-order correction to the phase shifts, can, however, be solved with the help of Langer's substitution. Some of the relevant points in this connection have already been mentioned in I. The purpose of the present paper is to present some additional results. In particular, the calculations for the first-order correction to the spheroidal phase shifts for a specific case of two equal point charges are given. The dependence of the calculated phase shifts on the choice of the model equation will also be considered. The variation of the phase shifts with the

0305-4470/79/030329+08$01.00

separation between the two point charges will be studied. We shall follow mostly the notations of I and work, as in I, with the prolate spheroidal coordinates (ξ, η, ϕ) defined in (1.1) of I.

2. First-order correction to spheroidal phase shifts

We first consider the effect of Langer's substitution in the radial equations (5.2) and (5.4) of I. We define

$$y - c = e^x \tag{2.1}$$

$$G_{ml}(y) = e^{x/2} F_{ml}(x) \tag{2.2}$$

$$s = e^z \tag{2.3}$$

$$U_l(s) = e^{z/2} F_l(z). \tag{2.4}$$

The radial equations (5.2) and (5.4) of I can be rewritten as

$$d^2F_{ml}(x)/dx^2 + (q_1(x)/\hbar^2)F_{ml}(x) = 0 \tag{2.5}$$

where

$$\frac{1}{\hbar^2} q_1(x) = \frac{e^x}{e^x + 2c}\left(e^{2x} + 2(b+c)\,e^x + 2bc + c^2 - \lambda_{ml}(c) - \frac{(m^2-1)c^2}{e^{2x} + 2c\,e^x}\right) - \frac{1}{4} \tag{2.6}$$

and

$$d^2F_l(z)/dz^2 + (q_2(z)/\hbar^2)F_l(z) = 0 \tag{2.7}$$

with

$$q_2(z)/\hbar^2 = e^{2z} + 2b\,e^z - (l+\tfrac{1}{2})^2. \tag{2.8}$$

In the above, b and c have the same significance as in I, and $\lambda_{ml}(c)$ is the separation constant, whose properties have been studied, in particular, by Stratton *et al* (1956), Flammer (1957) and Mott and Massey (1965). In calculating the phase shifts up to terms of order $\hbar^2$, we follow the semiclassical method of Miller and Good (1953) with the modifications introduced by Wald and Lu (1974). An outline of the method has already been given in § 4 of I. The method consists of comparing the solutions of a pair of equations of the type (4.1) and (4.2) of I. Equation (4.2) is assumed to be exactly solvable. The variable s is now looked upon as a function of y, with the assumption that as $y \to \infty$, $s \to \infty$. The assumption (4.3), the consequent consistency conditions (4.4) and (4.5) of I, and the known form of the functions $t_1(y)$ and $t_2(s)$, both of which tend to 1 asymptotically, as is expected with the radial equation of a physical problem, lead to the determination of the desired phase shifts. With Langer's substitution, we have to deal with the transformed equations (2.5) and (2.7), given above, in the variables x and z respectively, but the method can still be applied in a straightforward manner. The consistency condition which determines the phase shifts is given by

$$\int_{x_t}^{x} p_1\,dx + \frac{\hbar^2}{8}\int_{x_t}^{x}\left(\frac{3p_1'^2}{p_1^3} - \frac{2p_1''}{p_1^2}\right)dx = \int_{z_t}^{z} p_2\,dz + \frac{\hbar^2}{8}\int_{z_t}^{z}\left(\frac{3p_2'^2}{p_2^3} - \frac{2p_2''}{p_2^2}\right)dz \tag{2.9}$$

where $p_1^2(x) = q_1(x)$, $p_2^2(z) = q_2(z)$, and x_t and z_t are the largest real roots of $q_1 = 0$ and

