Company, Cleveland, Ohio, 1970). For polyatomic molecules, binding energies were calculated on the assumption of the now fairly well established value of 170 kcal/mole for the heat of sublimation of carbon from data on heats of combustion and vapor pressures given in the latter reference.

[6]The author's mass-synchrometer values of excesses and differences involving the chlorine isotopes have been excluded as being so much in error (presumably because of kinetic energy effects) as not to fall within the ranges of the plots of Figs. 4 and 5. Also excluded is the value $H_2 - D = 1\,553\,100 \pm 10\,300$ nu of Ref. O, M '63. Errors of combinations of mass table values are calculated without regard to their correlations and hence are somewhat larger than if correlations were taken into account.

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Approximation to the Relativistic Scattering Problem

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We extend the calculation of the relativistic phase-shift problem, as given before, to second order in $\hbar$ by means of Miller and Good's modified WKB method. The scheme of Bertocchi, Fubini, and Furlan is used to avoid the divergences introduced in the second-order terms. The example indicates that the phase shifts are greatly improved at lower angular quantum numbers.

1. INTRODUCTION

This note is written to report some improvements over a previous paper[1] that result from taking into account the second-order contributions in $\hbar$. We use Miller and Good's[2] modified WKB method, choosing a solved problem to approximate the unsolved problem. The second-order terms were given in a previous paper.[3] However, they are divergent at the lower limit. This divergent property at the lower limit for the high-order terms in $\hbar$ is not new. It was discussed in the paper of Bertocchi, Fubini, and Furlan[4] for the high-order terms in the ordinary WKB problem. They succeeded in avoiding the difficulty by means of contour integrals. In Sec. II, we discuss this in detail.

As an example, in Sec. III, we choose a point nucleus together with the pure Coulomb potential as the solved problem. We then solved for the phase shifts in a supposedly unsolved problem with another potential – for example, the shell distribution for the same amount of nuclear charge. These potentials are chosen for illustrative purposes. A comparison can readily be made with the numerical values for the phase shifts given by Ravenhall and Yennie.[5] In Ref. 1, the uniform distribution of the nuclear charge was used as the solved part, and the shell distribution as the unsolved part. Because these two distributions are remarkably similar, our lowest-order-in-$\hbar$ approach did yield some meaningful results. These results agree to the third decimal place for the phase shifts with the numerical ones, which are accurate to the fifth decimal place. In the problem considered here, however, the agreement for the lowest order in $\hbar$ is less good, especially for the first few phase shifts where the angular momentum quantum number is small. By carrying the calculation to the second order in $\hbar$, we see that substantially better agreement can be achieved. This fact actually is independent of the particular example chosen.

2. GENERAL THEORY OF THE RELATIVISTIC SCATTERING PROBLEM

From the Dirac radial equations at the high-energy limit, by taking the rest mass to be zero, we get

$$\frac{d}{dr}u - \frac{l+1}{r}u - \frac{W-V(r)}{\hbar c}v = 0\ , \tag{1a}$$

$$\frac{d}{dr}V + \frac{l+1}{r}v + \frac{W-V(r)}{\hbar c}u = 0\ . \tag{1b}$$

In the notation of Rosen and Yennie, these equations become

$$\frac{d}{dr}M = \frac{f(r)}{\hbar}N\ , \tag{2a}$$

$$\frac{d}{dr}N = \frac{-g(r)}{\hbar}M\ , \tag{2b}$$

with

$$M = u + v, \quad N = u - v\ ,$$

and

$$f(r)=\frac{(l+1)\hbar}{r}-\frac{W-V(r)}{c}, \quad g(r)=-\frac{(l+1)\hbar}{r}-\frac{W-V(r)}{c}.$$

We will solve the above set of equations for the scattering phase shifts using the known solutions of the following set of equations, which are solved by means of either a numerical method or other kinds of approximations:

$$\frac{d}{dS}M_0=\frac{f_0(S)}{\hbar}N_0, \tag{3a}$$

$$\frac{d}{dS}N_0=-\frac{g_0(S)}{\hbar}M_0, \tag{3b}$$

with $f_0(S)=(l+1)\hbar/S-[W-V_0(S)]/c$ and $g_0(S)=-(l+1)\hbar/S-[W-V_0(S)]/c$. In comparison with what we have done in Ref. 1, here we only require that $V_0(S)$ should be reasonably close to $V(r)$. The calculation is then carried to the second order, where use is made of the formula[3]:

$$\int_{r_0}^{r}[(fg)^{1/2}+\hbar^2\{f,g\}]=\int_{S_0}^{S}[(f_0g_0)^{1/2}+\hbar^2\{f_0,g_0\}]\,dS. \tag{4}$$

