Generalization of the Modified WKB Approximation for Phase Shifts

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A generalization of the modified WKB method proposed by Good and by Rosen and Yennie as applied to the scattering problem is presented. In the formulation of this problem the main equation connects two parts, the solved part and the part to be solved. We consider not only the case where the radical wave function of the solved part has the form of the three-dimensional free-particle solution, as is done by the authors mentioned above, but also where it has the form given by an explicit solution with a known potential. The closer the resemblance between the potentials of the unsolved and the solved parts, the better the result is.

1. INTRODUCTION

THIS note is a generalization of the work by Miller and Good[1] to the three-dimensional phase-shift problem. The formulation in that paper was limited to the problems of a one-dimensional bound state and tunneling through the one-dimensional barrier. In particular, it was pointed out that the ordinary WKB method takes a one-dimensional free-particle solution as its basis. The three-dimensional phase-shift problem was treated by Good[2] and later by Rosen and Yennie[3] by choosing the three-dimensional free-particle solution instead of the one-dimensional free-particle solution as the solved part in the WKB approximation. A treatment of the three-dimensional phase-shift problem in the spirit of Miller and Good seems not to have been made as yet. This note is intended to supply some information on the question.

TABLE I. Phase shifts for scattering from gold.

l	(a)	(b)	(c)
0	−0.82006	−0.82032	−0.83553
1	−0.83525	−0.83268	−0.85289
2	−0.85521	−0.85369	−0.88136
3	−0.88041	−0.88518	−0.92116
4	−0.92664	−0.92823	−0.97034

[a] Numerical data for shell distribution of the nuclear charges with $WR/\hbar c = 5.6$, where R is the boundary of the shell as given in Ref. 4.
[b] Numerical data from this method, the δ_r.
[c] Input data as given in Ref. 4, the δ_g.

The solved part need not be the free-particle solution. It may be any solvable problem. For the calculation to be successful, the unknown part should be as close to the known part as possible. In Sec. 2 a general criterion for success is developed.

The phase shifts from a supposedly unknown part (e.g., the shell distribution of the nuclear charges) are calculated from those of the known part (e.g., the uniform distribution). Ravenhall and Yennie[4] have reported numerically calculated phase shifts for all of these potentials, so a comparison can be made easily. Even though we only consider the contribution of the lowest order, our results for the phase shifts agree with those given by Ravenhall and Yennie to within a few parts in a thousand. The agreement can be made better if we go to a higher order of approximation. However, in order to keep the illustration simple, we shall not do so.

2. RELATIONSHIP BETWEEN TWO SETS OF PHASE SHIFTS OF TWO DIFFERENT POTENTIALS

We start from the Dirac radial functions at the high-energy limit by neglecting the rest-mass term:

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

$$\frac{d}{dr}G+\frac{l+1}{r}G+\frac{W-V(r)}{\hbar c}F=0. \tag{2}$$

Following the development in Rosen and Yennie, we get

$$(d/dr)M=[f(r)/\hbar]N, \tag{3}$$

$$(d/dr)N=-[g(r)/\hbar]M, \tag{4}$$

with $M(r)=F(r)+G(r)$, $N(r)=F(r)-G(r)$, and

$$f(r)=[(l+1)\hbar/r]-[W-V(r)/C],$$

$$g(r)=-[(l+1)\hbar/r]-[W-V(r)/C].$$

The above is the problem to be solved. We have, however, the following set of equations with potential V_0, which is already solved by either numerical integration or by some other approximations:

$$\frac{dM_0}{dS}=\left(\frac{(l+1)\hbar}{S}-\frac{W-V_0}{C}\right)\frac{N_0}{\hbar}\equiv\frac{f_0(S)}{\hbar}N_0, \tag{5}$$

$$\frac{dN_0}{dS}=\left(\frac{(l+1)\hbar}{S}+\frac{W-V_0}{C}\right)\frac{M_0}{\hbar}\equiv-\frac{g_0(S)}{\hbar}M_0. \tag{6}$$

Here we ask $V_0(S)$ to be close to $V(r)$, and we can recover everything from Rosen and Yennie if we put $V_0(S)=0$. However, in general V_0 is considered as nonzero here. In the example given below, we take the

[1] S. C. Miller, Jr., and R. H. Good, Jr., Phys. Rev. **91**, 174 (1953).
[2] R. H. Good, Jr., Phys. Rev. **90**, 131 (1953).
[3] M. Rosen and D. R. Yennie, J. Math. Phys. **5**, 1505 (1964).
[4] D. G. Ravenhall and D. R. Yennie, Proc. Phys. Soc. (London) **70A**, 857 (1957).

shell distribution of the nuclear charge together with the Coulomb potential outside as the unknown part $V(r)$, and the uniform distribution of the nuclear charge together with the Coulomb part outside as the known part $V_0(S)$. The phase shifts of the unknown part can be found in terms of the phase shift of the known part. The numerical part can be found in the paper by Ravenhall and Yennie.