$q_2 = 0$ respectively. The primes indicate the number of times the p_i are differentiated WRT the respective arguments. Since the p_i occur in the denominator, the integrals in the second term on each side appear to be divergent at the lower limit of integration. This apparent divergence may be easily removed in some cases by the method of Bertocchi *et al* (1965) and Wald and Lu (1974). This consists of converting the second integral on each side of (2.9) into a contour integral in the complex x or z plane. The contour is taken from $\infty - i\epsilon$ to $\infty + i\epsilon$ in a clockwise direction around the turning point (avoiding any other complex root). Integrating by parts, we can now eliminate the function from the denominator. One can convert the contour integral back into the definite integral along the real axis to obtain

$$\int_{x_t}^{x} \sqrt{q_1(x)}\,\mathrm{d}x + \frac{\hbar^2}{12}\int_{x_t}^{x} \mathscr{D}[q_1(x)]\sqrt{q_1(x)}\,\mathrm{d}x = \int_{z_t}^{z} \sqrt{q_2(z)}\,\mathrm{d}z + \frac{\hbar^2}{12}\int_{z_t}^{z} \mathscr{D}[q_2(z)]\sqrt{q_2(z)}\,\mathrm{d}z \tag{2.10}$$

where

$$\mathscr{D}[q_i] = \frac{q_i'''}{q_i'^2} - 4\frac{q_i''' q_i''}{q_i'^3} + 3\frac{q_i''^3}{q_i'^4}. \tag{2.11}$$

The integrands in (2.10) have no divergence at the respective turning points. However, a divergence is introduced every time the functions q_i have an extremum beyond the corresponding turning point. In the problem under consideration ($b = 0{\cdot}5$, $c \times 0{\cdot}3$), there is no real point of extremum beyond the classical turning point, and hence the divergence problem is solved up to first order in $\hbar^2$. It may be pointed out that the divergences, even when present, should mutually cancel out, so that a numerical method to cut off the singular point of the integrand may also lead to the correct results (Wald and Lu 1974).

It is convenient to express (2.10) in terms of the old variables y and s:

$$\int_{y_t}^{y} \sqrt{t_1^{\mathrm{L}}(y)}\,\mathrm{d}y + \frac{\hbar^2}{12}\int_{y_t}^{y} \mathscr{D}[\tau_1(y)]\sqrt{t_1^{\mathrm{L}}(y)}\,\mathrm{d}y = \int_{s_t}^{s} \sqrt{t_2^{\mathrm{L}}(s)}\,\mathrm{d}s + \frac{\hbar^2}{12}\int_{s_t}^{s} \mathscr{D}[\tau_2(s)]\sqrt{t_2^{\mathrm{L}}(s)}\,\mathrm{d}s \tag{2.12}$$

where

$$\tau_1(y) = (y-c)^2 t_1^{\mathrm{L}}(y) \tag{2.13}$$

$$\tau_2(s) = s^2 t_2^{\mathrm{L}}(s) \tag{2.14}$$

with $t_1^{\mathrm{L}}(y)$ and $t_2^{\mathrm{L}}(s)$ defined by (5.8) and (5.10) of I. The second integral on the RHS of (2.12) can be written as

$$\int_{s_t}^{s} \mathscr{D}[\tau_2(s)]\sqrt{t_2^{\mathrm{L}}(s)}\,\mathrm{d}s = -\frac{3b}{2}\int_{s_t}^{s} \frac{[s^2 + 2bs - (l+\frac{1}{2})^2]^{1/2}}{(s+b)^4}\,\mathrm{d}s \tag{2.15}$$

which is easily evaluated. The phase shifts σ_{ml} up to terms linear in $\hbar^2$ can now be written as

$$\sigma_{ml} = \sigma_{ml}^{0} + \Delta_{ml} \tag{2.16}$$

where

$$\sigma_{ml}^{0} = \sigma_{l}^{0} + \left(l+\frac{1}{2}\right)\left(\sin^{-1}\frac{b}{[b^2+(l+\frac{1}{2})^2]^{1/2}}+\frac{\pi}{2}\right)$$
$$-\sqrt{\lambda_{ml}}\left(\sin^{-1}\frac{b}{(b^2+\lambda_{ml})^{1/2}}-\sin^{-1}\frac{b\tilde{y}-\lambda_{ml}}{\tilde{y}(b^2+\lambda_{ml})^{1/2}}\right)$$
$$-b\ln\left(\frac{b+\tilde{y}+(\tilde{y}^2+2b\tilde{y}-\lambda_{ml})^{1/2}}{(b^2+(l+\frac{1}{2})^2)^{1/2}}\right)$$
$$-(\tilde{y}^2+2b\tilde{y}-\lambda_{ml})^{1/2}+\int_{y_t}^{\tilde{y}}\sqrt{t_1^{L}(y)}\,dy \tag{2.17}$$

with

$$\sigma_{l}^{c} = \arg\Gamma(l+1-ib) \tag{2.18}$$

and Δ_{ml}, the first-order correction term to the phase shift, is given by

$$\Delta_{ml} = \frac{b}{24[b^2+(l+\frac{1}{2})^2]}+\frac{1}{12}\int_{y_t}^{\infty}\mathscr{D}[\tau_1(y)]\sqrt{t_1^{L}(y)}\,dy. \tag{2.19}$$

$\tilde{y}$ is some large value of y so that the term $(m^2-1)c^2/(y^2-c^2)^2$ can be neglected in comparison with the other terms in $t_1^{L}(y)$. The integral on the RHS of (2.19) can be easily evaluated numerically, the integrand being a rapidly decreasing function of y.