With the following definitions:

$$\{f,g\}\equiv\frac{2F'-F^2}{8(fg)^{1/2}}+\frac{1}{8(fg)^{1/2}}\left[3\left(\frac{1}{(fg)^{1/2}}\frac{d}{dr}(fg)^{1/2}\right)^2-2\left(\frac{1}{(fg)^{1/2}}\frac{d^2}{dr^2}(fg)^{1/2}\right)\right],$$

$$\{f_0,g_0\}\equiv\frac{2G'-G^2}{8(f_0g_0)^{1/2}}+\frac{1}{8(f_0g_0)^{1/2}}\left[3\left(\frac{1}{(f_0g_0)^{1/2}}\frac{d}{dS}(f_0g_0)^{1/2}\right)^2-2\left(\frac{1}{(f_0g_0)^{1/2}}\frac{d^2}{dS^2}(f_0g_0)^{1/2}\right)\right],$$

and

$$F=\frac{1}{f}\frac{df}{dr}, \quad G=\frac{1}{f_0}\frac{df_0}{dS}.$$

The upper limit r will eventually be pushed to infinity for the scattering case discussed here. And because of this the upper limit S will also go to infinity. This can easily be seen by performing the integration to the lowest order in $\hbar$ for two closely similar potentials. However, for the present, we consider it to be finite but large. Here r_0 and S_0 are the turning points of the problem under consideration, or $f(r_0)=0$, $f_0(S_0)=0$. So the higher-order terms diverge at these lower limits individually. However, since they are higher-order terms, their algebraic sum should be a finite value. This condition holds for the conventional WKB approximation in accordance with Bertocchi *et al.* (Sec. 3.4 of Ref. 4). We generalize the concept here and ask that although these high-order terms diverge themselves, they should yield a finite difference in general. The result, then, is equivalent to taking the contour integral as shown in Fig. 1 together with the formula given below. In so doing we have the advantage that the integrals are already finite before the subtraction and their difference has the value that we want. This replacement may have some deeper significance so that one might say that the contour integral might be more basic than the definite integral given in Eq. (4). Now it may be better to regard this as a postulate. We wish to know whether this postulate is reasonable. In fact, it seems to be; for we can obtain numerical improvements for the phase shifts for some specific chosen potentials, as shown in the next section. We have, then,

$$\int_{r_0}^{r}(fg)^{1/2}dr+I_1=\int_{S_0}^{S}(f_0g_0)^{1/2}dS+I_2, \tag{5}$$

with

$$I_1=\frac{\hbar^2}{2}\int_{C_1}\{f,g\}\,dr$$

and

$$I_2=\frac{\hbar^2}{2}\int_{C_1'}\{f_0,g_0\}\,dS.$$

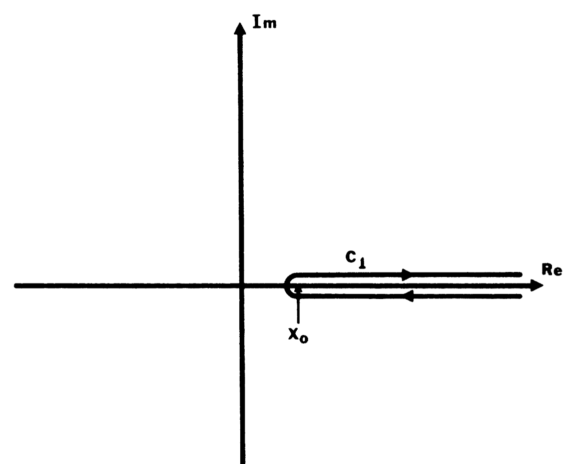

FIG. 1. The integration path C_1 or C_1'.

Here the contour integrals C_1, C_1' are around the turning points, respectively, and going from infinity to infinity (Fig. 1). The assumption made here is that the potentials used are analytic inside the contour C_1 or C_1'. The validity of Eq. (5) was demonstrated in its application to a specific problem.[6] In the example chosen in the next section, we used the shell distribution of the nuclear charge as the unsolved part. The resulting potential will be piece wise continuous. Let the discontinuity of the potential be at distance R from the origin, and let $\int_{C_2}$ indicate the integration along the path C_2 which is given in Fig. 2. It is a path like C_1 but does not extend to infinity; it ends at R around the turning point and with the upper and lower parts of the real axis, i.e., C_2 is the portion of C_1 lying to the left of R. The second-order term, which has a discontinuity at R, can be written as:

$$I_1=\frac{\hbar^2}{2}\int_{C_2}\{f,g\}dr+\hbar^2\int_R^r\{f_0,g_0\}dS$$
$$=\frac{\hbar^2}{2}\left(\int_{C_2}\{f,g\}dr-2\int_R^r\{f,g\}dr\right) \tag{6}$$
$$+\hbar^2\int_R^r\{f_0,g_0\}dS,$$

where f, g contain V_c, where $V_c=-Ze^2/R$, a constant differing from zero. What we have done above is to insure that the integrand of the contour integral $\int_{C_1}\{f,g\}dr$ is analytic. Notice that we extend the integration to infinity (path C_1) and then the additional parts are to be subtracted. To obtain a convergent integral, we repeatedly apply the following formula:

$$\int_{\infty-i\epsilon}^{\infty+i\epsilon}udv=-\int_{\infty-i\epsilon}^{\infty+i\epsilon}vdu+uv\Big|_{\infty-i\epsilon}^{\infty+i\epsilon}. \tag{7}$$

By denoting the phase-shift difference by $\Delta\delta=\delta_r-\delta_S$, we have

$$\Delta\delta=\lim_{r\to\infty}\left(\frac{W}{\hbar c}(S-r)+\frac{Ze^2}{\hbar c}(\ln 2S-\ln 2r)\right). \tag{8}$$

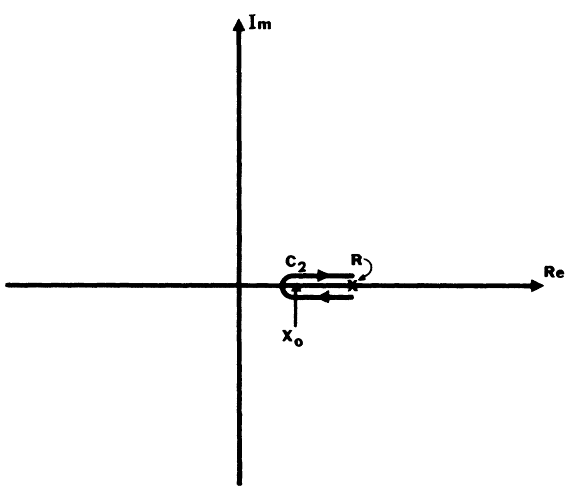

FIG. 2. The integration path C_2.

3. COMPARISON OF THE PHASE SHIFTS FOR THE SHELL DISTRIBUTION OF NUCLEAR CHARGE WITH THE PHASE SHIFTS FOR POINT DISTRIBUTION OF NUCLEAR CHARGE

Here we choose the phase shifts of the shell distribution of the nuclear charge as the unsolved part. We are going to solve for these phase shifts using those of the point distribution as the solved part. Ravenhall and Yennie give numerical values of the phase shifts for both of these distributions for a set of parameters. This choice is made for two reasons. The first one is that in both sides the differences between the phase shifts can be integrated out and expressed in terms of simple functions. They are easier to handle and they exhibit the properties that we want without necessary complications in mathematics. The second reason is that from the charge distribution we see that the phase shifts will be greatly improved if we include the contributions of second order in $\hbar$. Or in other words, the second-order terms are important, especially in those places where the angular quantum numbers are small. We only calculate, therefore, the cases corresponding to the small angular momentum numbers, or $l=0, 1, 2$ cases are reported in Table I. We see that there is also an upper limit for the l value. Since the assumed shell distribution of charge has a radius of shell R, the incident particle can only feel the Coulomb part if the impact parameter is greater than R. However, before this limit is reached, we may have to include some higher-order terms

TABLE I. Phase shifts for scattering from gold.

l	0	1	2
δ_1 [a]	−0.774 71	−0.820 86	−0.848 44
δ_2 [b]	−0.822 10	−0.831 37	−0.850 86
δ [c]	−0.820 06	−0.832 53	−0.855 21
δ_3 [d]	+0.407 36	−0.237 97	−0.533 03

[a] Phase shifts by the lowest-order calculation for shell distribution of the nuclear charges with $WR/\hbar c=5.6$, where R is the boundary of the shell.

[b] Corresponding phase shifts including the $\hbar^2$ order terms.

[c] Numerical data as given by Ravenhall and Yennie.

[d] Input data corresponding to the point-nucleus cases as given by Ravinhall and Yennie.

than $\hbar^2$ to get a closer check. This includes of course the small angular momentum quantum numbers too. But we can see that there is a large contribution to the phase shift at small values of l due to the $\hbar^2$ terms without carrying out the calculations in detail. Therefore, we can conclude from this example that the inclusion of the $\hbar^2$ terms is important especially when the potentials are less similar.