Following the derivation of Rosen and Yennie, we get, similar to their Eq. (2–11),

$$\int_{S_t}^{S}(-f_0g_0)^{1/2}d\sigma=\int_{r_t}^{r}(-fg)^{1/2}d\zeta \tag{7}$$

with r_t and S_t, respectively, being the turning points given by setting $f(r_t)=0$ and $f_0(S_t)=0$. This is the lowest-order approximation formula. All the discussions in this paper are limited to this order of approximation, to demonstrate the principle and at the same time keep things simple. By denoting the phase-shift difference $\Delta\delta$, we have

$$\Delta\delta=\lim_{r\to\infty}(W/\hbar c)(S-r)+(Z\mid e^2\mid/\hbar c)(\ln 2S-\ln 2r) \tag{8}$$

with $\Delta\delta=\delta_r-\delta_S$, where δ_r is the phase shift to be found and δ_S is the phase shift known already by some other method.

Here we use the phase shifts from numerical integrations in the paper of Ravenhall and Yennie, and we choose the uniform nuclear-charge distribution as the known part and the shell distribution of the nuclear charge as the unknown part. Then comparison is made from the numerical integration data. In Table I we present the results of the calculation. What is given below is a brief account of the formulas used in the modified WKB calculation.

It is easy to derive the expression of the potential for an electron with charge $-e$ inside a homogeneously distributed sphere of charge Ze as

$$V(r)=-(Z\mid e^2\mid/2S_1)[3-(r^2/S_1^2)] \tag{9}$$

with S_1 being the radius of the sphere. The outside potential as $r\geq S_1$ is $V(r)=-Z\mid e^2\mid/r$; the integral on the left side of Eq. (7) becomes

$$\int_{S_t}^{S1}\left\{\left[\frac{W}{\hbar c}+\frac{Z\mid e^2\mid}{2S_1\hbar c}\left(3-\frac{r^2}{S_1^2}\right)\right]^2-\frac{(l+1)^2}{r^2}\right\}^{1/2}dr+\int_{S1}^{S}\left[\left(\frac{W}{\hbar c}+\frac{Z\mid e^2\mid}{\hbar cr}\right)^2-\frac{(l+1)^2}{r^2}\right]^{1/2}dr.$$

Call the first part I_1, which has to be evaluated numerically by a computer. The integral on the other side, for the shell-type distribution is

$$\int_{r_t}^{R}\left[\left(\frac{W-V_c}{\hbar c}\right)^2-\frac{(l+1)^2}{r^2}\right]^{1/2}dr+\int_{R}^{r}\left[\left(\frac{W}{\hbar c}+\frac{Z\mid e^2\mid}{\hbar cr}\right)^2-\frac{(l+1)^2}{r^2}\right]^{1/2}dr$$

with $V_c=-Z\mid e^2\mid/R$, where R is the boundary of the shell. By equating both sides we get, after some easy integrations,

$$\delta_r=\delta_S-I_1+I_1'-I_2+I_2' \tag{10}$$

with the following definitions:

$$I_1=\int_{S_t}^{S_1}\left\{\left[\frac{W}{\hbar c}+\frac{Z\mid e^2\mid}{2S_1\hbar c}\left(3-\frac{r^2}{S_1^2}\right)\right]^2-\frac{(l+1)^2}{r^2}\right\}^{1/2}dr,$$

$$I_1'=\int_{r_t}^{R}\left[\left(\frac{W-V_c}{\hbar c}\right)^2-\frac{(l+1)^2}{r^2}\right]^{1/2}dr=\left[\left(\frac{WR}{\hbar c}\right)^2-(l+1)^2\right]^{1/2}-(l+1)\tan^{-1}\frac{[(WR/\hbar c)^2-(l+1)^2]^{1/2}}{l+1},$$

$$I_2=\left[\left(\frac{WS_1}{\hbar c}+\frac{Z\mid e^2\mid}{\hbar c}\right)^2-(l+1)^2\right]^{1/2}+\frac{Z\mid e^2\mid}{\hbar c}\ln\left\{\left[\left(\frac{WS_1}{\hbar c}+\frac{Z\mid e^2\mid}{\hbar c}\right)^2-(l+1)^2\right]^{1/2}+\frac{WS_1}{\hbar c}+\frac{Z\mid e^2\mid}{\hbar c}\right\}$$
$$-\left[(l+1)^2-\left(\frac{Z\mid e^2\mid}{\hbar c}\right)^2\right]^{1/2}\tan^{-1}\frac{(Z\mid e^2\mid/\hbar c)(WS_1/\hbar c+Z\mid e^2\mid/\hbar c)-(l+1)^2}{[(l+1)^2-(Z\mid e^2\mid/\hbar c)^2]^{1/2}[(WS_1/\hbar c+Z\mid e^2\mid/\hbar c)^2-(l+1)^2]^{1/2}}.$$

I_2' is the same as I_2 except for replacing S_1 by R.

It is seen by Table I that the error involved is very small, even to the lowest order of approximation.

3. CONCLUSION

It is very difficult to establish a criterion for the property of the so-called similarity discussed. Probably, we must work out the problem. Then we know which one gives the better resemblance; the example given here is capable of illustrating the principle. In this we take the uniform nuclear-charge distribution as the known part. We might as well, for example, choose the point-Coulomb potential as the known part. However, this is not done here, for what has been done is enough to illustrate the method.

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