We have shown in table 1 the spheroidal phase shifts calculated from (2.16) for $b=0{\cdot}5$ and $c=0{\cdot}3$. The m dependence of the phase shifts, though small, is an interesting feature of the results. Also, the first-order correction term to the phase

Table 1. The spheroidal phase shifts up to first order in $\hbar^2$ ($b=0{\cdot}5$, $c=0{\cdot}3$).

l	m	σ_{ml}^{0}	Δ_{ml}	σ_{ml}	σ_{l}^{c}
0	0	+0·0323	+0·7658	+0·7981	+0·2441
1	0	−0·2628	+0·0465	−0·2163	−0·2196
1	1	−0·2627	+0·0350	−0·2277	−0·2196
2	0	−0·4795	+0·0151	−0·4644	−0·4646
2	1	−0·4801	+0·0144	−0·4657	−0·4646
2	2	−0·4821	+0·0124	−0·4696	−0·4646
3	0	−0·6377	+0·0073	−0·6304	−0·6297
3	1	−0·6379	+0·0072	−0·6307	−0·6297
3	2	−0·6385	+0·0069	−0·6316	−0·6297
3	3	−0·6394	+0·0064	−0·6330	−0·6297
4	0	−0·7592	+0·0043	−0·7549	−0·7541
4	1	−0·7593	+0·0043	−0·7550	−0·7541
4	2	−0·7595	+0·0042	−0·7553	−0·7541
4	3	−0·7599	+0·0040	−0·7559	−0·7541
4	4	−0·7604	+0·0039	−0·7565	−0·7541
5	0	−0·8573	+0·0028	−0·8545	−0·8537
5	1	−0·8573	+0·0028	−0·8545	−0·8537
5	2	−0·8574	+0·0028	−0·8546	−0·8537
5	3	−0·8576	+0·0027	−0·8549	−0·8537
5	4	−0·8578	+0·0027	−0·8551	−0·8537
5	5	−0·8581	+0·0026	−0·8555	−0·8537

shifts for $l = 0$ is very high. The reason can be seen easily. Because of the particular choice of b and c ($b = 0{\cdot}5$, $c = 0{\cdot}3$), the function $t_1^{\mathrm{L}}(y)$ for $l = 0$ has a root at $y_2 = 0{\cdot}36851$ which is very close to the singular point $y = c = 0{\cdot}3$. The main contribution to the first-order term comes from small values of y. For $l \geqslant 1$ the correction term is small, and it decreases with increasing l.

3. Another model equation

The choice of an appropriate model equation is of considerable importance in the present method. It is therefore desirable to study the dependence of the calculated results on the particular choice of model equation made. This motivated us to repeat the calculations with another model equation, which we choose to be the free-particle radial equation. In spheroidal coordinates, the free-particle radial equation can be written as

$$\frac{\mathrm{d}^2 f_{ml}(z)}{\mathrm{d}z^2} + \frac{Q_2(z)}{\hbar^2} f_{ml}(z) = 0 \tag{3.1}$$

with

$$\frac{Q_2(z)}{\hbar^2} = \frac{\mathrm{e}^z}{\mathrm{e}^z + 2c}\left(\mathrm{e}^{2z} + 2c\,\mathrm{e}^z + c^2 - \lambda_{ml} - \frac{(m^2-1)c^2}{\mathrm{e}^{2z} + 2c\,\mathrm{e}^z}\right) - \frac{1}{4} \tag{3.2}$$

where Langer's substitution has already been made use of. Equation (3.1) satisfies all the requirements of a model equation for the two-centre problem under consideration. We define, as before,