Below is a brief account of the results that lead to such a conclusion. To the lowest order, we see that

$$\int_{r_0}^{r}(fg)^{1/2}dr=\int_{S_0}^{S}(f_0g_0)^{1/2}dS\ . \tag{9}$$

If we let r stand for the radial distance of the shell distribution of charge in a nucleus and S stand for that of the point nucleus, and let R be the radius of the shell, the above equation will read

$$\int_{r_0}^{R}(fg)^{1/2}dr+\int_{R}^{r}(f_0g_0)^{1/2}dr=\int_{S_0}^{S}(f_0g_0)^{1/2}dS\ . \tag{10}$$

We then have the following formulas:

$$\int_{S_0}^{S}(f_0g_0)^{1/2}dS=\hbar\int_{S_0}^{S}\left[\left(\frac{W}{\hbar c}+\frac{Ze^2}{\hbar c}\frac{1}{S}\right)^2-\left(\frac{l+1}{S}\right)^2\right]^{1/2}dS$$
$$=\hbar\left[\frac{W}{\hbar c}S+\frac{Ze^2}{\hbar c}\ln\left(\frac{2WS}{\hbar c}\right)+A_1\right], \tag{11}$$

where

$$A_1\equiv\frac{Ze^2}{\hbar c}\left[1-\ln(l+1)\right]-\left[(l+1)^2-\left(\frac{Ze^2}{\hbar c}\right)^2\right]^{1/2}\left\{\frac{\pi}{2}+\tan^{-1}\frac{Ze^2/\hbar c}{[(l+1)^2-(Ze^2/\hbar c)^2]^{1/2}}\right\},$$

$$\int_{r_0}^{R}(fg)^{1/2}dr=\hbar\int_{r_0}^{R}\left[\left(\frac{W}{\hbar c}+\frac{Ze^2}{\hbar c}\frac{1}{R}\right)^2-\left(\frac{l+1}{r}\right)^2\right]^{1/2}dr$$
$$=\hbar\left\{\left[\left(\frac{WR}{\hbar c}+\frac{Ze^2}{\hbar c}\right)^2-(l+1)^2\right]-(l+1)\tan^{-1}\frac{[(WR/\hbar c+Ze^2/\hbar c)^2-(l+1)^2]^{1/2}}{l+1}\right\}$$
$$\equiv\hbar A_2\ ; \tag{12}$$

and

$$\int_{R}^{r}(f_0g_0)^{1/2}dr=\hbar\int_{R}^{r}\left[\left(\frac{W}{\hbar c}+\frac{Ze^2}{\hbar c}\frac{1}{r}\right)^2-\left(\frac{l+1}{r}\right)^2\right]^{1/2}dr$$
$$=\hbar\left[\frac{W}{\hbar c}r+\frac{Ze^2}{\hbar c}\ln\left(\frac{2Wr}{\hbar c}\right)+A_3\right], \tag{13}$$

where

$$A_3\equiv\frac{Ze^2}{\hbar c}-\left[(l+1)^2-\left(\frac{Ze^2}{\hbar c}\right)^2\right]^{1/2}\tan^{-1}\left[\frac{Ze^2/\hbar c}{[(l+1)^2-(Ze^2/\hbar c)^2]^{1/2}}\right]-\left[\left(\frac{WR}{\hbar c}\right)^2+\frac{2WZe^2}{(\hbar c)^2}R-(l+1)^2+\left(\frac{Ze^2}{\hbar c}\right)^2\right]^{1/2}$$
$$-\frac{Ze^2}{\hbar c}\left(\ln\left\{\left[\left(\frac{WR}{\hbar c}+\frac{Ze^2}{\hbar c}\right)^2-(l+1)^2\right]^{1/2}+\frac{WR}{\hbar c}+\frac{Ze^2}{\hbar c}\right\}\right)$$
$$+\left[(l+1)^2-\left(\frac{Ze^2}{\hbar c}\right)^2\right]^{1/2}\tan^{-1}\left\{\frac{(WR/\hbar c)(Ze^2/\hbar c)-(l+1)^2+(Ze^2/\hbar c)^2}{[(l+1)^2-(Ze^2/\hbar c)^2]^{1/2}[(WR/\hbar c+Ze^2/\hbar c)^2-(l+1)^2]^{1/2}}\right\}.$$

To the order of $\hbar^2$, we evaluate the integrations involved in the following way: There is no problem in evaluating the point-charge side, since

$$I_2=\frac{\hbar}{16}\int_{C_1'}dS\frac{(W/\hbar c)(l+1)}{[(WS/\hbar c+Ze^2/\hbar c)^2-(l+1)^2]^{5/2}}\left\{-4\left(\frac{W}{\hbar c}\right)^2S^2-\frac{W}{\hbar c}\left((l+1)+\frac{2Ze^2}{\hbar c}\right)S-2\left[(l+1)^2-\left(\frac{Ze^2}{\hbar c}\right)^2\right]\right\}, \tag{14}$$

where the integral C_1' is evaluated above and below the real axis around the turning point $X_0=(l+1-Ze^2/\hbar c)/(W/\hbar c)$ and the connection of the other end will be made at infinity (Fig. 1). In so doing, we have

$$I_2=\frac{\hbar}{2}\left((l+1)^2\frac{Ze^2}{\hbar c}\,\frac{1}{8}-\frac{3}{4}(l+1)^3\right)\oint\frac{dY}{[Y^2-(l+1)^2]^{5/2}}$$

$$=\frac{\hbar}{2}\left((l+1)^2\frac{Ze^2}{\hbar c}\frac{1}{8}-\frac{3}{4}(l+1)^3\right)\oint\frac{dY}{Y^4[Y^2-(l+1)^2]^{1/2}}\,, \tag{15}$$

with

$$\oint\frac{dY}{Y^4[Y^2-(l+1)^2]^{1/2}}=\frac{4}{3}\,\frac{1}{(l+1)^4} \tag{16}$$

around the turning point. It is easy to see that, since there is no problem of divergence, on the other side we have

$$\lim_{r\to\infty}\hbar\int_R^r\{f,g\}\,dr=\lim_{r\to\infty}\int_R^r dr\,\frac{W'(l+1)/\hbar c}{[(W'r/\hbar c)^2-(l+1)^2]^{5/2}}\left[-4\left(\frac{W'}{\hbar c}\right)^2 r^2-\frac{W'}{\hbar c}(l+1)r-2(l+1)^2\right]$$

$$=\frac{-3(l+1)^3}{4}\int_{(WR/\hbar c)+(Ze^2/\hbar c)}^{\infty}\frac{dY}{[Y^2-(l+1)^2]^{5/2}}+\frac{1}{2(l+1)}$$

$$-\frac{(WR/\hbar c)+(Ze^2/\hbar c)}{2(l+1)\{[(WR/\hbar c)+(Ze^2/\hbar c)]^2-(l+1)^2\}^{1/2}}-\frac{(l+1)^2}{24}\,\frac{1}{\{[(WR/\hbar c)+(Ze^2/\hbar c)]^2-(l+1)^2\}^{3/2}}\,, \tag{17}$$

where $W'=W+Ze^2/R$, and the lower limit of the integration is

$$Y=\left(\frac{W-V_c}{\hbar c}\right)R=\frac{WR}{\hbar c}+\frac{Ze^2}{\hbar c},\qquad \text{with } V_c=-\frac{Ze^2}{R}\;.$$

Thus,

$$\lim_{r\to\infty}\hbar\int_R^r\{f_0,g_0\}\,dr=\left(\frac{(l+1)^2}{8}\,\frac{Ze^2}{\hbar c}-\frac{3(l+1)^3}{4}\right)\int_{(WR/\hbar c)+(Ze^2/\hbar c)}^{\infty}\frac{dY}{[Y^2-(l+1)^2]^{5/2}}+\frac{1}{2(l+1)}$$

$$-\frac{(WR/\hbar c)+(Ze^2/\hbar c)}{2(l+1)[(WR/\hbar c+Ze^2/\hbar c)^2-(l+1)^2]^{1/2}}+\frac{(l+1)[(6Ze^2/\hbar c)-(l+1)]}{24[(WR/\hbar c+Ze^2/\hbar c)^2-(l+1)^2]^{3/2}}\;. \tag{18}$$

The contour integral simply leads to

$$\hbar\int_{C_1}\{f,g\}\,dr=-\frac{3(l+1)^3}{4}\oint\frac{dY}{[Y^2-(l+1)^2]^{5/2}}$$

$$=-1/(l+1)\,, \tag{19}$$

where we have used Eq. (16). Notice here C_1 and C_1' are actually the same curve. The phase shifts for specifically chosen parameters, calculated here together with those given by Ravenhall and Yennie are shown in Table I. We see that we have

$$\Delta\delta=\delta_r-\delta_S$$

$$=-A_1+A_2+A_3+I_1/\hbar-I_2/\hbar\;. \tag{20}$$

And indeed we have substantial improvement here.

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