$$s - c = \mathrm{e}^z \tag{3.3}$$

$$T_2^{\mathrm{f}}(s) = (s-c)^{-2} Q_2(z)/\hbar^2 \tag{3.4}$$

and note that $T_2^{\mathrm{f}}(s)$ has only one real physical turning point for all l, m and no extremum beyond that. The phase shifts can be calculated as before. The phase shifts in the zeroth order in $\hbar^2$ are given by

$$\begin{aligned}\sigma_{ml}^{0\mathrm{f}} = b - \sqrt{\lambda_{ml}}\Bigg(&\sin^{-1}\frac{b}{(b^2+\lambda_{ml})^{1/2}} - \sin^{-1}\frac{b\tilde{y} - \lambda_{ml}}{\tilde{y}(b^2+\lambda_{ml})^{1/2}} - \frac{\pi}{2}\Bigg) \\ &- \sqrt{\lambda_{ml}}\cos^{-1}(\sqrt{\lambda_{ml}}/\tilde{s}) - b\ln[b + \tilde{y} + (\tilde{y}^2 + 2b\tilde{y} - \lambda_{ml})^{1/2}] \\ &- (\tilde{y}^2 + 2b\tilde{y} - \lambda_{ml})^{1/2} + (\tilde{s}^2 - \lambda_{ml})^{1/2} + \int_{y_t}^{\tilde{y}} \sqrt{t_1^{\mathrm{L}}(y)}\,\mathrm{d}y - \int_{s_t}^{\tilde{s}} \sqrt{T_2^{\mathrm{f}}(s)}\,\mathrm{d}s. \end{aligned} \tag{3.5}$$

where $\tilde{y}$ and $\tilde{s}$ are some suitably chosen large values of y and s respectively. Note that there is no s-dependent logarithmic phase term in this case. The integrals in (3.5) are evaluated numerically.

The first-order correction to the lowest-order results is given by

$$\Delta_{ml}^{\mathrm{f}} = \tfrac{1}{12}\int_{y_t}^{\infty} \mathscr{D}[\tau_1(y)]\sqrt{t_1^{\mathrm{L}}(y)}\,\mathrm{d}y - \tfrac{1}{12}\int_{s_t}^{\infty} \mathscr{D}[\tau_2(s)]\sqrt{T_2^{\mathrm{f}}(s)}\,\mathrm{d}s. \tag{3.6}$$

The integrals involve long expressions and require numerical evaluation. The expressions occurring in the second integral can, however, be obtained easily by putting $b = 0$

and changing y to s. The corrected phase shifts

$$\sigma^{f}_{ml} = \sigma^{0f}_{ml} + \Delta^{f}_{ml} \tag{3.7}$$

are shown in table 2, where the results obtained with the Coulomb radial equation as the model equation are also shown for the sake of easy comparison. It is interesting to note that, whereas the lowest-order phase shift and the correction term separately are quite different in the two cases, the corrected phase shifts show fairly good agreement with each other. It may be pointed out that the accuracy of the results obtained depends to a great extent on the similarity of the 'potentials' in the two equations, the given problem, and the model equation. Thus, when b is small, perhaps both the free-particle equation and the Coulomb equation are equally good as a model equation for the two-centre problem. For large b, the Coulomb radial equation will naturally be a better choice.

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

l	m	σ^{0f}_{ml}	Δ^{f}_{ml}	σ^{f}_{ml}	σ_{ml}
0	0	+0·2068	+0·5737	+0·7805	+0·7981
1	0	−0·2201	+0·0100	−0·2101	−0·2163
1	1	−0·2285	+0·0028	−0·2257	−0·2277
2	0	−0·4629	+0·0008	−0·4621	−0·4644
2	1	−0·4640	+0·0005	−0·4635	−0·4657
2	2	−0·4673	−0·0004	−0·4677	−0·4696
3	0	−0·6285	−0·0001	−0·6286	−0·6304
3	1	−0·6288	−0·0002	−0·6290	−0·6307
3	2	−0·6296	−0·0003	−0·6299	−0·6316
3	3	−0·6310	−0·0005	−0·6315	−0·6330

4. Discussion

We have presented in this paper the results of a semiclassical calculation for phase shifts for high-energy electron scattering from a two-centre potential (two fixed point charges). Some general features of these phase shifts studied in I remain true qualitatively even when the first-order correction calculated in this paper is introduced. The small dependence of σ_{ml} on m, however, is sensitive to the correction term. In general, the difference $|\sigma_{ml} - \sigma_l|$ increases slightly as m increases. For large values of l, the m dependence is almost washed out, as expected, and one can replace σ_{ml} by the central Coulomb phase shift σ_l. However, the particular value of l beyond which this can be done depends on b and c, i.e. the separation R, the strength of the two charges, and the energy of the incident electron.

It is interesting to note the variation of σ_{ml} with the internuclear distance R, holding other parameters constant. We have shown in figure 1 the variation of σ_{ml} (for $l = 3$) with R for a 50 MeV electron beam, with $b = 0{\cdot}5$. As the separation between the two charges is made to vanish, σ_{ml} tends towards the central Coulomb phase shift σ_l. With a change in scale, the same figure will exhibit the energy dependence of the phase shifts for a fixed separation.

We have presented in this paper, and in I, a simple method of studying the problem of high-energy electron scattering from a two-centre potential. The first part of the

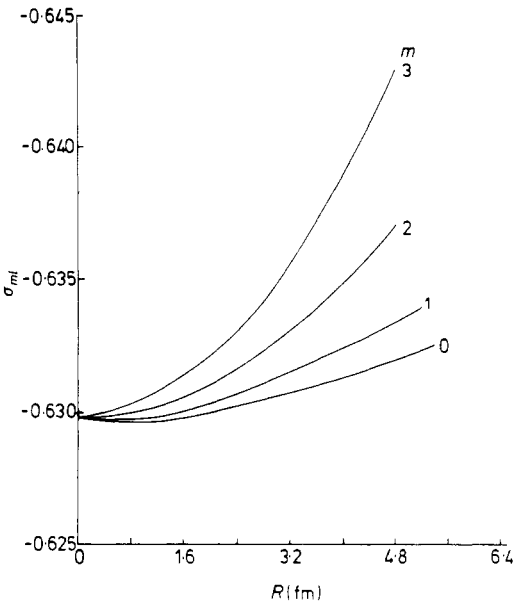

Figure 1. Variation of σ_{ml} with R for a 50 MeV electron beam, with $b = 0{\cdot}5$.

method involves the reduction of the problem to a Schroedinger-like radial equation by an approximation, and has been studied in detail in I. The second part involves the use of a modified JWKB method and calls for some explanation. As pointed out in I, with the semiclassical method we could avoid considerable calculation, involved in a direct numerical method to determine the phase shifts, without any significant loss of accuracy attainable by our method. The method, however, may not be useful for every two-centre problem, because a simple and solvable model equation may not be available. A complicated two-centre function $t_1(y)$, with many turning points, may make a semiclassical approach too complicated, if not impossible. A direct numerical method will be the only way out in those cases. Given a two-centre potential, it will therefore be useful first to locate the zeros and the extrema of the two-centre function $t_1(y)$ to see if a suitable model equation is readily available or not.

Acknowledgment

One of us (SSC) would like to acknowledge the financial assistance from the University Grants Commission, New Delhi, in the form of a Junior Research Fellowship.

References

Berry M V and Mount K E 1972 *Rep. Prog. Phys.* **35** 315
Bertocchi L, Fubini S and Furlan G 1965 *Nuovo Cim.* **35** 599–632
Flammer C 1957 *Spheroidal Wave Functions* (Stanford: Stanford University Press)
Langer R E 1937 *Phys. Rev.* **51** 669
Lu P and Measure E M 1972 *Phys. Rev.* D **5** 2514–8
Marinov M S, Popov V S and Stolin V L 1975 *J. Comput. Phys.* **19** 241–56

Miller S C and Good R H Jr 1953 *Phys. Rev.* **91** 174–9
Mott N F and Massey H S W 1965 *The Theory of Atomic Collisions* 3rd edn (London: Oxford University Press)
Mukherjee S and Chandel S S 1978 *J. Phys. A: Math. Gen.* **11** 1257–70
Mukherjee S and Majumdar S D 1965 *Ann. Phys., Lpz.* **16** 360–9
Müller B, Rafelski J and Greiner W 1973 *Phys. Lett.* B **47** 5–7
Rosen M and Yennie D R 1964 *J. Math.* **5** 1505–15
Stratton J A, Morse P M, Chu L J, Little J D C and Corbato F J 1956 *Spheroidal Wave Functions* (New York: Wiley)
Wald S S and Lu P 1974 *Phys. Rev.* D **9** 2254–8